UNIVERSIDAD POLITÉCNICA DE MADRID
ESCUELA TÉCNICA SUPERIOR DE INGENIERÍA Y
DISEÑO INDUSTRIAL

Traceable Characterization of Areal Topography of
Structured Surfaces using Confocal Microscopy

TESIS DOCTORAL

Chen Wang
Máster Universitario en Ingeniería de Producción

Directores: Dr. Emilio Gómez García
Dr. Jesús Caja García

2019

UNIVERSIDAD POLITÉCNICA DE MADRID
ESCUELA TÉCNICA SUPERIOR DE INGENIERÍA Y
DISEÑO INDUSTRIAL

Traceable Characterization of Areal Topography of
Structured Surfaces using Confocal Microscopy

TESIS DOCTORAL

Chen Wang
Máster Universitario en Ingeniería de Producción

Directores: Dr. Emilio Gómez García
Dr. Jesús Caja García

2019

Título de la Tesis: TRACEABLE CHARACTERIZATION OF AREAL TOPOGRAPHY OF STRUCTURED SURFACES USING CONFOCAL MICROSCOPY

Autor: Chen Wang

Directores: Dr. Emilio Gómez García y Dr. Jesús Caja García

Tribunal aprobado por la Comisión de Doctorado de la Universidad Politécnica de Madrid, el día 22 de julio de 2019:

Presidente: Dr. Alfredo Sanz Lobera (UPM)

Vocal: Dra. Eva María Rubio Alvir (UNED)

Vocal: Dr. Lorenzo Sevilla Hurtado (UMA)

Vocal: Dr. Pedro José Núñez López (UCLM)

Secretario: Dr. Roque Calvo Iranzo (UPM)

Suplente: Dr. Juan José Aguilar Martín (UNIZAR)

Suplente: Dr. Santiago Ferrándiz Bou (UPV)

Realizado el acto de defensa y lectura de Tesis el día 9 de septiembre de 2019 en la E.T.S. de Ingeniería y Diseño Industrial.

Calificación:

EL PRESIDENTE

LOS VOCALES

EL SECRETARIO

致敬我最亲爱的祖国以及我的家人，

月是故乡明。

To my beloved motheland, China &

To my family,

Miss you so much.

Abstract

This PhD thesis addresses, from an analytical and experimental point of view, the characterization of structured surfaces through 3D roughness parameters.

The thesis includes novel models for the determination of outliers and develops an original method to ensure the traceability of the measurements made by confocal microscopy in the X, Y, Z axes.

The experimental validation of the models and the proposed methodology has been made from different files with synthetic data provided by the National Institute of Standards and Technology (NIST), available on its Website, and also through the use of physical standards calibrated by external laboratories.

The uncertainties associated with the different parameters evaluated, such as Sa, Sq, Ssk, Sku, St, Sp, Sv..., have been estimated by applying the Monte Carlo Method to surface finish measurements. For this, the most significant sources of uncertainty: kinematic, geometric, optical, environmental... and those due to the mathematical models used, have been taken into account. The calculation algorithms have been developed in Matlab and their validation have been carried out using the supercomputer “Magerit” of the Centro de Supercomputación y Visualización of the Universidad Politécnica de Madrid.

Keywords: Metrology - Confocal microscopy

Resumen

Esta tesis doctoral aborda desde un punto de vista analítico y experimental la caracterización de superficies estructuradas a través de parámetros de rugosidad 3D. Incluye modelos novedosos para la determinación de “outliers” y desarrolla un método original para garantizar la trazabilidad de las medidas realizadas mediante microscopía confocal en los ejes X, Y, Z. La validación experimental de los modelos y la metodología propuesta se ha realizado a partir de diferentes ficheros con datos sintéticos elaborados por el National Institute of Standards and Technology (NIST), accesibles a través de internet y también mediante el empleo de patrones físicos calibrados por laboratorios externos.

La incertidumbre asociada a los distintos parámetros evaluados, tales como S_a , S_q , S_{sk} , S_{ku} , S_t , S_p , S_v ..., se ha estimado mediante la aplicación del Método de Monte Carlo a medidas de acabado superficial, y para ello se han tomado en consideración las fuentes de incertidumbre más significativas: cinemáticas, geométricas, ópticas, ambientales... y las debidas a los modelos matemáticos empleados. Los algoritmos de cálculo se han desarrollado en Matlab y su validación se ha realizado utilizando el supercomputador “Magerit” del Centro de Supercomputación y Visualización de la Universidad Politécnica de Madrid.

Palabras Clave: Metrología - Microscopía confocal

Contents

Abstract.....	i
Contents	v
Contents of Figure	xi
Contents of Table	xx
Chapter 1: Introduction.....	1
1.1 Introduction to the investigation and application of surface metrology	1
1.2 Introduction to the 3D measurement techniques for confocal microscopy	5
1.3 Introduction to the challenges and trends in measurement technology	10
1.4 References of Chapter 1	12
Chapter 2: Objectives and Justification.....	15
2.1 Objectives.....	15
2.2 Justification.....	16
2.3 References of Chapter 2	18
Chapter 3 Thesis Structure.....	21
Chapter 4: Review of current literature	23
4.1 An introduction to areal surface metrology.....	23
4.2 An overview of surface topography measurement techniques.....	27
4.3 An introduction to roughness parameters	34
4.4 Approaches to outlier identification in areal surface metrology.....	35

4.5 Calibration methods for surface metrology system	42
4.6 Assessment of measurement uncertainty	62
4.6.1 Modeling the measurement by GUM method	63
4.6.2 Monte Carlo Method for model development	64
4.7 Summary	67
4.8. References of Chapter 4	67
Chapter 5: Algorithms for areal roughness parameterization and filtration	73
5.1 Algorithms for 3D roughness parameterization	73
5.1.1 Areal height parameters	74
5.1.2 Areal spatial parameters	77
5.2 Algorithm for surface Gaussian filtration	80
5.3 Verification with synthetic data	92
5.3.1 Verification of the parameterization algorithm	92
5.3.1 Verification of the filtration algorithm	112
5.4 References of Chapter 5	115
Chapter 6: Comparison of statistical methods for outlier identification in surface metrology	117
6.1 Introduction	117
6.2 Statistical methods for outlier identification	121
6.2.1 Interquartile range (IQR)	121
6.2.2 Median absolute deviation (MAD)	122

6.2.3 The Q_n Estimator.....	124
6.2.4 The Trimmed Mean method	125
6.2.5 Grubbs' Test	126
6.2.6 The Extreme Studentized Deviate method (<i>ESD</i>)	127
6.2.7 Dixon-type tests	129
6.2.8 Chauvenet's Criterion	130
6.2.9 The Pauta Criterion (also named 3σ criterion)	132
6.2.10 Tukey's test.....	133
6.3 Methodology of the experimental study.....	133
6.4 Experimental study and comparison of those methods for surface measurement.....	137
6.4.1 Experimental study of IQR.....	137
6.4.2 MAD.....	138
6.4.3 The Q_n estimator.....	140
6.4.4 The Trimmed Mean.....	142
6.4.5 Grubbs' test.....	142
6.4.6 The extreme studentized deviate.....	143
6.4.7 Dixon-type test.....	143
6.4.8 Chauvenet's criterion	144
6.4.9 The Pauta criterion	144
6.4.10 Turkey's test	144
6.4.11 Combination of IQR and Dixon-type Test	145
6.5 Analysis and comparison of the ten methods.....	145

6.6 Comparison of the 10 methods by a standard artefact	152
6.7 Summary	154
6.8 References of Chapter 6	155
 Chapter 7: Confidence Distance Matrix for surface outlier identification	 159
7.1 Introduction	159
7.2. Methodology for identifying outliers in surface measurement data	161
7.3 Mathematical model of the Confidence Distance Matrix	162
7.4 Methods and algorithms for outlier detection in surface measurement data	164
7.4.1 Proposal and validation of method and algorithms for random outlier identification, threshold determination	165
7.4.2 Proposal and validation of method and algorithms for identifying outliers in a stochastic surface	172
7.5. Experimental study	180
7.5.1 Experiment 1: measurement and data processing of a Type C1 spacing standard.	180
7.5.2 Experiment 2: measurement and data processing of a steel plate	184
7.6 Summary	187
7.7 References of Chapter 7	188
 Chapter 8: Calibration of the lateral stage of confocal microscopy	 193
8.1 Introduction to the X- and Y- axis scale calibration	193
8.2 Mathematical models for X- and Y- scale calibrations	196
8.3 Methodology and experimental procedures	207
8.4 Algorithms for data processing	211

8.4.1 Algorithm for separation of flat and cylinders.....	211
8.4.2 Algorithm for determination of dots center and distance	218
8.4.3 Algorithm for determination of coefficients.....	220
8.5 Uncertainty evaluation of the geometric error correction coefficients	225
8.6 Validation of the algorithm	229
8.6.1 Validation of the algorithm for determination of dots' centres and distance ..	229
8.6.2 Validation of the algorithm for determination of coefficients.....	231
8.7 Experimental study of the lateral calibration	241
8.7.1 Experiment 1: Determination of error coefficients using a dot pattern standard	241
8.7.2 Experiment 2: measurement correction of the dot grid targets standard.....	250
8.8 Summary	257
8.9 References of Chapter 8	259
Chapter 9 Vertical calibration.....	265
9.1 Introduction to the vertical axial calibration of the confocal microscopy	265
9.2 Mathematical models and algorithms for determination of the calibration factors	266
9.2.1 Mathematical models and algorithms for calculation of the correction coefficient.....	266
9.2.2 Mathematical models and algorithms for determination of depth heights	268
9.2.3 Algorithms for evaluation of the uncertainty produced by measurement positioning inclination.....	273
9.2.4 Algorithms for evaluation of the uncertainty produced by repeatability	274
9.2.5 Algorithms for evaluation of the uncertainty produced by reproducibility....	274

9.2.6 Algorithms for evaluation of the uncertainty produced by light source	275
9.3 Validation of the algorithms for depth determination	276
9.4 Mathematical model for axial scale calibrations of Z coordinate	282
9.5 Experiments and calibrations on z-axis coordinate.....	283
9.5.1 Experiments and calculation of step heights	283
9.5.2 Calculation of correction coefficients	285
9.5.3 Experimental study of the uncertainty contributed by positioning inclination	289
9.5.4 Experimental study of the uncertainty contributed by measurement repeatability	292
9.5.5 Experimental study of the uncertainty contributed by measurement reproducibility	294
9.5.6 Experimental study of the uncertainty contributed by illumination	296
9.6 Conclusions	298
9.7 References of Chapter 9	299
Chapter 10 Conclusions	301
References.....	303
Standards.....	303
Journals, conferences, books.....	305

Contents of Figure

Fig.1.1 Surface classification.	2
Fig.1.2 A new classification of surfaces.	2
Fig.1.3 Some attributes used to characterize areal surface texture. Source: Investigation and Evaluation of Methods for Measuring Surface [10].	3
Fig.1.4 Applications for manufacturing metrology. Source: Looking at the future of manufacturing metrology: The VDI/VDE roadmap manufacturing metrology 2020 [20].	4
Fig.1.5 The traceability chain of metrology.	5
Fig.1.6 General view of Leica Dual-core DCM 3D in Laboratory LIMIT.	6
Fig.1.7 Set-up of Leica Dual-core DCM 3D.	7
Fig.1.8 Advancement and benefits of the Dual-core Leica 3D DCM.	8
Fig.1.9 Microscopy modes (from left to right): colour bright field, confocal, unlimited depth of field, depth coded.	9
Fig.1.10 Challenges and trends in manufacturing metrology from VDI 2020 Manufacturing Metrology Roadmap (updated in 2015).	11
 Fig.2.1 Measurement procedure in the field of surface texture.	 18
 Fig. 4.1 The role of surface metrology.	 25
Fig. 4.2 Standards membership bodies.	27
Fig. 4.3 Schema to categorize surface topography measurement instrument.	31
Fig. 4.4 Typical bandwidth limits for stylus instruments: two cutoffs for two RC filters. Source: Tutorial in optics [5].	33
Fig. 4.5 Amplitude-wavelength plot of the working range of surface topography measurement instruments.	34
Fig. 4.6 Areal parameters introduced in ISO 25178-2:2012 [30].	35

Fig. 4.7 Left: only the light coming through zone 2 is reflected to the detector; Right: almost all light is reflected outside the detector [33].	36
Fig. 4.8 Reflection on a diffuse surface [34].	37
Fig. 4.9 Ghost focus on a circular Groove [34].	38
Fig. 4.10. The sensor ‘sees’ a depth d' while the true thickness is d [34].	39
Fig. 4.11 Pattern units (blue) and individual features (red) of a structural surface.	40
Fig. 4.12 Summary of the definitions of metrological traceability.	44
Fig. 4.13. Flow of operations of calibration of confocal measurement instrument.	46
Fig. 4.14 Relationships between the S-filter, L-filter, F-operator and S-F and S-L surfaces. Source: Good Practice Guide No.128 [20].	48
Fig. 4.15 Classes of recent significant development of filters.	48
Fig. 4.16 Example of a non-linear response curve. Source: ISO 25178-602: 2010 [47].	55
Fig. 4.17 Example of the linearization of a response curve. Source: ISO 25178-602:2010 [47].	56
Fig. 4.18 Hierarchy from traceable standards to quality [10].	59
Fig. 4.19 The error sources of the measurement uncertainty [56]]	60
Fig. 4.20 Graphical representation of the meaning of error and measurement uncertainty: (a) The axial system (scalar); (b) Spatial (vector) [61].	63
Fig. 4.21 Propagation and summarizing stages of uncertainty evaluation using MCM to implement the propagation of distributions when the vector output quantity can be expressed explicitly in terms of the input quantities. Source: GUM-S2 [63].	66
Fig.5.1 Definition of a profile. Source: ISO 4287: 1998 [1].	74
Fig.5.2 ACF of a turned surface along X Direction and Y Direction. Source: Michigan Metrology, LLC [5].	78
Fig.5.3 Spatial parameters of directional surface and isotropic surface. Source: Michigan Metrology, LLC [5].	80
Fig.5.4 Procedure to calculate S_{al} and S_{tr} . Source: ISO 25178-2:2012 [6].	80

Fig.5.5 Indication of the superposition of a surface with form, waviness, and roughness. Source: Characterisation of Areal Surface Texture [3].	81
Fig.5.6 Relationships between the S-filter, L-filter, F-operation and S-F and S-L surfaces. Source: ISO 25178 - 2: 2012 [6].	82
Fig.5.7 Weighting function of a Gaussian profile filter for an open profile.	85
Fig.5.8 Long wave transmission function of the Gaussian filter for an open profile.	86
Fig.5.9 Short wave transmission function of the Gaussian filter for an open profile.	87
Fig.5.10 Gaussian filtration ($\lambda_c = 0.8 \text{ mm}$) with the removal of the end effect regions. Source: ISO 16610-28 [10].	88
Fig.5.11 An illustrative example of Gaussian filtration ($\lambda_c = 0.8 \text{ mm}$) using the moment retainment criterion. Source: ISO 16610-28 [10].	89
Fig.5.12 The weighting function of a Gaussian areal filter.	90
Fig.5.13 Long wave transmission function of the areal Gaussian filter for planar surfaces with λ_c .	91
Fig.5.14 Short wave transmission function of the areal Gaussian filter for planar surfaces with λ_c .	92
Fig.5.15 The website of the Internet based surface Metrology Algorithm Tesing System of NIST.	93
Fig.5.16 Data files provided by the Internet based surface Metrology Algorithm Tesing System of NIST.	94
Fig.5.17 Surface height distribution.	99
Fig.5.18 Distributions of the areal height parameters of the Data base of SG_1-2.	103
Fig.5.19 Surface height distribution.	105
Fig.5.20 Distributions of the areal height parameters of the Data base of SG_1-4.	107
Fig.5.21 Surface height distribution.	109
Fig.5.22 Distributions of the areal height parameters of the Data base of SG_3-4.	111
Fig.5.23 Testing system for Surface filtration provided by NIST.	112
Fig.5.24 Reconstruction of the Surface calculated by NIST testing system: (a) raw surface; (b) waviness; (c) roughness.	113

Fig.5.25 Construction of surface of the waviness calculated by our developed algorithms.....	114
Fig.5.26 3D view construction of the waviness calculated by our developed algorithms.	114
Fig. 6.1. Pattern units (blue) and individual features (red) of a structural surface.	119
Fig. 6.2. Probability band for identification of outliers as Chauvenet's Criterion.....	131
Fig. 6.3 Images of surfaces from the standard databases: (a) SG_1-2; (b) SG_1-4.....	134
Fig. 6.4. Comparison of results processed by different thresholds.....	139
Fig. 6.5 Reconstruction of surface: (a) before deletion of outliers; (b) after deletion of outliers	140
Fig. 6.6 Comparison of the elapsed time by each method.	146
Fig. 6.7 Comparison of the difference between S_a processed by the ten methods and the combination method with a logarithmic scale on the y axis.	147
Fig. 6.8 Comparison of the number of missed outliers by each method.....	148
Fig. 6.9 Comparison of filtered surfaces of Experiment 2 by methods of: (a) IQR; (b) MAD; (c) Q_n Estimator; (d) Trimmed Mean; (e) Grubbs' Test; (f) ESD ; (g) Dixon-type tests; (h) Chauvenet's criterion; (i) Pauta criterion; (j) Tukey's test.	152
Fig. 6.10 The Type C1 spacing standard: (a) photograph of the standard; (b) surface processed by MAD method.	152
Fig. 6.11 Comparison of the difference of S_a and the elapsed time measuring the physical standard artefact.	153
Fig. 7.1 Confidence distance measures: (a) d_{ij} ; (b) d_{ji} [21].....	163
Fig. 7.2 Surface reconstruction of the data set SG_3-3 provided by NIST: (a) 2D contour plot; (b) 3D surf plot.	165
Fig. 7.3 Surface reconstruction of the data set SG_3-3 after adding outliers: (a) 2D contour plot; (b) 3D surf plot.	166
Fig. 7.4 Histogram of the surface heights: (a) original data set SG_3-3; (b) SG_3-3 with outliers.....	167
Fig. 7.5 Variation of S_a according to different threshold value.	168

Fig. 7.6 Surface reconstruction of the data set after deleting outliers: (a) 2D contour plot; (b) 3D surf plot.	169
Fig. 7.7 Histogram of the height distribution of the data set after deletion of outliers.....	169
Fig. 7.8 Detection window for screening outliers [13].	172
Fig. 7.9 Reconstruction of our generated artificial stochastic surface: (a) 2D contour plot; (b) 3D surf plot.....	174
Fig. 7.10 Surface reconstruction of our generated artificial surface after adding random outliers: (a) 2D contour plot; (b) 3D surf plot.....	174
Fig. 7.11 Histogram of our produced artificial surface heights: (a) original data; (b) Data with outliers.	176
Fig. 7.12 Reconstruction of the artificial stochastic surface after deletion of outliers: (a) 2D contour plot; (b) 3D surf plot.....	177
Fig. 7.13 Histogram of the heights of the artificial surface after deletion of outliers.	178
Fig. 7.14 Comparison of areal height parameters calculated from the original data, with outliers, and after deletion of outliers of the artificial stochastic surface.....	179
Fig. 7.15 The Type C1 spacing standard: (a) photograph of the standard; (b) Image by Dino-Lite Digital Microscope.	181
Fig. 7.16 Reconstruction of the measured surface: (a) original measurement data; (b) after removal of the form.	181
Fig. 7.17 Surface reconstruction of the data after removing from: (a) 2D contour; (b) 3D surf.	182
Fig. 7.18 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.	182
Fig. 7.19 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.	183
Fig. 7.20 Image of the specimen: (a) Photograph; (b) Image by Dino-Lite Digital Microscope.	184
Fig. 7.21 Surface reconstruction of the measured data: (a) 2D contour; (b) 3D surf.	185
Fig. 7.22 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.	185
Fig. 7.23 Histogram of the distribution of the areal heights: (a) The measured data; (b) Data after deletion of outliers.....	186
Fig. 7.24 QQ plot of the measured surface data versus the data after deletion of outliers.	186

Fig. 8.1 Image of the cross gratings: (a) glass substrate carrying three chrome grid patterns; (b) white light interferometer image of one of the grid pattern. Source: Recent advances in traceable nanoscale dimension and force metrology in the UK [20].	194
Fig. 8.2 One dimensional reference structure for lateral scale calibration of scanning microscopes. Source: A landmark-based 3D calibration strategy for SPM [21].	195
Fig. 8.3 Schematic of the 4 coordinate measuring machine configurations.....	196
Fig. 8.4 Schema of the metrology loop of the Confocal Optical Microscopy.	197
Fig. 8.5 Architecture of the 3D Image Confocal Microscopy.	197
Fig. 8.6 Illustration of the 21 rigid body errors.....	200
Fig. 8.7 Manifestation of the vectors on the 3D image confocal microscopy.	201
Fig. 8.8 Diagram of the axis chain vector of the 3D image confocal microscopy.	201
Fig. 8.9 Illustration of the standard artefact of dot grid targets.	208
Fig. 8.10 Indication of the measurement range for individual topography by Objective Magnification of 50X: (a) 2D image; (b) 3D image.	209
Fig. 8.11 Indication of the measurement range for stitching topography by Objective Magnification of 50X. ..	210
Fig. 8.12 Flowchart of the algorithm for geometric errors correction.	211
Fig. 8.13 Reconstruction of the measured surface by its raw measurement data: (a) 2D contour; (b) 3D surf. ..	212
Fig. 8.14 Reconstruction of the surface with trimmed raw data.	212
Fig. 8.15 Reconstruction of the rotated surface: (a) 3D line plot; (b) 3D surface plot uses Z for the colour data.	214
Fig. 8.16 Histogram of the Z values of the rotated surface.....	214
Fig. 8.17 The separated flat plane of the rotated surface: (a) 3D view (b) view from top down.....	215
Fig. 8.18 The separated cylinders of the rotated surface: (a) 3D view (b) View from top down	215
Fig. 8.19 Separation of cylinders into individuals.....	216
Fig. 8.20 Flowchart of the algorithm for data partition	217
Fig. 8.21 Flowchart of the algorithm for circle fitting.....	220

Fig. 8.22 Illustration of the propagation of distributions for input quantities and the obtained output quantities [50].	228
Fig. 8.23 Plot of the created data for algorithm validation: (a) The 3D view of the point cloud; (b) View of the vertical projection.	229
Fig. 8.24 The separation of cylinders into individual point clouds.	230
Fig. 8.25 Plots of the calculated centres of the generated data.	230
Fig. 8.26 Comparison of the positions of certified, measured and corrected points	232
Fig. 8.27 Contour of the errors between certified and measured points.	233
Fig. 8.28 Contour of the errors between certified and corrected points	233
Fig. 8.29 Comparison of the error vectors between the measured and corrected points	235
Fig. 8.30 Comparison of the certified, measured, and corrected positions of the 10 simulations.	236
Fig. 8.31 Comparison of the mean residuals before correction and after correction.	237
Fig. 8.32 Comparison of the squared residuals before correction and after correction.	238
The results of the Simulation N° 10 are shown. Fig. 8.29 compare the positions of the certified, measured, and corrected points of Simulation N° 10. Fig. 8.33 and Fig. 8.31 presents contours of the mean residual and the squared residual between certified and measured points of Simulation N° 10. Fig. 8.34 manifests the error vectors between the measured and corrected points of Simulation N° 10.	238
Fig. 8.35 Comparison of the positions of the certified, measured, and corrected points of Simulation N° 10.	239
Fig. 8.36 Contour of the mean residual between certified and measured points of Simulation N° 10.	239
Fig. 8.37 Contour of the mean residual between certified and corrected points of Simulation N° 10.	240
Fig. 8.38 Comparison of the error vectors between the measured and corrected points of Simulation N° 10.	240
Fig. 8.39 Surface reconstruction by the raw measurement data: (a) 2D plot; (b) 3D plot.	242
Fig. 8.40 Surface reconstruction after rotation of the raw measured surface: (a) 2D plot; (b)) 3D plot.	242
Fig. 8.41 Histograms of the X-, Y-, and Z-coordinates of the rotated surface.	242
Fig. 8.42 Surface reconstruction of the data of cylinders.	243
Fig. 8.43 Distribution of the X-coordinates values and the thresholds for outlier detection.	243

Fig. 8.44 Distribution of the Y-coordinates values and the thresholds for outlier detection.....	244
Fig. 8.45 Surface reconstruction of the data of cylinders with outliers removed.	244
Fig. 8.46 Separation of the cylinders.....	245
Fig. 8.47 Plot of the cylinders' centres and their corresponding certified positions.....	245
Fig. 8.48 Comparison of the positions of certified, measured and corrected points.	246
Fig. 8.49 Contour of the Euclidean residuals between each certified and measured points.....	247
Fig. 8.50 Contour of the Euclidean residuals between each certified and corrected points.	247
Fig. 8.51 Distributions of the uncertainties of some geometric error correction coefficients.	250
Fig. 8.56 The measured surface with form removed: (a) 3D reconstruction; (b) 2D reconstruction.	251
Fig. 8.57 Separation of the cylinders: (a) The separated cylinders from the base; (b) Separate cylinders into individual clusters.	251
Fig. 8.58 Histogram of the three coordinates of the separated cylinders.....	252
Fig. 8.59 Comparison of the fitted circle centre and the centroid of the data.	253
Fig. 8.60 Comparison of the certified, measured, and corrected positions.	256
Fig. 8.61 Contour of the Euclidean residuals between each certified and measured points.....	256
Fig. 8.61 Contour of the Euclidean residuals between each certified and corrected points.	257
Fig. 8.63 Comparison of the error vectors between the measured and corrected points.....	257
Fig. 9.1 Flow chart of the procedure for the calibration on z-coordinate.	266
Fig. 9.2 Assessment of values for a standard artefact of type PGR. Source: ISO 25178-70-2014 [2].....	269
Fig. 9.3 Indication of the evaluation areas for areal standard artefact.	270
Fig. 9.4 Error caused by inaccurate positioning [7].	274
Fig. 9.7 Illustration of the signal acquisition from the surface to the image plane [8].	276
Fig. 9.8 (a) Interaction between surface and incident light, (b) Lambertian surface, (c) Specular surface [8] ...	276
Fig. 9.7 The website of the Internet based surface Metrology Algorithm Tesing System of NIST.	277

Fig. 9.8	Data files provided by the Internet Based Surface Metrology Algorithm Testing System of NIST.	278
Fig. 9.11	Surface reconstruction of the synthetic data SG_1-2: (a) 2D surface; (b) 3D surface.....	278
Fig. 9.12	Reconstruction of the created data with step height of 10 μm	280
Fig. 9.13	Distributions of the coordinates values of the created data: (a) x-axis direction; (b) z-axis direction.	281
Fig. 9.14	Histogram of the distribution of the calculated step height of the created data.	282
Fig. 9.13	Photograph of the depth-setting standard.....	284
Fig. 9.14	General information of the depth-setting standard.....	284
Fig. 9.15	Distribution of the processed results of groove depths of the depth-setting standard.	285
Fig. 9.16	Certified values of the groove depths of the depth-setting standard.	286
Fig. 9.17	Comparison of the corrected and certified values of step heights of the depth-setting standard.....	287
Fig. 9.18	Comparison of the corrected and certified values of step heights of the depth-setting standard.....	288
Fig. 9.19	Comparison of the corrected and certified values of step heights of the depth-setting standard.....	289
Fig. 9.20.	Photograph of the Type C1 spacing standard.	290
Fig. 9.21	Photograph of the base for inclination.	290
Fig. 9.22	Reconstruction of the 4 inclined Surface.....	291
Fig. 9.23	Distribution of the measured height difference due to inclination.	292
Fig. 9.24	Reconstruction of the 4 surfaces measured under repeatability conditions.	293
Fig. 9.25	Distribution of the measured height difference due to repeatability.	294
Fig. 9.26	Reconstruction of the 4 surfaces measured under reproducibility conditions.....	295
Fig. 9.27	Distribution of the measured height difference due to reproducibility.....	296
Fig. 9.28	Reconstruction of the 4 surfaces measured under different illumination conditions.....	297
Fig. 9.29	Distribution of the measured height difference due to reproducibility.....	298

Contents of Table

Tab. 4.1 Information on surface topography measurement techniques [8].	29
Tab. 4.2 Maximum measureable slope against numerical aperture [34].	36
Tab. 4.3 Relationships between nesting index value F-operator/L-filter, S-filter nesting index, and bandwidth ratio. n is a positive or negative integer. [20].	49
Tab. 4.4 Physical measurement standard for areal material measures identified in ISO 25178-70:2014 [45].	50
Tab. 4.5 Template for summary of calibration results. Source: Good Practice Guide No.128 [20].	53
Tab. 4.6 Efficiency of detection algorithms. Source: ISO 25178-602:2010 [47].	57
Tab. 4.7 Metrological Characteristics of non-contact (confocal chromatic probe) instruments. Source: ISO 25178-602:2010.	58
Tab.5.1 Nesting index values between the F-operation or L-filter and S-filter and the bandwidth ratio [4].	82
Tab.5.2 Implementation errors for different truncation constants.	85
Tab.5.3 Results calculated by the program and comparsion with the values given by NISTof the data base SG_1-2.	100
Tab.5.4 The covariance of the height parameters.	101
Tab.5.5 The correlation coefficient of the height parameters.....	101
Tab.5.6 Results Calculated by the Program and Comparsion with the Values given by NISTof the data base SG_1-4.	104
Tab.5.7 The covariance of the Height Parameters.	105
Tab.5.8 The correlation coefficient of the height parameters.....	105
Tab.5.9 Results Calculated by the Program and Comparison with the Values given by NIST.	108
Tab.5.10 The covariance of the Height Parameters.	109
Tab.5.11 The correlation coefficient of the height parameters.....	109
Tab.5.12 Comparison of the results provided by NIST and calculated.....	113

Tab. 6.1 Critical value λ_i for $r = 1, 2$, or 3 and significance levels of $\alpha = 1\%$, 5% .	128
Tab. 6.2 Critical values of Q_{crit}	130
Tab. 6.3 Chauvenet's Criterion Table	131
Tab. 6.4 Areal surface parameters from the standard database SG_1-2.	134
Tab. 6.5 Areal surface parameters from the standard database SG_1-4.	135
Tab. 6.6 Arrangement of data sets.	135
Tab. 6.7 Results of the height parameters processed by IQR.	137
Tab. 6.8 Comparison of results processed by different thresholds.	138
Tab. 6.9 Results of the height parameters processed by MAD.	140
Tab. 6.10 Results of Experiment 2 processed by Q_n Estimator with threshold = 18.	140
Tab. 6.11 Results of the height parameters processed by the Q_n Estimator.	141
Tab. 6.12 Results of the height parameters processed by Fast Trimmed Mean with $p = 0.2$.	142
Tab. 6.13 Results of the height parameters processed by the Grubbs' Test with $t = 2.3530$.	142
Tab. 6.14 Results of the height parameters processed by ESD method with $\lambda i = 1.175$.	143
Tab. 6.15 Results of the height parameters processed by Dixon-type method with $Q = 0.7100$.	143
Tab. 6.16 Results of the height parameters processed by Chauvenet's Criterion.	144
Tab. 6.17 Results of the height parameters processed by the combination of the IQR and the Dixon-type test.	145
Tab. 6.18 The possibility of deletion of normal values by the Pauta Criterion.	150
Tab. 7.1 areal surface parameters of the specimen provided by NIST [32].	166
Tab. 7.2 Arithmetic mean height value Sa according to different threshold value.	167
Tab. 7.3 Comparison of height parameters of the original data, data with outliers, and data after deletion of outliers.	170

Tab. 7.4 Surface slopes and curvatures of the original data, data with outliers, and data after deletion of outliers.	171
Tab. 7.5 Areal height parameters of our generated artificial surface data.	175
Tab. 7.6 Covariance matrix of the height parameters of our produced artificial surface.	175
Tab. 7.7 Correlation matrix of the height parameters of our produced artificial surface.	175
Tab. 7.8 Areal height parameters of the artificial surface data with outliers.	176
Tab. 7.9 Covariance matrix of the height parameters of the artificial surface data with outliers.	176
Tab. 7.10 Matrix of the correlation coefficients of the height parameters of the artificial surface data with outliers.	177
Tab. 7.11 Areal height parameters of the artificial surface after deletion of outliers.	178
Tab. 7.12 Covariance matrix of the height parameters of the artificial surface after deletion of outliers.	178
Tab. 7.13 Matrix of the correlation coefficients of the height parameters of the artificial surface after deletion of outliers.	179
Tab. 7.14 Comparison of the surface slopes and curvatures	180
Tab. 7.15 Comparison of height parameters of the original data, data with outliers, and data after deletion of outliers.	183
Tab. 7.16 Comparison of the surface slopes and curvatures	184
Tab. 7.17. Comparison of the surface slopes and curvatures of the data of the steel plate.	187

Chapter 1: Introduction

Abstract: This chapter makes a general introduction to the surface metrology, including the introduction to the investigation and application of surface metrology, Introduction to the 3D measurement techniques for confocal microscopy, and Introduction to the challenges and trends in measurement technology

1.1 Introduction to the investigation and application of surface metrology

Metrology covers three parts: the first is the definition of internationally accepted units of measurement, such as the meter; the second is the realization of units of measurement by scientific methods; the last one is the establishment of traceability chains [1]. Metrology is essential for scientific research, and scientific research forms the basis for the development of the technologies of metrology [1].

Development of two dimensional profile measurement and roughness evaluation can be traced back to the 1930s [2, 3, 4]. With the improvement of the processing technology, variability of materials, etc., surface texture of the workpieces is more and more complicate. Therefore, two dimensional measurements cannot fulfil the requirements of industrial surface characterization. There is a demand for areal surface characterization to provide more information about the surfaces for production [5]. There are many classifications of surfaces, two of them is shown, as indicated in Fig.1.1 and Fig.1.2. [6]. The structured surfaces and freeform surfaces gains lots of research interests recently [7, 8].

Fig.1.1 Surface classification.

Fig.1.2 A new classification of surfaces.

Investigation on areal surface metrology mainly focused on instrument techniques, i.e. to develop metrological instruments, before the 1970s. Development of the laser and the large computer during the 1960s and 1970s promoted many changes in testing capabilities. Several commercial interferometers became available in 1970s [9]. After that, the developments of surface metrology shifted to quantitative analysis. Some attributes used to characterize areal surface texture can be found in Fig.1.3 [10].

Fig.1.3 Some attributes used to characterize areal surface texture. Source: Investigation and Evaluation of Methods for Measuring Surface [10].

Nowadays, surface metrology is further improved due to the development of instrumentation techniques, mathematical models and algorithms, computer processing technology, etc. [11]. Computer vision techniques have received increasing attentions from many researchers for surface roughness measurement. B. Y. Lee, *et al.* used a polynomial network to construct the relationships between the cutting parameters and cutting performance, i.e. surface roughness [12]. G. A. Al-Kindi, *et al.* explored experimentally the capability of a machine vision system to monitor the texture over a finite area as surface colour, lighting conditions, surface texture, surface geometry, tarnishing, all creating measurement problems [13]. P. M-Argüello, *et al.* presented a multiresolution method based on the processing of surface images for unmanned visual quality inspection and surface roughness discrimination, applying Haar wavelet transform to the original surface images obtaining four sub-images, and these images are used for the extraction of features [14]. Computer vision based surface roughness assessment, surface finish control in machining processes, measurement of surface roughness using image processing is gaining more and more attentions [15, 16, 17].

Surface metrology is commonly used for characterization of functional engineering surfaces [18]. Surface finish evaluation is crucial to solve many fundamental problems, such as friction, deformation of contact joints, positional accuracy, etc. [19]. Fig.1.4 shows some of the applications of the manufacturing metrology, such as for the areas of shape, material, function, and electricity.

Fig.1.4 Applications for manufacturing metrology. Source: Looking at the future of manufacturing metrology: The VDI/VDE roadmap manufacturing metrology 2020 [20].

Uncertainty is a quantitative evaluation of the quality of a measurement value, enabling the measurement results comparable with other results, references, specifications, or standards [1]. All measurements are subject to errors, and most sources of measurement error can be identified, quantified, and corrected, such as calibration. Measurement calibrations can be determined in many ways. One of them is the evaluation of measurements by the method of least squares. In 2002, L. Nielsen presented a general technique applying least squares in its more generalized form, fully compatible with the principles for measurement uncertainty evaluation [21, 22]. Despite the importance of this contribution, this method has hardly widespread due to the technicalities of its implementation [23].

The most widely used and accepted method is the Guide to the Expression of Uncertainty in Measurement (GUM) recommended by ISO. Fig.1.5 indicates the traceability chain. Definition of the unit is defined by Bureau International des Poids et Mesures (BIPM). Foreign national primary standards and national primary standards are defined by National Metrology Institutes or designated national institutes. Reference standards are usually offered by calibration laboratories. Working standards are often termed by industry, academia, regulators, hospitals, etc. Measurements are made by end users. As indicated in Figure 1.5, uncertainty increases from the top down to the final measurements.

Fig.1.5 The traceability chain of metrology.

Standards of surface roughness evaluations can be traced back to 1940s. In the mid-1960s, the techniques of digitizing surface height information rendered the enthusiasm of researchers for computation between data acquisition and data manipulation [4]. Due to the complication of the surface texture and the slowness of internationalization of those standards, there appeared 100 or so surface parameters. Those parameters were not unique and many of them had different names for the same form of evaluation [4]. In 1982, ISO/TC57 issued the surface roughness standards ISO 468:1982 [24], specifying the terms, definitions, parameters, etc., about profile roughness. The first ASME B46.1 standard was issued March 1940 and there are 9 revisions of the B46.1 since then [25, 26].

1.2 Introduction to the 3D measurement techniques for confocal microscopy

The laboratory LIMIT of UPM has a Confocal Dual Core 3D Measuring Microscopy, as shown in Fig.1.6.

The Leica DCM 3D system with dual core technology has been designed for fast, non-invasive assessment of micro and nanostructures of technical surfaces, in multiple configurations.

According to information given by Leica Company, the DCM 3D is designed to combine confocal and interferometry technology for high speed and high-resolution measurements, which are down to 0.1 nm of precision. It is necessary to note that this equipment is only

available with confocal measurements, but the functions are enough for the experiments of this work. The micro display confocal technology, no moving parts, measures a variety of materials and provides confocal and bright field images simultaneously [27].

Fig.1.6 General view of Leica Dual-core DCM 3D in Laboratory LIMIT

The Leica DCM 3D features vibration-free, long-lifetime scanning using micro display technology. Conventional confocal microscopies use movable mechanic parts inside scanning heads (scanning mirrors and spinning discs) that limit the instrument's lifetime, need a periodic re-adjustment to maintain optimum performance, and introduce mechanical vibrations that increase noise on the measurement. The Leica DCM 3D uses advanced micro display technology, a fast switching device with no moving parts inside that makes the scanning of confocal or interferometry images fast and stable with an extensive life time.

Fig.1.7 Set-up of Leica Dual-core DCM 3D.

The Leica Dual-core DCM 3D Measuring Microscopy has three systems in one, there forth brings us many benefits and convenience, especially when compared with traditional Laser Scan based systems. Fig.1.7 illustrates the set-up system of microscopy. The Leica DCM 3D has bright field and dark field colour digital microscopy, high resolution confocal imaging and measuring system, dual optical Interferometry Profiler. It incorporates confocal micro display (MD) technology, which gives non-moving part concept.

The non-moving part concept, the confocal micro display (MD), two light sources and two cameras (one colour and one monochromatic) achieve high accuracy 3D measurements and unlimited depth of focus.

Confocal MD technology is used to measure the topography of very rough to smooth surfaces. Even fine surface structures become visible without touching the sample surface. Within seconds the sample is scanned vertically in pre-defined steps during which every point on the surface passes through the focus level. All image information that is out of focus is eliminated, and acquired confocal images are providing detailed information of the sample in high resolution and contrast in all three dimensions. Measurement of topographical differences ranges from one nanometre to several millimetres, and up to 70 degrees of local slope. In comparison to Laser Scan based systems or Spinning Disc, MD confocal technology needs no moving mechanical parts, increasing both image stability at high magnifications and light efficiency, and enhancing reliability and flexibility [28]. Along with a LED based light

source, MD technology prolongs instrument lifetime, reducing servicing and avoiding the cost of expensive spare parts. Surface measurements are achieved in seconds. The system is easy to use. Just place your sample under the microscopy, focus and click “Acquire”. It only takes a few seconds (typically less than 5) to get a 3D view of the surface comparable to those acquired with a scanning electron microscopy, in a fraction of the time. Fig.1.8 indicates the summarization of advancement and benefits of the Dual-core Leica 3D DCM.

Fig.1.8 Advancement and benefits of the Dual-core Leica 3D DCM.

3D provides the highest lateral resolution within seconds. However, main reason for applying confocal imaging for surface profiling is the possibility to measure in the Z-dimension. Objectives with high NA (0.95) and high magnification are facilitating the measurement of smooth surfaces that may contain even steep local slopes with more than 70° inclination.

Covers the whole spectra from super smooth to rough surfaces Micro optical measurement technology fulfil two important requirements of metrology: non-destructive measurement combined with high accuracy. The measuring capabilities of the Leica DCM 3D range from a few nanometres to several millimetres and therefore they serve a wide variety of different applications. Besides the capabilities of adapting to the requirements of the application from

super smooth to very rough surfaces, the Leica DCM 3D is specifically designed to carry out measurements at extremely high speed. This does not only save valuable time, but also significantly improves the return of investment.

The integrated technologies of the Leica DCM 3D overcome the physical limits of conventional profiling systems. With a single system it is possible to analyse rough (confocal) as well as smooth (Vertical Scanning Interferometry or VSI) and super smooth (Phase Shift Interferometry or PSI) surfaces. Sub-micron lateral resolution and a vertical resolution in the nm range are obtained in confocal mode, while large fields of view in combination with sub-nanometre Z resolution are acquired in the Interferometry mode. Fig.1.9 shows the four measurement modes of the microscopy, i.e. colour bright field, confocal, unlimited depth of field, depth coded.

Fig.1.9 Microscopy modes (from left to right): colour bright field, confocal, unlimited depth of field, depth coded.

The Leica DCM 3D is designed to be maintenance-free. Two high-power LEDs are integrated into the beam path, which provides a long average lifetime of 20,000 hours in MTBF. A white light LED is used for colour bright field inspection, confocal images with real colour texture, and VSI. A blue light LED is used for high-resolution confocal imaging and PSI. The blue LED's short wavelength increases lateral resolution to 0.15 μm and improves PSI noise to 0.1 nm of vertical resolution. Making use of two integrated camera systems, the main metrology image sensor of the Leica DCM 3D is an integrated high-resolution CCD camera, which delivers black and white images at high speed. Cost of ownership is significantly reduced when compared to other spinning disk or laser-based systems. Information about the system parameters and general specifications of Leica DCM 3D can be found in Tab.1.1.

Tab.1.1 System parameters and general specifications of Leica DCM 3D.

Measuring principle	Dual Core Optical Imaging Profilometry (Confocal and Interferometry) non-contact, 3 dimensional
Maintenance	Maintenance free
Sample preparation	No specific sample preparation required
Capabilities	Imaging, 3D-Topography, Profiles, Coordinates, Thickness, Roughness, Volume, Surface Texture, etc.

Contrasting modes	Confocal, Interferometry (PSI, Epsi, VSI), Brightfield Color, Brightfield Greyscale (high resolution), Darkfield.				
Objectives	from 2.5X up to 150X in confocal from 5X up to 50X in interferometry				
Nosepiece	6-fold objective revolver manual/ 6-fold objective revolver motorized				
Stage travel range (x,y)	Manual: 200X100 mm (others on request). Manual stitching available Motorized: From 114X75 mm to 302×302 mm (others on request). Automatic stitching available over the full scanning range Closed loop encoded stages for high precision stitching				
Illumination	High power white LED 530 nm for coaxial light, controllable High power blue LED 460 nm for coaxial light, controllable				
Image Acquisition	2 Sensors: Metrology Sensor (B&W), Colour Sensor (both high resolution CCD)				
Vertical Scanning Range	40 mm				
Sample Reflectivity	From 0.1% up to 100%				
Operating temperature	5 °C to 40 °C				
Ambient humidity	< 80% relative humidity				
Vibration Isolation	active or passive (recommended for Interferometry)				
Confocal mode					
Objective magnification	5X	10X	20X	50X	150X
Numerical Aperture	0.15	0.30	0.50	0.90	0.95
FOV (μm)	2550×1910	1270×950	636.61×477.25	254.64×190.90	84.83×63.60
Optical Resolution (X/Y) (μm)	0.94	0.47	0.28	0.16	0.14
Vertical resolution (nm)	< 150	< 30	< 15	< 3	< 2
Vertical Scanning speed (μm/s)	20-320	10-160	5-80	1-16	0.5-8
Full Resolution Confocal Frame Rate	12.5 fps				
Typical measurement time	3–5 seconds				
Due to the Interferometry mode is not available, neither is experimented, its parameters are not listed here					

1.3 Introduction to the challenges and trends in measurement technology

According to the report by NPL [29], metrology will be used to assess and guarantee the fit, performance and functionality of every part. The technological progress in the 2020s will be driven and constrained by the need to achieve scientific discovery.

Stylus methods for surface measurement seems likely going to be replaced by optical methods, and white light interferometry and confocal microscopes are the most promising techniques [30]. However, due to the errors that instruments will add to the measurements, stylus methods are mostly likely to be treated as a reference technique. The best solution is the combination of both optical and stylus methods [30].

A German group of experts from researches and industries prepared a forecast relating to future development of metrology and published it in the form of roadmap as shown in Fig. 1.10. The roadmap covers four topics as fast, accurate, safe and flexible [31]. Trends of production are concluded as resource efficiency, flexibility, transparency, and new processes. The topic fast includes challenges of increasing integration, reducing measuring time, automatic data processing. The topic of accurate aims at reducing measuring errors/uncertainty. The area of safe emphasizes verification of measuring uncertainty. The topic flexible underlines increasing variety of measuring techniques and information density.

Fig.1.10 Challenges and trends in manufacturing metrology from VDI 2020 Manufacturing Metrology Roadmap (updated in 2015).

Based on this context the thesis is developed, which aims to improve the characterization of manufactured parts with structured surfaces, using confocal microscopy, with the measurement traceability ensured.

1.4 References of Chapter 1

- [1] P. Howarth, F. Redgrave, Metrology - in short 3rd Edition, EURAMET project 1011, participants: DFM Denmark, NPL United Kingdom, PTB Germany, 2008.
- [2] A. Godi, A. Kuhle, and L. D. Chiffre, A new procedure for characterizing textured surfaces with a deterministic pattern of valley features, *Measurement Science and Technology* 24 (8) (2013) 085009.
- [3] K. H. Lin, Y. H. Hu, White-light interferometric techniques in microstructure measurement, *Proceedings of the SPIE*, Volume 6280, id. 62800X (2006).
- [4] K. J. Stout, L. Blunt, Three-dimensional Surface Topography, 2nd Edition, Penton Press, 2000.
- [5] Interagency working group on manufacturing research and development, Instrumentation, metrology, and standards for nanomanufacturing, Tech. rep., National Institute of Standards and Technology, U.S. Department of Commerce, National Science Foundation, Office of Naval Research (2008).
- [6] X. J. Jiang, D. J. Whitehouse, Technological shifts in surface metrology, *CIRP Annals - Manufacturing Technology* 61 (2012) 815–836.
- [7] K. A. Cychosz, R. G. Nicolas, J. G. Mart 柳 nez, M. Thommes, Recent advances in the textural characterization of hierarchically structured nanoporous materials, *Chemical Society Reviews* 46 (2017) 389 – 414.
- [8] C. F. Cheung, M. Liu, R. Leach, X. Feng, C. Zhao, Hierarchical information based characterization of multiscale structured surfaces, *CIRP Annals* 67 (1) (2018) 539 – 542.
- [9] J. C. Wyant, Guest Editorial Precision Surface Metrology, *Optical Engineering* 23 (4) (1984) 349.
- [10] A. S. Soy, C. Ohrstrom, Investigation and Evaluation of Methods for Measuring Surface Texture on Worktops and Kitchen Fronts, mathesis, Lund University (2013).
- [11] D. G. Abdelsalam, B. Yao, Interferometry and its Applications in Surface Metrology, Chapter 5 in *Optical interferometry*, InTech, 2017.
- [12] B. Y. Lee, H. Juan, S. F. Yu, A study of computer vision for measuring surface roughness in the turning process, *The international journal of advanced manufacturing technology* 19 (2002) 295–301.

- [13] G. A. Al-Kindi, R. M. Baul, K. F. Gill, An application of machine vision in the automated inspection of engineering surfaces, *International Journal of Production Research* 30 (2) (1992) 241–253.
- [14] P. M-Arguello, J. Barreiro, E. Alegre, An evaluation of surface roughness classes by computer vision using wavelet transform in the frequency domain, *The International Journal of Advanced Manufacturing Technology* 59 (2012) 213–220.
- [15] S. I. Chang, J. S. Ravathur, Computer Vision Based Non-contact Surface Roughness Assessment Using Wavelet Transform and Response Surface Methodology, *Quality Engineering* 17 (2005) 435–451.
- [16] E. Alegre, J. Barreiro, M. Castejon, and S. Suarez, Computer Vision and Classification Techniques on the Surface Finish Control in Machining Processes, *Image Analysis and Recognition*, 5th International Conference, ICIAR 2008.
- [17] S. Sophia, A. Vicithra, S. Sangeetha, V. Mahitha, S. Hedayathbasha, Measurement of Surface Roughness Using Image Processing, *IOSR Journal of Electronics and Communication Engineering* (2017) 20–24.
- [18] X. A. Zheng, J. A. Soons, T. V. Vorburger, J. F. Song, T. B. Renegar, R. M. Thompson, Applications of Surface Metrology in Firearm Identification, *Surface Topography: Metrology and Properties* 2 (014012) (2014) 10pp.
- [19] A. Srivania, M. A. Xaviorb, Investigation of Surface Texture Using Image Processing Techniques, *12th Global Congress on Manufacturing and Management, GCMM*.
- [20] D. Imkamp, Looking at the future of manufacturing metrology: The VDI/VDE roadmap manufacturing metrology 2020, in: *Proceedings of the 5th Manufacturing Engineering Society International Conference - Zaragoza - June 2013*, 2013.
- [21] L. Nielsen, Evaluation of measurements by the method of least squares, J. Levesley, I. J. Anderson, J. C. Mason (Eds.), *Algorithms for Approximation IV*, University of Huddersfield (2002) 170–186.
- [22] L. Nielsen, Least-squares estimation using Lagrange multipliers, *Metrologia* 35 (2) (1998) 115–118.
- [23] M. S. Fernandez, MATLAB implementation for evaluation of measurements by the generalized method of least squares, *Measurement* 114 (2018) 218–225.
- [24] ISO 468:1982 Surface roughness – Parameters, their values and general rules for specifying requirements.

- [25] D. K. Cohen, Introduction To ASME B46.1-2009: surface texture (surface roughness, waviness, and lay), Tech. rep., Michigan Metrology, LLC (2011).
- [26] ISO 25178-2: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 2: Terms, definitions and surface texture parameters.
- [27] L. cooperation., 3D Optical Surface Metrology System Leica DCM 3D, 2015.
- [28] L. cooperation., Dual Core 3D Profiler combines Confocal Imaging and Interferometry, 2015.
- [29] K. Hossain, M. Milton, B. Nimmo, Metrology for the 2020s, Fiona Auty, the NPL Graphics Team, 2013.
- [30] T. G. Mathia, P. Pawlus, M. Wiczorowski, Recent trends in surface metrology, *Wear* 271 (3-4) (2011) 494–508.
- [31] D Imkamp, J. Berthold, M. Heizmann, K. Kniel, E. Manske, M. Peterek, R. Schmitt, J. Seidler, and K. D. Sommer, Challenges and trends in manufacturing measurement technology - the "Industrie 4.0" concept, *Journal of sensors and sensor systems* 5 (2016) 325–335.

Chapter 2: Objectives and Justification

Abstract: This chapter introduces the objectives that this thesis will achieve and make a justification for explanation of the necessities and importance of the work. Objectives of this thesis mainly include outlier identification and confocal system calibration. The rapid development of precision manufacturing technologies and the diversity of materials lead to higher and higher demands for precision metrology.

2.1 Objectives

This work consists mainly of five objectives:

- First, review the current literature of the science and technology of surface metrology. Surface metrology mainly embraces surface roughness characterization. It is determined by both the surface topographic measurement techniques and the relevant roughness parameters. The part of current literature review makes studies mainly about these two points. That is an introduction to the general concept, history, applications, etc. to the areal surface metrology, then focuses on the study of the two important topics which determine the characterization of surface roughness. Moreover, current literature of outlier identification methods, calibration approaches, and measurement uncertainty evaluation assessment, which determine the quality and the reliability of the surface metrology, are also should be studied.
- Second, study the mathematical models and develop the algorithms for 3D roughness parameterizations and for filtrations. Parameterization is to characterize the parameters of surface data, such as height parameters, spatial parameters, hybrid parameters, etc. Those parameters indicate various characteristics of surface textures. Filtration is feature operation used to create a non-ideal feature from a non-ideal feature or to transform one variation curve to another by reducing the level of information, separating surfaces into different wave components.
- Third, compare and implement the statistical methods for identifying outliers in raw measurement data. Data pre-processing is a very important part for surface roughness

characterization. Pre-processing of areal data includes treatment of non-measured points and treatment of measurement artefacts, as well as levelling and form removal, and filtering. There are two ways for the treatment of non-measured points, i.e. left them as non-measured or replace them with a plausible height value. The first method needs algorithms capable of excluding non-measured points and has an advantage of not introducing additional error. To replace non-measured points with a plausible height value needs compute them from interpolation of neighbouring points, interpolation or fitting of the surrounding valid pixels by median interpolation, splines, kriging, etc., all will introduce uncertainties. This work excludes non-measured points and investigates the identification of outliers for achievement of a better and more accurate characterization of structured surfaces.

- Four, calibrate the lateral and vertical scales of the system of confocal microscopy. Measurement deviations in the Z-coordinate and X- and Y-coordinate deteriorate the accuracy of surface characterizations, for which the lateral and vertical calibrations are evidently important. For the vertical calibration, a step-height standard artefact is implemented. For the lateral calibration, the theory of kinematic modelling for geometric errors is applied. A dot target grid standard is measured for data processing by algorithms.
- Five, make some experimental study to validate the proposed surface evaluation methodology. Several structured surfaces are measured by confocal microscopy. The measurement data is processed by all the methods proposed in this thesis, including outlier identification, filtration, calibration of the X- and Y-coordinate, calibration of the Z-coordinate, parameterization, uncertainty evaluation using Monte Carlo method. Final parameterizations with uncertainty evaluations are presented.

2.2 Justification

Recently the methods of surface characterizations have gained a lot of attentions by investigators and a big amount of investigation and application of surface characterizations are published. Science is completely dependent on measurement [1]. Metrology plays a fundamental part in sustaining a fair, efficient and technological society. To develop new products, services and processes, companies need to measure quantity, quality and performance [29]. Over the last decades, nano fabrication, micro fabrication, micro actuation, ultra precision engineering, etc. have enabled the development of Micro Electro Mechanical Systems (MEMS) for a wide variety of applications [3, 4]. Because of the increasingly strict

demands for precision measurement in industrial manufacturing, this thesis carries out the work aims at improving the precision of surface measurement using Confocal Microscopy.

Due to the rapid development of manufacturing technologies and diversity of materials, the surface texture of workpieces is more and more complicated. In this case, three-dimensional areal surface characterizations are becoming crucial and necessary, as which can provide information links the surface and its corresponding functions. Traceable results with uncertainty evaluations are much more reliable and applicable than the results given directly and simply by the measurement instrument. In current industry, where nanofabrication and ultraprecision machining are prevailing, many materials are required with atom-scale planarization, such as micro motors, semiconductor wafers, 3D printings, etc. Therefore, the uncertainties of measurement results will count a lot for the surface functions.

The reliability of a surface measurement result with uncertainty evaluations is highly dependent on the measurement procedures implemented. Fig.2.1 shows the measurement procedure in the field of surface texture. Every step of the measurement has significant impact on the reliability of the final result. Due to the limitation of the time for the development of this work, two important parts of the measurement procedure are investigated. One is the investigation of the statistical outlier identification methods; the other is the investigation of the calibration of the confocal microscopy system. Outlier identification is part of pre-processing areal data. Pre-processing areal data contains mainly four areas: treatment of non-measured points, treatment of measurement artefacts, levelling and form removal, and filtering. Outlier identification and system calibration lead to a more accurate and better characterization of structural surfaces.

Fig.2.1 Measurement procedure in the field of surface texture.

Areal characterization of surfaces is necessary in the area of industry and engineering. With the rapid increasing requirements on precision for manufacturing, it is notably necessary to improve the measurement procedures and techniques. This thesis proposes methods and algorithms for identifying outliers in surface measurement data, aiming at improving the accuracy of topography characterization by decreasing the impact of outliers. Methods and algorithms for calibration of the vertical and lateral coordinates of the confocal microscopy are also presented. This will allow more precise measurements and therefore better areal characterizations of the structured surfaces.

2.3 References of Chapter 2

- [1] P. Howarth, F. Redgrave, Metrology - in short 3rd Edition, EURAMET project 1011, participants: DFM Denmark, NPL United Kingdom, PTB Germany, 2008.
- [2] K. Hossain, M. Milton, B. Nimmo, Metrology for the 2020s, Fiona Auty, the NPL Graphics Team, 2013.

- [3] Y. Jia, and Q. Xu, MEMS Microgripper actuators and sensors: The state-of-the-art survey, Recent Patents on Mechanical Engineering 6 (2013).
- [4] PRIME Faraday Partnership, An Introduction to MEMS, Prime Faraday Technology Watch , 2002.

Chapter 3 Thesis Structure

Abstract: This chapter introduces the structure of the thesis.

The work of this doctoral thesis is divided into 11 chapters. The first chapter makes a general introduction of the surface metrology, such as the 3D measurement techniques for confocal microscopy, challenges and trends in measurement technology. The second and third chapters describe the objectives, the importance and necessity of this work, and the methodology as well as the structure of this work. The forth chapter review the current literature of the science and technologies. From chapter five on, is the realization of the study and research of areal characterizations of structural surfaces.

Chapter 5 makes a study of the mathematical models of 3D roughness parameterizations and filtrations. This chapter develops the corresponding algorithms for parameterization and filtration, as well as presents the results.

Chapter 6 introduces the statistical methods for outlier identification and makes a comparison of those methods for processing measurement data of structured surfaces.

Chapter 7 proposes a new method for outlier identification, introducing the statistical method, confidence distance matrix, for processing outliers in data measured by confocal microscopy. Confidence distance matrix has widely been used in statistics and many engineering areas, such as signal processing, but no bibliographies can be found until now that implementing confidence distance matrix for surface metrology.

Chapter 8 calibrates the X- and Y- axis of confocal microscopy system. This chapter presents a method for characterizing and correcting the geometric errors of the movement of the lateral stage of Imaging Confocal Microscopy in extended topography measurement.

Chapter 9 calibrates the Z- axis of confocal microscopy system. The influence factors on the calibration of Z coordinate include correction coefficients for raw measured heights, positioning inclinations, repeatability, reproducibility, light intensity, etc. Mathematical models and algorithms are developed and validated for the vertical calibration of the system.

Chapter 10 makes a conclusion about the work of this doctoral thesis.

Chapter 11 presents the references referred to by this thesis. The references shown in this chapter are organized separately as books, journals, standards, conferences, etc. by alphabetic order.

Chapter 4: Review of current literature

Abstract: Surface metrology mainly embraces surface roughness characterization, which is determined by two important things: the surface topographic measurement techniques and the relevant roughness parameters. This chapter first makes an introduction to the general concept, history, applications, etc. to the areal surface metrology, then focuses on the study of the two important topics which determine the characterization of surface roughness. Moreover, current literature of outlier identification methods, calibration approaches, and measurement uncertainty evaluation assessment, which determine the quality and the reliability of the surface metrology, are also introduced.

4.1 An introduction to areal surface metrology

Surface metrology is the science of measuring small-scale geometrical features on the surface, i.e. the topography of the surface [1]. From an engineering standpoint, it is the measurement of the deviations of a workpiece from its intended shape. It takes into account of features such as deviations from roundness, straightness, flatness, cylindricity, etc. [2]. Measurement of marks left on the workpiece in trying to get to the shape, which is the surface texture formed during machine process, as well as surface deviations on naturally formed objects are also included in surface metrology.

The first question for the surface metrology is the definition of the geometric extent of the surface layer, which is often termed as the layer from which the information is obtained by measurement instruments. But the depth that one technique can specify varies a lot from another. In material science, the surface layer will extend from atomic dimensions to micrometres [3]. Therefore, for some surface studies it is necessary to ensure that the bulk signal is small compared to the surface signal. Other definition about the surface is the

boundary that separates an object from another, substance, space, etc. Texture is defined as the composite of certain deviations that are typical of the real surface, including roughness and waviness, etc. [25]

Surface topography is important to the appropriate functions of many industrial products and with the increasing number of applications, the need for adequate control of surfaces and understanding of surface topography measurements is more and more important than ever [5]. To understand the role of surface metrology, considering how a workpiece fulfils its design could be the best way. Supposing a material has been selected correctly and the workpiece has been machined from it, the first thing to do is to measure its dimensions which should be conformed to its drawing to a tolerance. Dimensional measurement measures geometric features of an artefact, including length, position, radius, angle, form, or co-ordinate of a feature [6]. It should be the first aim because it assures that the size of the workpiece complied with its design and make sure that this workpiece can be assembled into a gearbox, an engine, etc., which are static characteristics of engineering products.

Although dimensional metrology assures static characteristics of products, it is not sufficient to make sure those pieces will function well, for example, they might not rotate or move. This is where the surface metrology becomes important, as it ensures all the aspects of the surface geometry are known and preferably controlled. When both their shape and surface texture are compliant with the corresponding design, workpieces would be able to move at the speeds, loads, and temperatures specified by their designers. Surface metrology assures dynamic characteristics. Surface metrology was essentially a mechanical engineering discipline, but with its rapid development it has broaden into other disciplines. Recent years, surface metrology has been interwoven with tribology, nanotechnology, etc., since surface geometry and texture have significant influence on the performance of these subjects [7].

The third measurement is the physical metrology which is to know the long-term characteristics. It concerns the physical and chemical condition of workpieces, including the hardness of the materials, the residual stress of the surfaces, metallurgical structure, chemical constructions, etc. These characteristics contribute to the durability of the components, such as resistance to corrosion or fatigue. Surfaces play crucial role in many thermal, chemical, physical, and mechanical processes, such as oxidation, adhesion, corrosion, friction, wear, erosion, etc. [8].

Fig. 4.1 The role of surface metrology

Summary of the roles of the surface metrology is shown in Fig. 4.1. Within the scope of surface geometry, metrology can be classified as dimensional metrology, surface metrology, and physical metrology. Each assures static, dynamic, and long-term characteristics of workpieces from an engineering standpoint.

This thesis focus on investigation of surface metrology, but it should be noticed that all three types of metrology are necessary to ensure a workpiece function well. As a matter of fact, all these three types of metrology influence mutually, none of them can divorce itself completely from the others. To characterize a solid surface, information is searched on the topography of the surface, on its structure, chemical composition, and its quantitative distribution of the elements [3].

With the development of surface metrology, it is undergoing a paradigm shift from profile to areal, from traditional stochastic to structured surfaces and from simple geometries to complex free-form geometries. This shift of surface metrology was together with three historical paradigm shifts, i.e., instrumentation, digital methods, form and texture instruments [1]. For most materials, the surface composition is different from the bulk. This phenomenon might be intentional, such as coatings, or unintentional, for example contaminations [3]. This difference can be an advantage or a disadvantage. The importance of surfaces, interfaces, and boundaries increase markedly in recent time and as a consequence surface texture and features take on a significant important role [9].

Measurement standards are those artefacts, devices, procedures, systems, instruments, protocols, processes, etc. that are used to define measurement units and on which all less accurate measurements depend [10]. In 1875, the United States and 16 other countries signed the ‘Treaty of meter’ to establish a common set of units for measure and established the

International Bureau of Weights and Measures (BIPM). The units set up by BIPM were based on kilogram and meter instead of pound and yard. This system of units is called the International System of Units, known as its abbreviation SI, compiled by BIPM [11]. However, SI cannot guarantee measurement agreement due to lack of the knowledge of accuracy in measurement. Therefore, standards for measurement are necessary. The earliest standards were based on human body, later were based on natural phenomena. Due to the improvement of scientific sophistication, the basis for the measurement system changed significantly. Now in the world there are lots of standards bodies such as International Organization for Standardization (ISO), American Society of Mechanical Engineering (ASME), Institute of Electrical and Electronic Engineers (IEEE), etc., as shown in Fig. 4.2.

Among all the standard organizations, ISO, BIPM, ASME, JCGM are mostly referenced by works developed in this thesis. The series of ISO 25178 defines areal surface parameters and the related standards and metrological characteristics [12]. Filtration methods are specified in the series of ISO 16610 [13]. These two series as well as some other standards, such as ISO/TR 13587:2012 [14], ISO 13565 [15], etc., are organized by ISO. Guide to the Expression of Uncertainty in Measurement (GUM) [16] and International Vocabulary of Metrology (VIM) [17] are two guides administrated by Joint Committee for Guides in Metrology (JCGM) and were developed by ISO Technical Advisory Group 4 (TAG 4) [17]. The JCGM has two working groups. The first group (JCGM/WG 1) is responsible for promotion of utilization of GUM and preparation of supplements for GUM for its wide applications. The second group (JCGM/WG 2) has the task of revising VIM and promoting its application. JCGM reports to BIPM and BIPM is under the supervision of International Committee for Weights and Measures (CIPM) [11]. For algorithm validation, standard data base provided by National Institute of Science and Technology (NIST) can be used through the Internet Based Surface Metrology Algorithm Testing System [18]. Good practice guides (NPL GPGs) and standard artefacts provided by National Physical Laboratory are referred to for the development of this work [19] [20].

Fig. 4.2 Standards membership bodies.

4.2 An overview of surface topography measurement techniques

Developments of instruments for surface metrology can be traced back to the early 1930s when G Schmalz, J Abbott and A Firestone first introduced a stylus instrument for scanning over a surface picking up information from workpieces [2] [30]. The assessment of surfaces in those early days employed two-dimensional surface profiles [23]. Due to the increasing enquiry of surfaces and demands for new assessment techniques, surface measurement instrument undergoes lots of evolutions to higher orders. The sophistication of industrial practice in measuring surface roughness is increasing steadily with the improvements in instrumentations. Metrologic techniques have advanced from central-tendency and dispersion statistics of surface-topographic profiles of metal bearings, through modelling of two-dimensional samples to a major shift now underway [24]. Surface measurement techniques now are available for characterizing surface textures, shapes, chemical, physical, and micromechanical properties, as well as composition and chemical states of any solid surface [8]. For surface characterization, such as film thickness, plastic deformation, and fracture damage, there are optical profiler and laser interferometry, confocal microscopy, optical scatterometry, light microscopy, stylus profilometry, scanning tunnelling microscopy (STM), atomic force microscopy (AFM) or scanning force microscopy (SFM), variable-angle spectroscopic ellipsometry (VASE), X-ray fluorescence (XRF), etc. For physical metrology, such as hardness, mechanical strength measurements, etc., exist mechanical strength

microprobe for microhardness and nanohardness measurements, micrometre and nanometre scratch hardness measurements. For elemental composition and chemical state measurements, there are scanning electron microscopy (SEM), electron probe x-ray microanalysis (EPMA), energy-dispersive x-ray spectroscopy (EDS) or wavelength-dispersive x-ray spectroscopy (WDS), high-resolution electron energy-loss spectroscopy (EELS), auger electron spectroscopy (AES), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, etc. Tab. 4.1 summarizes the information on surface topography measurement techniques. K. Miyoshi [8] has concluded three types of popular analytical techniques, including profilometry and quantitative measurements of film thickness, plastic deformation, and fracture damage, surface microprobes for hardness and mechanical strength measurements, and instruments for elemental composition and chemical state measurements

Tab. 4.1 Information on surface topography measurement techniques [8].

Technique	Main information	Vertical resolution (depth probed, typical)	Lateral resolution (typical)	Types of solid specimen (typical)	Use (Popularity)
Optical profiler and laser interferometry	3D and 2D imaging Morphology Profilometry Topographic mapping Film thickness Wear volume Scar and crater depth Defects	-0.1 nm	A few sub μm to a few tens of μm	All	Medium
Confocal microscopy	3D and 2D imaging Morphology Profilometry Topographic mapping Film thickness Wear volume Scar and crater depth Defects	Variable (from a few nm to a few μm)	Optical, 0.5 to 4 μm ; SEM, 1 to 50 μm	Almost all	Medium
Optical scatterometry	Profilometry Topographic imaging/mapping	≥ 0.1 nm	A few sub μm to a few tens of μm ;	Almost all	Not common

Traceable Characterization of Areal Topography of Structured Surfaces using Confocal Microscopy

	Periodic structure		$\geq$ laser		
	Morphology		wavelength $\lambda/2$		
	Defects		for topography		
Light microscopy (general)	Imaging	Variable	Variable	All	Extensive
	Morphology				
	Damages				
	Defects				
Stylus Profilometry	Profilometry	0.5 nm	100 nm	Almost all; Flat smooth films	Extensive
	Topographic tracing				
	Film thickness				
	Morphology				
	Scar and crater depth				
	Wear volume				
Scanning tunnelling microscopy	Topographic imaging	< 0.03 to 0.05 nm	Atomic	Conductors	Medium
	Compositional mapping				
	Morphology				
	Profilometry				
	Film thickness				
	Spectroscopy				
	Structure				
	Defects				

Developments of instrumentation for surface metrology evolved in two methods. One is the optical methods which focus on lateral structure, namely spaces and details in the plane; the other is the stylus methods, examining heights in the plane perpendicular to the surface [7]. The two different evolutions have become one of the main classification methods of those current measurement instruments, that is, according to the data collection mechanism, measurement instruments can be classified into contacting systems and non-contacting ones. The contacting systems mainly include mechanical stylus instruments, such as Scanning Tunneling Microscope, Atomic Force Microscopy, etc. The non-contacting systems incorporate optical focus detection, optical interferometry, light scattering, capacitance scanning-probe techniques, etc. [23] Categorisation of those surface topography measurement instruments is shown in Fig. 4.3.

Fig. 4.3 Schema to categorize surface topography measurement instrument.

Optical focus detection, interferometry, and capacitance scanning probe techniques are most popular ones among the non-contacting systems. Optical focus detection system are used when contacting with specimen surface are not allowed or adorned. This system projects strong convergent laser beams onto the surface of the workpiece and a focusing lens move vertically to maintain focus. Focusing lens is controlled by a focus error signal from a piezo electric circuit. This signal detects the variations in the distance to its true focal point. Movements of the lens represent the areal heights deviations of the surface. Areal measurements are realized by either raster scanning on the surface of workpieces by laser sensor or in a converse way by raster scanning the laser head. It works in a way

similar to the stylus instruments which only measure a single point at a time. While optical instruments incorporate another type of instruments, which use a CCD or similar devices to measure the entire field of view similar to a camera [25]. Caution should be paid when using the optical focus detection system for the following reasons. First, this system requires sufficient reflection of laser beam for which opaque surfaces cannot be measured. Second, when the focusing lens encounters with steep slopes, it will lose its focal point and rapidly searches for focus in the z plane before finding again the surface in its next scan position, which renders spurious sparks and sharpening pits registered in its collected data. Last but not least, the interference between reflected beam lights upon measuring smooth surfaces as well lead to spikes in the surface data.

Interferometry systems are used where nanometre scale resolution is required. This system works on the principle of interference of two beam lights and one of the beam lights is required as reflected off from the workpiece surface. A reference surface is built into the interferometer, lights from the surface of workpieces and from the reference surfaces interfere with each other, generating interference pattern. Phase deviations in the fringe pattern represent the height deviations of the surface. Two most widely used interferometry techniques are phase shifting interferometry and scanning differential interferometry. Although the optical interferometry systems can be of nanometre scale resolution, it is difficult to measure rapid slope changes. In addition, environmental vibration isolations are required for maintenance stable optical path.

Scanning tunnelling microscopes (STMs) and Atomic Force Microscopes (AFMs) can achieve sub-angstrom scale of resolution. Both two microscopes utilize a tiny probe tip raster scanning workpiece surfaces. The difference between these two systems is that STM requires the probe tip be conducting material, while AFM has no such requisition. This difference comes from their different working principle, as STM works on a bias voltage of 2 mV – 2V, while AFM depends on the deviation of the reflective light beam from the probe tip [26]. The major problem of stylus instruments is that they require direct contact with the surface which might cause scratches and slow measuring speed [27]. Other disadvantages of stylus instruments include that the instrument readings are based on a limited number of line samplings, which might not represent the real characteristics of the

surface under investigation. Besides these, the limits of the sampling length could as well render errors in the instrument readings. Fig. 4.4 shows typical lateral ranges of sensitivity for stylus profiling instruments [5]. The sensitivity is the unity in the middle of the range.

Fig. 4.4 Typical bandwidth limits for stylus instruments: two cutoffs for two RC filters.

Source: Tutorial in optics [5].

Those surface topography instruments have various working range of vertical and lateral resolutions. Amplitude-wavelength plot for the above instruments are presented in Fig. 4.5. The two axes represent the lateral and vertical resolutions, the orthogonal lines drawn from point P to points Pt, Pl, Pr (top, left, right) indicates the ratio of range to resolution, the greater the length, the bigger the ratio. Each block with colours gives an indication of the working range of instruments, the bigger the block, the larger application of the working range. Diversity of the measurement instruments give a good resolution to the problem of the wide range of texture obtained during manufacture, from milling, which produces sub-millimetre roughness, to polishing, which produces nanometre values [1]. Optical instruments provide versatile working ranges, from capacitance-based methods for rougher surfaces, to interferometry for nanometre scale resolution. Although this thesis deals with confocal optical microscopy, it is also important to know that optical instruments cannot fulfil all the requirements of measurement and this is why stylus methods also prevailed for general use.

Fig. 4.5 Amplitude-wavelength plot of the working range of surface topography measurement instruments.

4.3 An introduction to roughness parameters

Surface roughness is highly related with many fundamental problems, such as friction, contact deformation, heat and electric current conduction, tightness of contact joints, positional accuracy, etc. [28]. Parameters extracted from surface profiles and areal topographies constitute actual information that can be used as the link between surface functionality, processing variation, and surface texture [29]. Therefore, a variety of parameters have been defined over years, some are very specific to certain applications, others more generally used in a number of situations. Surface parameters generally include height parameters, spatial parameters, hybrid parameters, functions and related parameters, miscellaneous parameters, as introduced in ISO 25178-2: 2012 [26], and this classification can be found in Fig. 4.6. These parameters from the texture can describe the areal amplitude characteristics, spacing characteristics, or some characteristics associated with the general shape of the profile. This is the purpose of defining parameters, succinctly extract meaningful information from surface texture that could then be related to the

functional performance of the part. Height parameters provide a measure of the height or depth of the profile elements from the mean line, and spatial parameters provide a measure of the spacing between the peaks and valleys.

The introduction of the definitions and parameters for the determination of surface texture by areal methods are part of ISO 25178-2: 2012 specifies terms [26]. All areal height parameters are defined over the definition area.

Fig. 4.6 Areal parameters introduced in ISO 25178-2:2012 [26].

Roughness parameters can be described both in two-dimensional and three-dimensional forms. The two-dimensional roughness parameters are calculated based on information from a profile and indicate only the information of a profile, while the three-dimensional parameters have information on areal surface.

Specifications, definitions, mathematical models, etc. of the currently used 3D parameters are described in detail in section 5.1 in Chapter 5. Those parameters are implemented in the subsequent experimental work of the thesis.

4.4 Approaches to outlier identification in areal surface metrology

Outlier detection has attracted considerable interest because misuse of outliers deteriorates substantially the outcome of model updating, leading to erroneous and drastically misleading predictions [31]. Removing data points on the basis of statistical analysis without an assignable cause is not sufficient to throw data away [32].

Raw measurement data file obtained from optical instruments are often affected by local measurement defects due to limitation of techniques. It is necessary to remove these defects before metrological analysis. Defects of raw measurement data mainly include unmeasured points and measurement artifacts. These defects are usually caused by local slopes, scanning speed, light intensity, material transparency, circular groove, etc. [33]. Optical instruments analyse lights received by the detector. However, due to the limitation of objective lens, only lights reflected from zone 2 can be received, as shown in Fig. 4.7. A ray coming from zone 1 will be reflected outside the objective lens. The detector needs sufficient light for the detection algorithm be able to detect the peak position, otherwise it will generate unmeasured points.

Fig. 4.7 Left: only the light coming through zone 2 is reflected to the detector; Right: almost all light is reflected outside the detector [33].

The maximum slope, $\alpha_{\max}$ is related with numerical aperture of the lens, as shown in Equation 4.1 and Tab. 4.2.

$$\alpha_{\max} = \sin^{-1} A_N \quad (4.1)$$

Tab. 4.2 Maximum measurable slope against numerical aperture [34].

Numerical aperture	Maximum slope (specular case)
--------------------	----------------------------------

0.3	$\pm 18^\circ$
0.4	$\pm 24^\circ$
0.5	$\pm 30^\circ$
0.6	$\pm 37^\circ$
0.7	$\pm 44^\circ$

In fact, surfaces such as matt metal, plastics, rubber, etc., often have roughness creating diffusion reflection, as shown in Fig. 4.8. In this case, some part of those light will reach the objective lens even if the slope exceeds $\alpha_{\max}$. Besides the surface slope, material reflectivity, power of light source, and acquisition frequency also influence the amount of light received by measurement system detector.

Fig. 4.8 Reflection on a diffuse surface [34].

Scanning speed is a parameter usually chosen by operator during measurement. This speed is limited by acquisition frequency of the probe f_{probe} . This frequency determines the exposure time during which the detector accumulates light coming back from the sample. The exposure time t_{exp} is inverse of the acquisition frequency as indicated by Equation 4.2.

$$t_{\text{exp}} = \frac{1}{f_{\text{probe}}} \quad (4.2)$$

Light intensity received by detector must be within a low boundary and a high boundary. If the light intensity is too low, there will be no peak detected above the noise level and results in a non-measured point. If the light is too bright, the detector will be saturated and the peak will be truncated leading to erroneous calculation of the height.

If the material has a circular groove, then the detected point will be in the centre of the circle as shown in Fig. 4.9, instead of on the surface. Therefore, this will generate an outlier which is known as ghost foci.

Fig. 4.9 Ghost focus on a circular Groove [34].

When the material is transparent, the refractive index must be taken into account as which changes the true height of the surface point as shown in Fig. 4.10. The depth must be corrected by Equation 4.3:

$$d = \frac{d'n'}{n} \quad (4.3)$$

Where, n is the refractive index outside the material, n' is the refractive index of the measured material.

Fig. 4.10. The sensor ‘sees’ a depth d' while the true thickness is d [34].

Outlier detection has attracted considerable interest because misuse of outliers deteriorates substantially the outcome of model updating, leading to erroneous and drastically misleading predictions [31]. Removing data points on the basis of statistical analysis without an assignable cause is not sufficient to throw data away [32].

Raw data provided by measurement instruments like confocal microscopy often contains non-measured points and measurement artefacts. Treatment of these abnormal points is necessary for a high accuracy. Series of ISO 16610 define various types of filters to separate surfaces into different scales [35]. However, linear filters often follow outliers [36]. Although some robust filters do not, they were designed mainly for the conventional stochastic surfaces. Because of the existence of micro and nano-scale feature patterns, many statistical methods which worked very well with the conventional stochastic surfaces do not perform the same to the structured surfaces [25], as shown in Fig. 4.11. For example, some methods for interpolation of spatial data, such as nearest neighbour, natural neighbour, they interpolate a point based on its neighbour point, which is unreliable for structured surfaces as whose point of background and features usually differ significantly.

Fig. 4.11 Pattern units (blue) and individual features (red) of a structural surface.

Confocal microscopy is used in this work, it is very common having unmeasured points and measurement artefacts together in one surface measurement, especially measuring structured surfaces, such as hydrophobic materials, which are constructed with complicated pattern units.

There are two ways for treatment of unmeasured points: left them as unmeasured and the calculation algorithms need to be able to exclude those points; or replace those unmeasured points with a plausible height value, using methods of interpolation of neighbouring points, or methods of interpolation or fitting of the surrounding valid pixels for determination of a best fit value. Some investigators prefer the first method for not introducing additional error [25]; Some others tend to fill in small unmeasured areas for obtain a complete measured surface, but left large unmeasured areas for which might be holes [33].

A surface topography can be viewed as a superposition of different scales of geometrical features and these features are usually scaled as form, waviness, and roughness [36]. Besides these three components an engineering surface might also have data inclination, noise, and outliers. All of these features can be separated by filters while outliers are managed as part of noise [37]. Series of ISO 16610 has defined three kinds of areal filters, i.e. linear areal filters, robust areal filters, and morphological areal filters [38]. Areal Gaussian filter is the default linear areal filter, it is widely used by almost all the instrument manufacturers, however, this filter is not robust against outliers and in fact it

often follows outliers [37, 36]]. Robust areal filters are defined as Gaussian Regression Filters. As indicated in ISO 16610-30 [39] robustness is not an absolute property of a filter but a relative one. One can only say that some filter is robust compared to an alternative filter against a particular phenomenon. In series ISO 16610 Robust Areal Filters are named reference to their defined Linear Areal Filters, which does not mean the Robust Areal Filters defined by series ISO 16610 are absolutely robust against outliers. In fact, some previous investigators have presented that those robust filters neither can completely remove those outliers from the dataset [37].

Another disadvantage of those linear areal filters is that they map each point on a surface to a weighted average of its neighbour points, as shown in Equation 4.4 [34], where $z(s)$ is the unfiltered profile or surface, and $K(x, s)$ is the kernel function. $K(x, s)$ is required to be real, symmetric and space invariant, and it is the weighting applied to average those input data. Different choices of the kernel function will lead to different linear filters.

$$y(x) = \int_{-\infty}^{+\infty} K(x, s)z(s)ds \quad (4.4)$$

For the traditional stochastic surfaces those linear areal filters or robust areal filters might work well by mapping a point to a weighted average or its neighbour point, but for structural surfaces, those filters are very likely to fail as features and background on a pattern unit often vary a lot. However, shift from stochastic to structured surfaces is among the three important aspects of current paradigm shifts in surface metrology, while the other two aspects are shift from profile to areal characterization and from simple geometries to complex freeform geometries [40].

ISO 16610-30 [39] also declared the importance of data pre-processing, indicating that pre-processing followed by a filter results in a robust filter and it has an advantage that once a method has been found to be capable of remove unwanted phenomena, then it will work with any filter [39]. This standard also defined two pre-processing methods, i.e. scale-space pre-processing and wavelet pre-processing. However, these two methods are aimed at removing profile discontinuities before filtration, but not used to remove outliers.

M. F. Ismail, *et al.* proposed an outlier correction procedure applied to areal surface data measured by optical instruments [37]. Their procedure includes two stages: outlier candidates' detection and outlier verification. For outlier candidates' detection, they first determine the sufficient size of an outlier detection window, and make the reference of the detection by the relative height between the median of the surrounding data and the observed data. The difference will be noticeable when the observed data is outlier and the surrounding data are normal data. To have the median value of the surrounding data arise from normal ones, the investigators have to enlarge the detection window. This makes their algorithm cumbersome and unreliable for various reasons. First, enlarged detection window might reach other clusters of outliers which against the expectation of normal data. Second, for structured surfaces points between background and features usually differ a lot, median value of the surrounding background might do not have obvious difference with outliers on the feature. They also defined methods for setting threshold value, outlier verification and correction, with illustrations of application for measurement of surface of dental implant, as well as compare their proposed method to Gaussian filter and median filter, and it shows that their proposed method function obviously better than those typical filtering methods. This method work well with stochastic surface with simple distribution of outlier clusters but might fail when applied to structured surfaces or to those surfaces containing adjacent outlier clusters.

Yutao Wang, *et al.* investigated the formation of outliers in scanning reflective surfaces and developed two outlier formation models due to mixed reflections and multi-path reflections [41]. Their developed outlier formation models can be applied to sensor view and scan path planning. Besides this, they also proposed an outlier detection method for scanned point clouds using majority voting [42]. The main feature of their method is the majority voting scheme to reliably remove connections between non-isolated outlier clusters and the scanned surface even when these outlier clusters form planar patches.

4.5 Calibration methods for surface metrology system

In order to substantiate or validate those measurements by metrological instruments, it is very important to assure those measurements are correct and comply to the international or

national standards, or are compliant with both [43]. With the development of nanotechnology, there is a growing requirement of using traceable measurement and verification systems from the metrological point of view, in order to ensure a reasonable level of confidence conformity specifications to make sure that the final products will operate smoothly as well as good interchangeability between their components. It is necessary that the measurement results are traceable from the metrological point of view, and this indicates that [44]:

- a) The instrument which is used to measure has been previously calibrated with traceable physical measurement standards;
- b) The calibration correction of the instrument has been determined;
- c) Uncertainties of the calibration of the instrument have been estimated and the measurement results are calculated by the method described in the guide ISO-GUM or other equal standards.

Current industrial demand is that areal surface topography measuring instrument should provide traceable measurement result. In 2002, the International Organization for Standardization (ISO) Technical Committee, dealing with Dimensional and Geometrical Product Specifications and Verifications (TC213), formed Working Group 16 to address standardization of areal (three dimensional) surface topography measurement methods. Working Group 16 develops a number of draft standards (the ISO 25178 series) encompassing definitions of terms and parameters, calibration methods, file formats and characteristics of instruments. Under this process, a project team is developing specification standards for areal surface topography measurement including calibration techniques.

According to the International vocabulary of metrology — Basic and general concepts and associated terms (VIM) [17], metrological traceability is the “*property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty*”.

A complete traceability route for areal surface texture measurements requires the following elements:

- i. *calibrated areal physical measurement standards (ISO/FDIS 25178-70: 2012) [45] or standard artifacts for calibrating areal surface topography measuring instruments or means for calibrating the geometric deviations of the x and y axes and the probe movement;*
- ii. *software measurement standards for calculating areal surface texture parameters; and*
- iii. *Methods for calculating the uncertainties associated with areal surface topography measuring instruments and surface texture parameters.*

There is a summary of necessary elements of metrological traceability in Fig. 4.12.

Fig. 4.12 Summary of the definitions of metrological traceability.

Besides this, it is recommended that the instrument calibration of the confocal systems should be separated, for example, measurement of slopes should be separated from the measurement of planes, and measurement of different materials should be complied with different instrument calibration. Moreover, calibrating an instrument for all possible measuring conditions is difficult and lengthy. Therefore, the solution is to calibrate the instrument for task specific applications. For instance, choosing of the physical measurement standard and the spatial width as well as measurement precision are decided by the surface features to be measured, in addition to other measurement conditions, such as environmental temperature and sample cleanliness. It is necessary to emphasise that the environmental conditions of the instrument calibration should be similar to the

measurement working environmental conditions; otherwise the calibration process will not assess the true performance of the instrument.

Areal surface texture measurements involve a simple task of measuring a set of points across the surface of a component, but the difficulty of instrument calibration lies in the assessment of the effect of multitude factors that contributes to the measurement uncertainties. The effect of the factors that contributes to the measurement uncertainties can be determined by the metrological characteristics of instruments. These metrological characteristics generally involve [46]:

- Measurement noise;
- Flatness deviation;
- Linearity errors;
- Amplification coefficient;
- Perpendicularity of the axes; and
- Resolution of the measurements along the axis of operation.

It is only general introduction of metrological characteristics of measurement instrument. ISO 25178-602: 2010 [47] have a detailed study about the characteristics, which will be introduced here in the latter part. Before the study of the metrological characteristics which contributes to the measurement uncertainties, it is important to have an overview of the method of conducting the instrument calibration which is the essential step for acquirement of traceable metrologies. Operations of instrument calibration can mainly be classified into four steps, which is stated below and also summarized in Fig. 4.13.

Fig. 4.13. Flow of operations of calibration of confocal measurement instrument.

Step 1: Establish the measurement conditions for the surfaces to measure, such as sampling interval, environmental conditions, etc. Choose the appropriate set-up parameters of the confocal microscopy suitable for the spatial bandwidth of the surface, such as magnification lens and numerical aperture. Generally to say, establish the measurement conditions that are directly related to a particular function of the surface. These measurement conditions for calibration of the instrument and for measure surfaces should be similar. Otherwise the calibration will be meaningless as the measurement conditions contribute to the sources of metrological characteristics, which in turn generates different uncertainty sources.

Step 2: Make appropriate configurations of the optical confocal microscopy. This part mainly includes the appropriate application of surface texture filters, optical nesting index combinations, and physical measurement standards. The meaning of the majority of the areal parameters depends on the type of scale-limited surface used. ISO 25178 part 3 [48] defines two categories of filters: the S-filter and the L-filter, as shown in Fig. 4.14. The S-filter is defined as a filter that removes the unwanted small-scale lateral components, such as measurement noise, spikes, or functionally irrelevant unwanted small features. The L-filter is defined as a filter that removes the large-scale lateral components of the surface. Besides the S-filter and L-filter, F-operator is also used, which is the nominal form removal, achieved typically by using a least-square method. Recently there is a significant development of the filter types and systems, as shown in Fig. 4.15 it has been necessary to produce a standardized framework for filters, and information about these filters has been published as a series of technical specifications in ISO/TS 16610 series. The classes of filters involve:

First, linear filters, which include the mean line filters (M-system), as well as Gaussian filters, spline filter, and the spline-wavelet filter.

Second class involves morphological filters, which include the envelope filters (E-system), and closing and opening filters.

Third, robust filters, they are robust respect to the filtration of specific phenomenon such as spikes, scratches, and steps. This class includes the robust Gaussian filter and the robust spline filter.

Finally, segmentation filters. These class of filters partition surfaces into parts according to specific rules. The motif approach belongs to this class and now has been put on firm mathematical basis.

Fig. 4.14 Relationships between the S-filter, L-filter, F-operator and S-F and S-L surfaces.

Source: Good Practice Guide No.128 [20].

Fig. 4.15 Classes of recent significant development of filters.

The scale at which the filters operate is controlled by the nesting index. The nesting index is an extension of the cut-off wavelength used in profile analysis and is suitable for all types of filters. The S-filter nesting index (equivalent to λ_s filter in the profile case) allows the selection of the maximum sampling distance (the sampling distance is at least three times the S-filter nesting index). The selection of the S-filter nesting index should be based on the instrument lateral resolution and the lower limit of the measurement spatial bandwidth of interest. The L-filter (equivalent to λ_c filter in the profile case) or the F-operator nesting index could be based on the size of the measured area and their values should be smaller than the upper limit of the measurement bandwidth of interest and at least five times the scale of the coarsest structure of interest. Tab. 4.3 reproduces proposed recommended sets of nesting indices from ISO 25178-3:2012 [48].

Tab. 4.3 Relationships between nesting index value F-operator/L-filter, S-filter nesting index, and bandwidth ratio. n is a positive or negative integer. [20].

Nesting index value (F-operator/L-filter) / 10^n mm	S-filter nesting index / 10^n μ m	Bandwidth ratio between F-operator/L-filter and S-filter nesting index
1	10	100:1
	5	200:1
	2	500:1
	1	1000:1
2	20	100:1
	10	200:1
	5	400:1
	2	1000:1
2.5	25	100:1
	8	300:1*
	2.5	1000:1
5	50	100:1
	20	250:1
	10	500:1
	5	1000:1
8	80	100:1
	25	300:1*
	8	1000:1
*Rounded value		

The physical measurement standard, which is also known as standard artefact, is very important to the instrument calibration. ISO 25178-70:2014 [45] identifies thirteen types of profile standard artefact and eleven types of areal standard artefacts. Tab. 4.4 has a list of the areal physical measurement standard.

Tab. 4.4 Physical measurement standard for areal material measures identified in ISO 25178-70:2014 [45].

Number	Type	Name
1	AGP	Grooves, perpendicular
2	AGC	Grooves, circular
3	ASP	Hemisphere
4	APS	Plane-sphere
5	ACG	Cross grating
6	ACS	Cross sinusoidal
7	ARS	Radial sinusoidal
8	ASG	Star-shape grooves
9	AIR	Irregular
10	AFL	Flat plane
11	APC	Photochromic pattern

Step 3: The third step of the instrument configuration lies in the determinations and measurement of metrological characteristics contributing to uncertainties, which is one of the most important parts. The metrological characteristics can be mainly classified into groups of measurement noise, flatness deviation, amplification, linearity, perpendicularity, resolution. ISO 25178-602: 2010 [47] identifies amount number of metrological characteristics.

Step 4: The forth step, also the final work of instrument calibration is the data processing and uncertainty calculation. This process should follow the software standard and specifications described in Guide to the Expression of Uncertainty in Measurement (GUM) [16], the International Organization for Standardization (ISO), etc. or other equivalent level of standardizations. Uncertainties can be calculated according to the classifications of the metrological characteristics, and each contribution has different statistical propagation distribution, and different mathematical calculation method.

a. Measurement noise and flatness deviation contribution

If the measurement noise and flatness deviation are estimated separately, the measurement noise contribution to the overall measurement uncertainty is propagated in the form of normal distribution with the expectation equal to zero and a variance equal to the square of the value of the measurement noise. The flatness deviation contribution to the overall measurement uncertainty is propagated in the form of a rectangular distribution that has the variance equal to $Sz_{\text{flatness}}^2/12$. The combined measurement uncertainty is given by

$$\mu_{NF} = \sqrt{Sq_{noise}^2 + \frac{Sz_{flatness}^2}{12}} \quad (4.5)$$

Where, μ_{NF} is the combined uncertainty of measurement noise and flatness deviation contribution, Sq_{noise} is the uncertainty of measurement noise contribution, $Sz_{flatness}$ is the flatness deviation contribution.

b. Amplification, linearity, and perpendicularity contribution

The calculated amplification coefficients (αx , αy and αz) are either used to adjust the instrument or the instrument is used without correction. Also, the adjustment process implies that the amplification and linearity tests have to be repeated, which means that the uncertainty contribution of the amplification and linearity can be calculated as the combined uncertainty of the measurement errors, traceability, reproducibility and repeatability.

The contribution of the measurement errors to the overall measurement uncertainty (u_{error}) is propagated in the form of a rectangular distribution that has a variance equal to the square of the value of the error divided by three ($\delta_{error}^2/3$). The contribution of the measurement traceability and reproducibility and repeatability to the overall measurement uncertainty ($u_{traceability}$, u_{repeat} , u_{reprod}) are propagated in the form of a normal distribution that has an expectation equal to zero and a variance equal to the square of the value of the repeatability of reproducibility or traceability ($u_{traceability}^2$, u_{repeat}^2 , u_{reprod}^2). The combined effect of the measurement errors, traceability, repeatability and reproducibility on the coordinate measurement standard uncertainty u_{T-x} , u_{T-y} , u_{T-z} is given by

$$\mu_{T-i} = \sqrt{\mu_{traceability}^2 + \mu_{repeat}^2 + \mu_{reprod}^2 + \mu_{error}^2} \quad (4.6)$$

Where, $i = x, y, z$.

The perpendicularity between the x and y axis contribution to the measurement uncertainty is propagated in the form of a rectangular distribution that has a variance equal to the square of the value of the maximum possible length error produced by the cosine error divided by three.

c. Lateral resolution

The lateral resolution contribution to the measurement uncertainty (u_{Res}) is propagated in the form of a rectangular distribution that has a variance equal to the $Res^2/3$, where Res is the lateral topographical resolution.

Tab. 4.5 gives a summary of calibration results.

Tab. 4.5 Template for summary of calibration results. Source: Good Practice Guide No.128 [20].

Metrological characteristic (Unit)	Comments		Value /Unit	Uncertainty contribution /Unit
x y measurements				
amplification and linearity (.....)	Physical measurement standard SNo/Type: Nominal pitch:.....mm Calibration range: x range:mm y range:mm	Tested measurement range: x range: from.....% to% y range: from.....% to% z range: from.....% to%		
x and y perpendicularity (.....)	Physical measurement standard SNo/Type: Method used:	Tested measurement range: x range: from.....% to% y range: from.....% to%		
resolution (.....)	Physical measurement standard SNo/Type: Method used:	Tested measurement range: x range: from.....% to% y range: from.....% to%		
x y standard uncertainty (.....)				
z measurements				
Measurement noise (.....)	Filters nesting index: S-filter: μm L-filter:.....mm	Physical measurement standard S/No:..... Calibrated: YES/No		

	Method used: Subtraction Addition Calibrated flat	Tested measurement range: x range: from.....% to% y range: from.....% to% z range: from.....% to%		
Residual flatness (.....)	Filters nesting index: S-filter: μm L-filter:mm Method used: Average Calibrated flat	Physical measurement standard S/No:..... Calibrated: YES/No Tested measurement range: x range: from.....% to% y range: from.....% to% z range: from.....% to%		
amplification, linearity (.....)	Physical measurement standard(s) SNo/Type: Nominal Value(s):mm Calibrated range: z range: mm	Tested measurement range: x range: from.....% to% y range: from.....% to% z range: from.....% to%		
z standard uncertainty (.....)				

According to the ISO 25178-602: 2010 [47], characteristic of measuring equipment may influence the result of measurement, and this part gives two notes: Calibration of metrological characteristics may be necessary; the metrological characteristics have an immediate contribution to measurement uncertainty.

The metrological characteristics of non-contact instrument related in ISO 25178 involve:

i. Measuring volume

Measuring volume is defined as range of the instrument stated as simultaneous limits on all spatial coordinates measured by the instrument.

ii. Hysteresis

Hysteresis is defined as property of measuring equipment, or a characteristic whereby the indication of the equipment or value of the characteristic depends on the orientation of the preceding stimuli.

iii. Response curve F_x, F_y, F_z

Response curve is defined as graphical representation of the function that describes the relation between the actual quantity and the measured quantity. Fig. 4.16 gives an example of a non-linear response curve

Fig. 4.16 Example of a non-linear response curve. Source: ISO 25178-602: 2010 [47].

iv. Amplification coefficient $\alpha_x, \alpha_y, \alpha_z$

Amplification coefficient is defined as slope of the linear regression curve obtained from the response curve. Fig. 4.17 gives an example of the linearization of a response curve.

Fig. 4.17 Example of the linearization of a response curve. Source: ISO 25178-602:2010 [47].

v. Instrument noise

Instrument noise is defined as internal noise added to the output signal caused by the instrument if ideally placed in a noise-free environment.

vi. Static noise N_s

Static noise is defined as combination of the instrument and environmental noise on the output signal when the instrument is not scanning laterally.

vii Dynamic noise N_d

Dynamic noise is defined as noise occurring during the motion of the drive units on the output signal.

viii. Sampling interval in X D_x

Sampling interval in X is defined as distance between two adjacent measured points along the X-axis.

ix. Sampling interval in Y

Sampling interval in Y is defined as distance between two adjacent measured points along the Y-axis.

x. Digitization step in Z D_z

Digitization step in Z is defined as smallest height variation along the Z-axis between two ordinates of the extracted surface. Tab. 4.6 shows the summarization of the efficiency of detection algorithms.

Tab. 4.6 Efficiency of detection algorithms. Source: ISO 25178-602:2010 [47].

Algorithm	Accuracy	Speed
Simple detection of the pixel position of maximum intensity	Poor	High
Fitting of a known curve (Gaussian, Pearson, etc.)	Good	Low
Barycentre of the peak	Good	High

xi. Lateral resolution R_l

Lateral resolution is defined as smallest distance between two features which can be detected separately.

xii. Width limit for full height transmission W_l

Width limit for full height transmission is defined as width of the narrowest rectangular groove whose measured height remains unchanged by the measurement.

xiii. Maximum acceptable local slope

Maximum acceptable local slope is defined as greatest local slope of a surface feature that can be assessed by the probing system.

xiv. Spot size W_{spot}

Spot size is defined as maximum lateral size of the projected image of the source pinhole.

xv. Integration time T_i

Integration time is defined as time during which the incoming light is accumulated (integrated) on the detector in the spectrometer.

xvi. Measurement frequency f_m

Measurement frequency is defined as number of data points provided per second by the probing system.

A summary of these metrological characteristics can be found in Tab. 4.7.

Tab. 4.7 Metrological Characteristics of non-contact (confocal chromatic probe) instruments. Source: ISO 25178-602:2010.

Component	Element	Metrological characteristics		Can introduce error along
Probing system	Optical stylus	W_{spot}	spot size	X, Y and Z
		A_N	numerical aperture	X, Y and Z
		R_1	lateral resolution	X, Y and Y
	optoelectronic device	C_z	height adjustment coefficient	Z
		α_z	height amplification coefficient	Z
		z_{HYS}	vertical hysteresis	Z
		F_z	response curve	Z
		D_z	scanning step height	Z
		T_i	integration time	X and Z
		f_m	measurement frequency	X
Lateral scan system	Position sensor (linear encoder, micrometric screw)	F_x or F_y	response curve	X or Y
		α_x or α_y	lateral amplification coefficients	X or Y
		D_x or D_y	lateral sampling interval	X or Y
		x_{HYS}	X positioning hysteresis, between two adjacent profiles	X
		y_{HYS}	Y positioning hysteresis	Y
		v_x	measuring velocity X	X and Z
	Reference guide areas (height component)	$Z_{\text{FLT}(X,Y)}$	height component of the flatness of the movement in the XY plane	Z
			$Z_{\text{FLT}(X,Y)}$ contains in particular	
		$Z_{\text{STR}(X)}$	height component of the straightness along the axes X	
Lateral scan system	Reference guide areas (lateral component)	$Z_{\text{STR}(Y)}$	height component of the straightness along the axes Y	
		Δ_{PER}	perpendicularity between axis X and Y	X and Y
		$y_{\text{STR}(X)}$	Y lateral component of the straightness along the axes X	X and Y
Instrument		$y_{\text{STR}(Y)}$	X lateral component of the straightness along the axes Y	X and Y
		N_s	static noise	Z
		N_d	dynamic noise	Z

As stated above, instrument calibration is a complicated and lengthy work, which incorporates a number of metrological characteristics and requires the consistence with numerous international standards related with mathematical calculation and software of data processing. Fig. 4.18 presents the hierarchy from traceable standards to quality.

Fig. 4.18 Hierarchy from traceable standards to quality [10].

Confusion often arises over the subject of accuracy and repeatability as they do not have the same origin. The repeatability is a function of the instruments' design while the accuracy is a function of calibration [43]. The repeatability conditions of measurement include the same measurement procedure, same operators, same measuring systems, same operating conditions and locations, and replicate measurements on the same or similar objects over a short period of time [17].

A high percentage of the uncertainties come from the measuring optical or tactile probe. The behaviour of the measuring probe has to be characterized under similar environmental conditions to reduce the contribution of the uncertainties related to the behaviour of the instrumentation probes [49].

For 3D confocal microscopy, axial distances can be distorted by the point spread function (PSF), as well as a refractive index (RI) mismatch between the sample and immersion material which are difficult to separate [50]. The RI mismatch not only deteriorates the PSF with increasing focus depth, but also introduces a decrease in intensity and a shift of the objective focus [51].

The difference in axial and lateral resolution affects the shape of any micronized or sub-micronized feature in a 3D measurement. Every image system distorts the object by PSF, but the distortions are negligible when the objects under study are much larger than the resolution limit [52]. Little attention is devoted to the axial-distance calibration which is indispensable for precise measurements. Accurate calibration of the axial

distances in confocal microscopy remains cumbersome, although several high-precision methods exist [53, 54, 55]. Accurate three dimensional measurements require precision pixel-to-micrometer conversion factors in all three dimensions. This is very difficult for optical axis, the z-direction, since scanning in this direction is very different from that in the x- and y- directions. The 3D images are acquired by adding 2D images with step heights along the z-axis, while the whole 2D images are taken in the x-y plane at once by a CCD array or by a raster scan of the plane. Although it is vital to reconcile these two physically different scanning mechanisms to ensure consistent distance measurements in all directions, the system software uses nominal pixel-to-micrometer conversion factors, which are usually incorrect by as much as 40%. An independent calibration is essential to ensure accuracy of results [55].

Fig. 4.19 The error sources of the measurement uncertainty [56]]

H Noura, N El-Hayek, X Yuan, *et al* identified the main error sources of chromatic confocal probes for dimensional measurement [56]. The major error sources include, for example, the relative axial and radial motions of the probe, properties of the materials of the measured sample, the relative deviations of the probe, the scanning speed of the measurement system, etc. The general conclusion of the error sources of the measurement uncertainty can be found in Fig 4.19. Results of the experimental tests shown in their work indicate that the chromatic confocal probes are sensitive to these errors and that their measurement behaviors highly depend on them.

S. Carmignato, *et al.* carried out the comparisons of measurements of a set of standards by coordinate measuring machines (CMMs) equipped with optical sensors [57]. This

comparison was performed in Europe from August 2007 to January 2009 involving 21 optical CMMs. The participants included industrial users and manufacturers of measuring systems as well as research institutions. They presented that the interactions of optical sensors with material and surface of parts are among the most important error sources. On measuring the diameter of the three selected holes, they found that the small dust particles on the holes were the major error sources. The diameter measurement is very much influenced by image processing and filtering algorithms used by optical CMMs. The plate thickness is higher than the tiny chromium depositions on the glass scale, making the holes measurements more sensitive to the type of illumination used. On measuring the plastic bricks, they studied the effect of different colours and optical properties as well as the impact of feature types. Translucent materials, such as plastic, can transmit or reflect the light depending on the material properties, for example the colour of the measurand, or on the type of light used, causing an effect of shrinkage or distortion of the measured features. Specimen that does not have sharp edges, which are round off, makes the measurements more difficult for image processing sensors. Plastic bricks are more sensitive to thermal effects than other artefacts due to much higher CTE ($8 \times 10^{-5} \text{ K}^{-1}$).

F. R. Boddeke, *et al.* provided a method for the calibration of the z-axis of the optical microscopy [53]. Quantitative analysis requires calibration of the image sensor and the automated axes. The image sensor converts a light intensity pattern into a digital image. Its important characteristics include sampling density, linearity of photometric response, signal-to-noise ratio, sensitivity, and spatial resolution. To calibrate the focus axis, the physical distance of each step must be known as the automated axes are driven by stepping motors with position coders. For the *xy* stage calibration, a camera with known sampling density could be used. Owing to the mismatch of refractive index and the unknown depth of the bead in the surrounding medium, calibrations of z axis cannot be related to that of the *xy* stage. To overcome this problem, they offered an alternative solution based on focus functions.

J.C. Mullikin, *et al.* presented some methods for CCD camera characterization [58]. For example, to calculate signal-to-noise ratio Equation 4.7 and 4.8 are used,

$$SNR = 10 \log(\bar{I}^2 / \text{var}(I)) \quad (4.7)$$

$$\text{var}(I) = \frac{1}{2} \text{var}(I_1 - I_2) = \frac{1}{2} \left(\frac{1}{N-1} \sum (I_d - \bar{I}_d)^2 \right) \quad (4.8)$$

where I_d represents the difference between two images with the same exposure time. The mean of the difference image, $\bar{I}_d$, and its variance, $\text{var}(I_d)$, are calculated over a

sub-set of all pixels in the image, and normalized by the number of pixels in the sub-image, N .

To calculate the sensitivity, the equation is used

The sensitivity can be calculated by Equations 4.9 and 4.10 [58]:

$$S = \frac{\bar{I} - \bar{I}_{dark}}{\Phi_f A_i t_e} \quad (4.9)$$

$$A_i = \Delta_{x,i} \Delta_{y,i} \quad (4.10)$$

Where t_e is the exposure time, A_i is the area of a pixel, Φ_f is the photon flux at the focal plane of the camera port, $\Delta_{x,i}$ and $\Delta_{y,i}$ are the sample spacing along the horizontal and

vertical axis in the image plane.

4.6 Assessment of measurement uncertainty

Roughness measurement is the common method of characterization of surface morphologies, including surface texture, features such as deviations from roundness, straightness, flatness, cylindricity, all the aspects of surface geometry, etc. For surface roughness characterization, two important things have to be sure. One is the surface topographic measurement techniques and the other is the relevant roughness parameters [59]. The roughness parameters can be determined by numerical methods, but data of the topography must be measured by suitable measurement techniques. However, roughness parameters might differ obviously by different techniques [60].

Measurement of any quantity is correlated with its evaluations. The measurement result as a single value has little practical meaning, only except when it is combined with its accuracy evaluation [61]. The generally accepted interpretation of accuracy is the range on the value axis, set around the true value x_t :

$$[x_t - \Delta_{\min} x, x_t + \Delta_{\max} x] \quad (4.11)$$

Where, x_t is the true value of the measurand, $\Delta_{\min} x$ is the minimum value of the measurement result, and $\Delta_{\max} x$ is the maximum value of the measurement. Both $\Delta_{\min} x$, and $\Delta_{\max} x$ are positive values.

Accuracy of measurement is defined as the closeness of the agreement between the result of a measurement and a true value of the measurand by GUM [16], while error of

measurement is the result of a measurement minus a true value of the measurand [16]. Uncertainty is defined as a parameter that characterizes the dispersion of the values that could reasonably be attributed to the measurand [16]. Fig. 4.20 shows the graphical representation of the relationship between measurement uncertainty, measurement error, measured quantity, and true value.

Fig. 4.20 Graphical representation of the meaning of error and measurement uncertainty:
(a) The axial system (scalar); (b) Spatial (vector) [61].

4.6.1 Modeling the measurement by GUM method

Mostly the measurand Y is not measured directly but determined from N other quantities $X_1, X_2, \dots, X_N$ through a functional relationship f :

$$Y = f(X_1, X_2, \dots, X_N) \quad (4.12)$$

The estimate of X_i is denoted as x_i , and the estimate of the measurand Y , is denoted as y , using input estimates $x_1, x_2, \dots, x_N$, for the values of the N quantities $X_1, X_2, \dots, X_N$. The result of the measurement y is given by

$$y = f(x_1, x_2, \dots, x_N) \quad (4.13)$$

Sometimes y can be obtained from

$$y = \bar{Y} = \frac{1}{n} \sum_{k=1}^n Y_k = \frac{1}{n} \sum_{k=1}^n f(X_{1,k}, X_{2,k}, \dots, X_{N,k}) \quad (4.14)$$

The evaluations of standard uncertainty are classified as Type A and Type B. For an input quantity X_i determined from n independent repeated observations $X_{i,k}$, the standard uncertainty $u(x_i)$ of its estimate $x_i = \bar{X}_i$ is $u(x_i) = s(\bar{X}_i)$. For convenience, $u^2(x_i) = s^2(\bar{X}_i)$ and $u(x_i) = s(\bar{X}_i)$ are sometimes called a *Type A variance* and a *Type A standard uncertainty*, respectively. For some input quantities that has not been obtained

from repeated observations, the associated estimated variance $u^2(x_i)$ or the standard uncertainty $u(x_i)$ is evaluated by scientific judgement based on all of the available information on the possible variability of X_i , which may include previous measurement data, experience with or general knowledge of the behaviour and properties of relevant materials and instruments, manufacturer's specifications, data provided in calibration and other certificates, uncertainties assigned to reference data taken from handbooks [16].

For uncorrelated input quantities, the standard uncertainty of y might be obtained by appropriately combining the standard uncertainties of the input estimates $x_1, x_2, \dots, x_N$. This combined standard uncertainty of the estimate y is denoted by $u_c(y)$, and given by

$$u_c^2(y) = \sum_{i=1}^N \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \quad (4.15)$$

When the input quantities are correlated, the combined variance $u_c^2(y)$ associated with the result of a measurement is:

$$u_c^2(y) = \sum_{i=1}^N \sum_{j=1}^N \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j) = \sum_{i=1}^N \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j) \quad (4.16)$$

The expanded uncertainty U is obtained by multiplying the combined standard uncertainty $u_c(y)$ by a coverage factor k :

$$U = k u_c(y) \quad (4.17)$$

Where $k = 3$ produces an interval having a level of confidence of $p \approx 99.73\%$, while $k = 2$ produces an interval having a level of confidence of $p \approx 95.45\%$ [16, 61].

The result of measurement is then conveniently expressed as

$$Y = y \pm U \quad (4.18)$$

4.6.2 Monte Carlo Method for model development

Monte Carlo method (MCM), which is introduced in the Supplement 1 of Guide to the Expression of Uncertainty in Measurement [62], is implemented in this work to propagate probability distributions, and using the propagated parameters to estimate the measurement uncertainties. MCM is a method to generate approximate numerical representation $\mathbf{G}$, for example, distribution function $\mathbf{G}_Y(\eta)$ for Y , the measurand. The

heart of this approach is to make repeated draws from the Probability Distribution Functions (PDFs) or joint PDF for X , observed value, and the evaluation of the vector outputs. Due to the distribution function $G_Y(\eta)$ contains all the information about the measurand Y , any property of Y can be approximated by G , such as expectations, variances, covariances, etc. The procedure is shown in Fig. 4.21, which is mainly divided into four steps.

First, determination of the MCM inputs, i.e. joint PDF $g_X(\xi)$ for input quantities X , measurement model $Y = f(X)$, coverage probability p , number M of Monte Carlo trials.

Second, generate the MCM propagation: draws from the joint PDF $g_X(\xi)$ for the input quantities and evaluation of the vector output quantity for these draws, $y_r = f(x_r)$, $r = 1, \dots, M$.

Third, calculate the primary MCM output: distribution function for the output quantity, i.e. discrete representation G of distribution function for output quantity Y .

Fourth, summarize the MCM, such as, estimate y of Y and associated covariance matrix U_y , calculate the coverage region for Y .

Fig. 4.21 Propagation and summarizing stages of uncertainty evaluation using MCM to implement the propagation of distributions when the vector output quantity can be expressed explicitly in terms of the input quantities. Source: GUM-S2 [63].

Normally, the quality of approximations improves with the increasing of the number of draws made. There are two ways to choose the value of M , one is to choose *a priori* which is adequately large to generate satisfied output results. However, this method does not directly control the quality of the numerical results. The other method is the Adaptive Monte Carlo procedure, which increasing the number of Monte Carlo trials until acquire the stabilized results in a statistical sense. The numerical results are deemed stabilized if twice the standard deviation associated with it is less than a stipulated numerical tolerance. The objective of the adaptive procedure is to provide:

- a) An estimate $y = (y_1, \dots, y_m)^T$ of $\mathbf{Y}$

- b) A vector $u(y) = (u(y_1), \dots, u(y_m))^T$ of standard uncertainties associated with the estimates,
- c) A positive definite matrix R_y of dimension $m \times m$ of correlation coefficients $r_{i,j} = r(y_i, y_j)$ associated with pairs of the estimates, and
- d) A coverage factor k_p defining a 100p% coverage region for Y in the form of a hyper-ellipsoid in m dimensions.

Therefore, each of these values can be expected to meet the stipulated numerical tolerance.

4.7 Summary

This chapter generally introduces the recent developments of scientific research and technology of areal surface measurements. Surface characterization means a lot in current industrial engineering. Based on the idea that two important things determine surface characterization, i.e. instrumentation and parameters, this chapter first make a general introduction to the areal surface measurement, then focus on the introductions of surface parameters, as well as approaches for outlier identification, measurement calibration methods, and uncertainty evaluation assessment, which contributes to the reliability and accuracy of the measurement result. Two methods for measurement uncertainty evaluation are introduced, one is the analytical methods provided by GUM, the other is the MCM introduced in the supplements.

4.8. References of Chapter 4

- [1] X. Jiang, P. J. Scott, D. J. Whitehouse, and L. Blunt, Paradigm shifts in surface metrology. Part I. Historical philosophy, Proceedings of the Royal Society, 2007.
- [2] David J. Whitehouse, Hand book of surface and nanotechnology. 2nd Edition, CRC Press, 2011.
- [3] M. Genevieve, B. Labrousse, Surface chatacterization, Physical methods, instruments and measurements 3.
- [4] D. K. Cohen, Introduction to ASME B46.1-2009: surface texture (surface roughness, waviness, and lay), Tech. rep., Michigan Metrology, LLC (2011).
- [5] T. V. Vorburger, Tutorial in optics: Chapter 8 Methods for characterizing surface topography, Optical society of America, 2010.

- [6] National Physical Laboratory, Good Practice Guide No. 80: Fundamental Good Practice in Dimensional Metrology, Queen's Printer and Controller of HMSO, 2005.
- [7] D. J. Whitehouse, Surface metrology, Measurement science and technology 8 (1997) 955–972.
- [8] K. Miyoshi, Surface characterization techniques: An overview, NASA/TM.
- [9] B. X. Jiang, and D. J. Whitehouse, Precision metrology, Philosophical transactions of the royal society A 370 (2012) 4154–4160.
- [10] D. B. Sharp, Measurement Standards, CRC Press LLC, 1999.
- [11] Bureau International des Poids et Mesures (BIPM), The International System of Units (SI), Organisation Intergouvernementale de la Convention du Metre, 2006.
- [12] ISO 25178 - 1: 2016 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 1: Indication of surface texture.
- [13] ISO 16610-22:2015. Geometrical product specifications (GPS) – Filtration – Part 22: Linear profile filters: Spline filters.
- [14] ISO/TR 13587:2012 (en) Three statistical approaches for the assessment and interpretation of measurement uncertainty.
- [15] ISO 13565-1:1996. Geometrical Product Specifications (GPS) – Surface texture: Profile method; Surfaces having stratified functional properties – Part 1: Filtering and general measurement conditions.
- [16] Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement (GUM).
- [17] International Vocabulary of Metrology - Basic and General Concepts and Associated Terms (VIM).
- [18] Internet Based Surface Metrology Algorithm Testing System, <https://physics.nist.gov/3DVSC/jsp/SurfaceParameter3D.jsp?ran=1679>.
- [19] S. Bell, Good Practice Guide No.11: The beginner's guide to Uncertainty of measurement, National Physical Laboratory, 1999.
- [20] C. L. Giusca, R. Leach, Good Practice Guide No.128: Calibration of the metrological characteristics of Imaging Confocal Microscopy (ICMs), 2012.

- [21] A. Godi, A. Kuhle, and L. D. Chiffre, A new procedure for characterizing textured surfaces with a deterministic pattern of valley features, *Measurement Science and Technology* 24 (8) (2013) 085009.
- [22] T. G. Mathia, P. Pawlus, M. Wiczorowski, Recent trends in surface metrology, *Wear* 271 (3-4) (2011) 494–508.
- [23] K. J. Stout (Ed.), *Development of methods for the Characterisation of Roughness in Three Dimensions*, Penton Press, 1993.
- [24] R. J. Pike, and T. R. Thomas, Quantitative characterization of micro-topography—A bibliography of industrial surface metrology, Tech. rep., U.S. Department of the interior and U.S. Geological survey (1988).
- [25] Gavin MacAulay, *Characterization of structured surfaces and assessment of associated measurement uncertainty*, NPL, 2015.
- [26] T. V. Vorburger, J. Raja, *Surface Finish Metrology Tutorial*, NISTIR 89-4088, 1990.
- [27] A. Murugarajan, G.L. Samuel, Measurement, modeling and evaluation of surface parameter using capacitive-sensor-based measurement system, *Metrology and measurement systems* 3 (2011) 403–418.
- [28] E.S. Gadelmawla, M.M. Koura, T.M.A. Maksoud, I.M. Elewa, H.H. Soliman, Roughness parameters, *Journal of Materials Processing Technology* 123 (2002) 133–145.
- [29] B. Muralikrishnan. J. Raja, *Computational Surface and Roundness Metrology*, Springer, 2009.
- [30] ISO 25178-2: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 2: Terms, definitions and surface texture parameters.
- [31] Gilberto A. Ortiz Ka Veng Yuen, Outlier detection and robust regression for correlated data, *Computer methods in applied mechanics and engineering*.
- [32] Steven Walfish, A review of statistical outlier methods, *Pharmaceutical Technology* 30 (2006) 1–5.
- [33] Richard Leach, *Optical measurement of surface topography*, Springer, 2011.
- [34] M. Krystek 1, P.J. Scott 2 and V. Srinivasan, Discrete linear filters for metrology, *Proceedings of the 16th IMEKO World Congress, Hofburg, Wien, Austria*.

- [35] ISO 16610-60: 2015. Geometrical Product Specimen (GPS) - Filtration - Part 60: Linear areal filters: Basic concepts.
- [36] R. Leach, Characterisation of Areal Surface Texture, Springer, 2013.
- [37] M. F. Ismail, K. Yanagi, A. Fujii, An outlier correction procedure and its application to areal surface data measured by optical instruments, Measurement science and technology 21 (10) (2010) 105105(11pp).
- [38] ISO 16610-1:2015. Geometrical product specifications (GPS) – Filtration – Part 1: Overview and basic concepts.
- [39] ISO 16610-30: 2015(en). Geometrical product specifications (GPS)-Filtration-Part 30: Robust profile filters: Basic concepts.
- [40] X. Jiang, P. J. Scott, D. J. Whitehouse, and L. Blunt, Paradigm shifts in surface metrology. Part II. The current shift, Proceedings of the Royal Society, 2007.
- [41] Y. Wang, H. Y. Feng, Modeling outlier formation in scanning reflective surfaces using a laser stripe scanner, Measurement 57 (2014) 108–121.
- [42] Y. Wang, H. Y. Feng, Outlier detection for scanned point clouds using majority voting, Computer-Aided Design 62 (2015) 31 – 43.
- [43] G. T. Smith, Industrial Metrology: Surfaces and Roundness, Springer, 2002.
- [44] J. Vicente, C. Molpeceres, O. Guarneiros, et al., Calibracion de Microscopios Confocales, XVII Congreso Nacional de Ingenier 柳 a Mec 谩 nica (2008) 307 – 312.
- [45] ISO 25178 - 70: 2014 (en). Geometrical product specification (GPS) - Surface texture: Areal - Part 70: Material measures.
- [46] C. L. Giusca, and R. K. Leach, Measurement Good Practice Guide No.128: Calibration of the Metrological Characteristics of Imaging Confocal Microscopes (ICMs), 2012.
- [47] ISO 25178 - 602: 2010 (en). Geometrical product specifications (GPS) -Surface texture: Areal-Part 602: Nominal characteristics of non-contact (confocal chromatic probe) instruments.
- [48] ISO 25178-3: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 3: Specification operators.

- [49] H. Nouira, J. A. Salgado, N. E. Hayek, S. Ducourtieux, A. Delvallee, and N. Anwer, Setup of a high-precision profilometer and comparison of tactile and optical measurements of standards, *Measurement Science and Technology* 25 (044016) (2014) 12pp.
- [50] T.H. Besseling, J. Jose, and A. Van Blaadenren, Methods to calibrate and scale axial distances in confocal microscopy as a function of refractive index, *Journal of Microscopy* 257 (2) (2015) 142–150.
- [51] T.D. Visser, J.L. Oud, G.J. Brakenhoff, Refractive index and axial distance measurements in 3-D microscopy, *Optik* 90 (1992) 17–19.
- [52] M.C. Jenkins, S.U. Egelhaaf, Confocal microscopy of colloidal particles: Towards reliable, optimum coordinates, *Advances in Colloid and Interface Science* 136 (2008) 65–92.
- [53] F. R. Boddeke, L. J. Van Vliet, and I. T. Young, Calibration of the automated z-axis of a microscope using focus functions, *Journal of Microscopy* 186 (3) (1997) 270–274.
- [54] H. Bornfleth, K. Saetzler, R. Eils, and C. Cremer, Distance measurements and volume-conserving segmentation of objects near and below the resolution limit in three-dimensional confocal fluorescence microscopy, *Journal of Microscopy* 189 (1998) 118–136.
- [55] K.E. Jensen, D.A. Weitz, and F. Spaepen, Note: A three-dimensional calibration device for the confocal microscope, *Review of Scientific Instruments* 84 (2013) 016108.
- [56] H. Nouira, N. E. Hayek, X. Yuan, and N. Anwer, Characterization of the main error sources of chromatic confocal probes for dimensional measurement, *Measurement Science and Technology* 25 (044011) (2014) 14pp.
- [57] S. Carmignato, A. Voltan, E. Savio, Metrological performance of optical coordinate measuring machines under industrial conditions, *CIRP Annals - Manufacturing Technology* 59 (2010) 497–500.
- [58] J.C. Mullikin, L.J. van Vliet, H. Netten, F.R. Boddeke, G. van der Feltz, and I.T. Young, Methods for CCD camera characterization, *SPIE* 2173 (1994) 73–84.
- [59] N. Jouini, A. Gautier, P. Revel, P-E. Mazeran, and M. Bigerelle, Multi-scale analysis of high precision surfaces by Stylus Profiler, *Scanning White-Light*

Interferometry and Atomic Force Microscopy, International Journal of Surface Science and Engineering 3 (4).

- [60] L. Richard, and A. Hart, A comparison of stylus and optical methods for measuring 2D surface texture, NPL Report CNTLM 15 (2002) 1–46.
- [61] J. Sladek, Coordinate Metrology: Chapter 2 Measurement Uncertainty and Requirements of Production System. Selected Issues of Measurement Uncertainty Theory, Springer-Verlag Berlin Heidelberg, 2016.
- [62] JCGM 101: 2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method.
- [63] JCGM 102: 2011 Evaluation of measurement data - Supplement 2 to the "Guide to the expression of uncertainty in measurement" - Extension to any number of output quantities.

Chapter 5: Algorithms for areal roughness parameterization and filtration

Abstract: This chapter mainly includes three parts: development of the original algorithms for 3D roughness parameterization, development of the Gaussian filter algorithms for surface filtration, and the validation of those two parts of algorithms with the data provided by the Testing System of NIST.

5.1 Algorithms for 3D roughness parameterization

Profile roughness parameters are introduced briefly here, in order to have a better understanding of the areal surface parameters, which are introduced in detail. Surface profile is defined as the profile that results from the intersection of the real surface by a specified plane according to ISO 4287 [1]. The arithmetic mean deviation of the assessed profile is defined by ISO 4287 [1] as the arithmetic mean of the absolute ordinate values $Z(x)$ within a sampling length, which can be calculated by Equation 5.1

$$R_a = \frac{1}{l} \int_0^l |Z(x)| dx \quad (5.1)$$

The root mean square deviation of the assessed profile is defined as the root mean square value of the ordinate values $Z(x)$ within a sampling length, calculated as shown by Equation 5.2:

$$R_q = \sqrt{\frac{1}{l} \int_0^l Z^2(x) dx} \quad (5.2)$$

$$R_a = \frac{1}{n} \sum_{i=1}^n |y_i| \quad (5.3)$$

$$R_q = \sqrt{\frac{1}{n} \sum_{i=1}^n y_i^2} \quad (5.4)$$

Fig.4.8 shows the mathematical definition and calculation of the two-dimensional average height parameters. The digital implementation of the arithmetic average height parameters are respectively indicated by Equations 5.3 and 5.4:

Fig.5.1 Definition of a profile. Source: ISO 4287: 1998 [1].

5.1.1 Areal height parameters

Arithmetical mean height of the scale limited surface, S_a , is defined as the arithmetic mean of the absolute of the ordinate values within a definition area (A):

$$S_a = \frac{1}{A} \iint_A |z(x, y)| dx dy \quad (5.5)$$

This integral equation cannot be used directly to program in Matlab, it is necessary to transform it equally to a discontinuous one, as shown in Equation 5.6, cited from Computational Surface and Roundness Metrology [29].

$$S_a = \frac{1}{nx \cdot ny} \sum_{i=1}^{nx} \sum_{j=1}^{ny} |z(j, i)| \quad (5.6)$$

Where $z(j,i)$ is the ordinate of the point at the j_{th} row and i_{th} column, and nx and ny are the number of points along the two directions.

Root mean square height of the scale-limited surface, S_q , is defined as the root mean square value of the ordinate values within a definition area (A):

$$S_q = \sqrt{\frac{1}{A} \iint_A z^2(x,y) d_x d_y} \quad (5.7)$$

Transform this integral equation into the discontinuous one as following [29]:

$$S_q = \sqrt{\frac{1}{nx \cdot ny} \sum_{i=1}^{nx} \sum_{j=1}^{ny} z(j,i)^2} \quad (5.8)$$

The S_a and S_q parameters are strongly correlated with each other. The S_q parameter has more statistical significance (it is the standard deviation) and often has a more physical grounding than S_a , for example, S_q is directly related to surface energy and the way light is scattered from a surface [36].

Skewness of the scale-limited surface, S_{sk} , is defined as the quotient of the mean cube value of the ordinate values and the cube of S_q within a definition area (A),

$$S_{sk} = \frac{1}{S_q^3} \left[\frac{1}{A} \iint_A z^3(x,y) dxdy \right] \quad (5.9)$$

Transform this integral equation into the discontinuous one as following [29]:

$$S_{sk} = \frac{1}{S_q^3} \frac{1}{nx \cdot ny} \sum_{i=1}^{nx} \sum_{j=1}^{ny} z(j,i)^3 \quad (5.10)$$

Parameter of skewness can be either positive, negative, or zero, and it is unit-less since this parameter is normalized by the cube of root mean square height. Skewness describes the shape of the topography height distribution, such as symmetric or asymmetric, with a left side tail or a right one. A surface with a random height distribution has a symmetric shape of the curve of its topography height distribution, and its skewness parameter is zero. Skewness derives from the amplitude distribution curve, and measures the symmetry of the profile about the mean line. It cannot indicate whether spikes are distributed evenly above or under the mean line, but represents the degree of bias of quantity of spikes above or under mean line. A symmetric profile gives a symmetric curve of amplitude distribution, while an asymmetric profile results in a skewed curve. For example, if the bulk of the material is above the mean line, this profile will have a negative skew, while it will have a positive skew if the bulk of the

material is below the mean line. This parameter has very useful applications in material science engineering, as it correlates well with porosity and load carrying ability. For instance, a porous, sintered or cast iron surface will have a large value of skewness. A good bearing surface should have a negative skew, which indicating comparatively less peaks that can be removed away quickly and relatively more valleys to retain lubricant traces. A surface with a positive skew is likely to have poor lubricant retention because of the lack of deep valleys in which to retain lubricant traces. Turned surfaces usually have positive skew as they have spikes that protrude above the mean line [36].

Kurtosis of the scale-limited surface, S_{ku} , is defined as the quotient of the mean quartic value of the ordinate values and the fourth power of S_q within a definition area (A):

$$S_{ku} = \frac{1}{S_q^4} \left[\frac{1}{A} \iint_A z^4(x, y) dx dy \right] \quad (5.11)$$

Transform this integral equation into the discontinuous one as following [29]:

$$S_{ku} = \frac{1}{S_q^4} \frac{1}{nx \cdot ny} \sum_{i=1}^{nx} \sum_{j=1}^{ny} z(j, i)^4 \quad (5.12)$$

The S_{ku} is the measure of the sharpness of the surface height distribution. This parameter is strictly positive and unit-less. A surface with normal distribution amplitude has S_{ku} value with 3. Unlike parameter S_{sk} , S_{ku} not only indicates whether the spikes are evenly distributed but also provides a measure of the spikiness of the area. A spiky surface will have a high kurtosis value and a bumpy surface will have a low kurtosis value.

The S_{sk} and S_{ku} can be less mathematically stable than other parameters, as they have higher order powers in their equations, leading to faster error propagation [36].

Maximum peak height of the scale limited surface, Sp , is defined as the largest peak height value within a definition area, i.e. the height of the highest point of the surface.

Maximum pit height of the scale limited surface, Sv , is defined as minus the smallest pit height value within a definition area, i.e. the height of the lowest point of the surface.

As heights are counted from the mean plane and signed, Sp is always positive while Sv is always negative.

Maximum height of the scale-limited surface, S_z , is defined as sum of the maximum peak height value and the maximum pit height value within a definition area, i.e. sum of the values of S_p and S_v .

$$S_z = S_p + |S_v| = S_p - S_v \quad (5.13)$$

The maximum height parameters must be used with caution as they might be sensitive to isolated peaks and pits which may not be significant. There are two main functions of S_z parameter. One is to characterize the amplitude of waviness on the work piece whose surfaces have been filtered with a low-pass filter. Another is to find unusual conditions such as a sharp spike or burr on the surfaces that may be indicative of poor material or poor processing.

5.1.2 Areal spatial parameters

All spatial parameters are defined over the definition area.

Autocorrelation length, Sal , is defined as horizontal distance of the $f_{ACF}(t_x, t_y)$, which has the fastest decay to a specified value s , with $0 \leq s \leq 1$,

$$Sal = \min_{t_x, t_y \in R} \sqrt{t_x^2 + t_y^2} \quad (5.14)$$

Where, $R = \{(t_x, t_y) : f_{ACF}(t_x, t_y) \leq s\}$

Note 1: If not otherwise specified, the default value of s is found in ISO 25178-3:2012 [48].

As the development of the spatial parameters involves the use of the mathematical technique of the autocorrelation function (**ACF**), here briefly introduce the **ACF** as well as area autocovariance function (**AACV**) since **AACV** is related with **ACF**.

The autocorrelation function (**ACF**) is found by taking a duplicate surface ($Z(x-Dx, y-Dy)$) of the measured surface ($Z(x, y)$) and mathematically multiplying the two surfaces together, with a relative lateral displacement (Dx, Dy) between the two surfaces. The function of multiplied surfaces is called autocovariance function (**AACV**). After multiplied together, the resulting function which is integrated and normalized to square of S_q is **ACF**, yielding a measure of the degree of overlap between the two functions.

AACV is a function that tracks the correlation of a texture against itself. A copy of a texture is first overlapped with the original and a coefficient is computed as the sum of the term-by-term product of texture elements in the original and duplicate textures. Then the copied texture shifted by some amount and a new coefficient is evaluated. These coefficients, plotted

as a function of shift distance, form the **AACV**. Formally, **AACV** is defined as the integral of the shifted and unshifted textures evaluated over the definition area [29].

The area autocovariance function (AACV) for 3D surfaces is defined as:

$$AACV(j', i') = \frac{1}{nx \cdot ny} \sum_{i=1}^{nx-i'} \sum_{j=1}^{ny-j'} z(j, i) z(j + j', i + i') \quad (5.15)$$

Where, $0 \leq j \leq ny - 1$, $0 \leq i \leq nx - 1$, (j, i) and (j', i') are autocovariance points.

ACF is the **AACV** normalized by the square of the root mean square roughness. Therefore,

$$ACF(k) = \frac{AACV(k)}{R_q^2} \quad (5.16)$$

If the shifted version of the surface is identical to the original surface then the **ACF** is 1.00. If the shifted surface is such that all peaks align with corresponding valleys then the **ACF** will approach -1.00.

Therefore, the **ACF** is a measurement of the similarity between the original texture and the copied one with a certain shifted distance. If the **ACF** value stays near 1.00 for a given amount of shift, it means the texture is similar along that direction. If the **ACF** value falls rapidly to zero along a given direction, then the surface is different and thus uncorrelated with the original measurement location. Fig.8.2 gives an example about the autocorrelation of a turned surface [5].

Fig.5.2 ACF of a turned surface along X Direction and Y Direction. Source: Michigan Metrology, LLC [5].

In the X direction, the **ACF** decrease to zero quickly, when the peak of the copied texture moves to align with the mean height of the original texture; **ACF** becomes negative when the peaks are aligned with valleys of the original surface. In the Y direction, **ACF** keeps near 1.00, as the surface texture almost does not change in the Y direction [5].

S_{al} , the Auto-Correlation Length, is a measure of the distance over the surface such that the new location will have minimal correlation with the original location. The direction over the surface chosen to find S_{al} is the direction which yields the lowest S_{al} value.

$$S_{al} = \text{Length of fastest decay of ACF in any direction} \quad (5.17)$$

Texture aspect ratio, S_{tr} , is defined as ratio of the horizontal distance of the $f_{ACF}(t_x, t_y)$, which has the fastest decay to a specified value s to the horizontal distance of the $f_{ACF}(t_x, t_y)$ which has the slowest decay to s , with $0 \leq s < 1$.

$$S_{tr} = \frac{\min_{t_x, t_y \in R} \sqrt{t_x^2 + t_y^2}}{\max_{t_x, t_y \in Q} \sqrt{t_x^2 + t_y^2}} \quad (5.18)$$

Where, $R = \{(t_x, t_y) : f_{ACF}(t_x, t_y) \leq s\}$, $Q = \{(t_x, t_y) : f_{ACF}(t_x, t_y) \geq s \text{ and } **\}$

where $**$ is the property that the $f_{ACF}(t_x, t_y) \geq s$ on the straight line connecting the point (t_x, t_y) to the origin.

Note 1: If not otherwise specified, the default value of s is found in ISO 25178-3: 2012 [48].

Note 2: A graphical representation of the procedure to calculate S_{tr} is given in Fig.8.5.

$$S_{tr} = \frac{\min(\frac{1}{n_x \cdot n_y} \sum_{i=1}^{n_x-i'} \sum_{j=1}^{n_y-j'} z(j, i) z(j + j', i + i'))}{\max(\frac{1}{n_x \cdot n_y} \sum_{i=1}^{n_x-i''} \sum_{j=1}^{n_y-j''} z(j, i) z(j + j'', i + i''))} \quad (5.19)$$

S_{tr} , is a measure of the spatial isotropy or directionality of the surface texture. For a surface with a dominant lay, the S_{tr} parameter will tend towards 0.00, whereas a spatially isotropic texture will result in a S_{tr} of 1.00. Fig.5.3 gives an example of spatial parameters of directional surface and isotropic surface.

$$S_{tr} = \frac{\text{Length of fastest decay of ACF in any direction}}{\text{Length of slowest decay of ACF in any direction}} \quad (5.20)$$

Highly Directional Surface with Str of 0.11 and Sal of 37mm

Highly isotropic surface with Str of 0.88 with an Sal of 21mm

Fig.5.3 Spatial parameters of directional surface and isotropic surface. Source: Michigan Metrology, LLC [5].

Fig.5.4 Procedure to calculate Sal and Str. Source: ISO 25178-2:2012 [26].

5.2 Algorithm for surface Gaussian filtration

Surfaces can be viewed as the superposition of different geometrical structures with different scales. Form or form deviations have large scales while roughness has small scales. Waviness is a periodic component which can have large and small scales respectively [36]. Fig.5.5 shows topography of a honed surface with form, waviness, and roughness. In ISO 25178-3:2012, there are two surfaces defined, i.e. S-L surface and S-F surface [26]. S-F surface is defined as surface derived from the primary surface by removing the form using an F-

operation. S-L surface is defined as surface derived from the S-F surface by removing the large scale components using an L-filter. Primary surface is defined as surface portion obtained when a surface portion is represented as a specified primary mathematical model with specified nesting index [26]. S-filter is a surface filter which removes small scale lateral components from the surface resulting in the primary surface. L-filter is a surface filter which removes large scale lateral components from the primary surface or S-F surface. F-operation is an operation which removes form from the primary surface. The relationships between the S-filter, L-filter, F-operation and S-F and S-L surfaces are shown in Fig.5.7. Some F-operations function differently from filtrations. Although F-operations can limit the larger lateral scales of a surface, this action is very fuzzy, as indicated in Fig.5.7. Moreover, many L-filters are sensitive to form and require an F-operation first before being applied [26].

Fig.5.5 Indication of the superposition of a surface with form, waviness, and roughness. Source: Characterisation of Areal Surface Texture [36].

Fig.5.6 Relationships between the S-filter, L-filter, F-operation and S-F and S-L surfaces.

Source: ISO 25178 - 2: 2012 [26].

The default surface is the mechanical surface, defined in ISO 14406 [7], obtained with a radius chosen in accordance with the F-operation or L-filter and S-filter nesting index given in Tab.5. 1 [48].

Tab.5.1 Nesting index values between the F-operation or L-filter and S-filter and the bandwidth ratio [48].

F-operation or L-filter nesting index value [mm]	S-filter nesting index value [mm]	Approximation bandwidth ratio between the F-operation or L-filter and S-filter nesting index values
...	...	...
0.1	0.001	100:1
	0.000 5	200:1
	0.000 2	500:1
	0.000 1	1 000:1
0.2	0.002	100:1
	0.001	200:1
	0.000 5	400:1
	0.000 2	1 000:1
0.25	0.002 5	100:1
	0.000 8	300:1
	0.000 25	1 000:1
0.5	0.005	100:1
	0.002	250:1

0.8	0.001	500:1
	0.000 5	1 000:1
	0.008	100:1
	0.002 5	300:1
1	0.000 8	1 000:1
	0.01	100:1
	0.005	200:1
	0.002	500:1
2	0.001	1 000:1
	0.02	100:1
	0.01	200:1
	0.005	400:1
2.5	0.002	1 000:1
	0.025	100:1
	0.008	300:1
	0.0025	1 000:1
5	0.05	100:1
	0.02	250:1
	0.01	500:1
	0.005	1 000:1
8	0.08	100:1
	0.025	300:1
	0.008	1 000:1
	...	...

Standardization of metrological filters currently mainly refers to the series of ISO 16610, which specifies Gaussian filters [8], Spline filters [13], End effects [10], Spline wavelets [11], Robust Gaussian regression filters [12], Robust Spline filters [13], Disk and horizontal line-segment filters [14], Scale space techniques [15], areal Gaussian filters [16], areal Gaussian regression filters [17], Morphological areal filters [18], etc. Before the implementation of the series of ISO 16610, ISO 11562 was applied for the specification of filtration for profile metrology [19]. This International Standard specifies the metrological characteristics of phase correct filters for the measurement of surface profiles, which in particular specifies how to separate the long and short wave content of a surface profile. The weighting function of this

filter corresponds to the equation of Gaussian density function, with the cut-off wavelength λ_{co} , is as following:

$$s(x) = \frac{1}{\alpha \lambda_{co}} e^{-\pi \left(\frac{x}{\alpha \lambda_{co}}\right)^2} \quad (5.21)$$

Where, λ_{co} is the cut-off wavelength of the profile filter, x is the position in relation to the centre of the weighting function, and:

$$\alpha = \frac{\ln 2}{\pi} = 0.4697 \quad (5.22)$$

There are two ways to realise the phase correct filter, one is the convolution, and the other is the fast Fourier transform (FFT). By the method of convolution, profile $z(x)$ can be separated into high frequency roughness $r(x)$ and low frequency waviness $w(x)$:

$$w(x) = \int_{-\infty}^{+\infty} z(\xi) s(x - \xi) d\xi \quad (5.23)$$

$$r(x) = z(x) - w(x) \quad (5.24)$$

By the method of FFT, first multiply the Fourier transformed profile mathematical model and the weighting function, then make an inverse Fourier transform (IFFT) to obtain its results. FFT for the discrete sample data $z(n)$ of profile $z(x)$ is:

$$Z(k) = DFT[z(n)] = \sum_{n=0}^{N-1} z(n) e^{-2\pi j \left(\frac{n}{N}k\right)} \quad (5.25)$$

Discrete Fourier transform for the weighting function is:

$$S(k) = DFT[s(n)] = \sum_{n=0}^{N-1} s(n) e^{-2\pi j \left(\frac{n}{N}k\right)} \quad (5.26)$$

According to Equation 5.23 and convolution theorem, there is:

$$W(k) = Z(k)S(k) \quad (5.27)$$

After the IDFT of the above equation, there is:

$$w(n) = IDFT[W(k)] \quad (5.28)$$

Therefore, the roughness profile is:

$$r(n) = z(n) - w(n) \quad (5.29)$$

Nowadays ISO 16610 has replaced ISO 11562 and the most popular filters are the linear profile Gaussian filter for profile filtering and the linear areal Gaussian filter for areal surface filtering. The Gaussian filter is probably the most widely used filter today [29].

ISO 16610-21 has specified the terms, definitions, characteristics of Gaussian profile filter for open profile and for closed profile. The weighting function defined in ISO 16610-21 is the same as indicated in Equation 5.21. Fig.5.8 shows the weighting function of a Gaussian profile for an open profile. For implementation, the weighting function equation is:

$$s(x) = \begin{cases} \frac{1}{\alpha \times \lambda_c} \times \exp \left[-\pi \left(\frac{x}{\alpha \times \lambda_c} \right)^2 \right] & \text{for } -L_c \times \lambda_c \leq x \leq L_c \times \lambda_c \\ 0 & \text{otherwise} \end{cases} \quad (5.30)$$

Where L_c is a truncation constant of the weighting function, α is calculated by Equation 5.22. Implementation errors for different truncation constants are listed in Tab.5.2.

Fig.5.7 Weighting function of a Gaussian profile filter for an open profile.

Tab.5.2 Implementation errors for different truncation constants.

Truncation constants L_c	Implementation error (%)
----------------------------	--------------------------

0.5	0.76
0.6	0.14
0.8	1.96×10^{-3}
1.0	9.47×10^{-6}

The transmission characteristic of the long wave component for an open profile is determined from the weighting function by means of the Fourier transformation, and it is given by:

$$\frac{a_1}{a_0} = \exp \left[-\pi \left(\frac{\alpha \times \lambda_c}{\lambda} \right)^2 \right] \quad (5.31)$$

Where a_0 is the amplitude of a sinusoidal wave profile before filtering, a_1 is the amplitude of this sinusoidal profile in the mean line, λ is the wavelength of this sinusoidal profile. Fig.5.8 shows the long wave transmission function of the Gaussian filter for an open profile.

Fig.5.8 Long wave transmission function of the Gaussian filter for an open profile.

The transmission characteristic is determined from the weighting function by means of Fourier transformation and is complementary to the transmission characteristic of the long wave profile component. The transmission characteristic of the short wave component is:

$$\frac{a_2}{a_0} = 1 - \exp \left[-\pi \left(\frac{\alpha \times \lambda_c}{\lambda} \right)^2 \right] \quad (5.32)$$

$$\frac{a_2}{a_0} = 1 - \frac{a_1}{a_0} \quad (5.33)$$

Where a_2 is the amplitude of the short wave component of a sinusoidal wave profile.

Fig.5.9 Short wave transmission function of the Gaussian filter for an open profile.

The method of convolution of the profile and the weighting functions usually cause end effects, which are the unintentional changes in the filtration response in the end portions of the profile. The end portion of an open profile where end effects are significant are called the end effect regions [8]. One strategy to solve this problem is to remove the end effect regions and leave a filtration response with insignificant end effects, as shown in Fig.5.10. An alternative strategy to reduce end effects is to use the techniques introduced in ISO 16610-28 [10], Fig.5.11 shows an illustrative example of this method.

Fig.5.10 Gaussian filtration ($\lambda_c = 0.8 \text{ mm}$) with the removal of the end effect regions. Source: ISO 16610-28 [10].

Fig.5.11 An illustrative example of Gaussian filtration ($\lambda_c = 0.8$ mm) using the moment retainment criterion. Source: ISO 16610-28 [10].

The areal Gaussian filter is just an extension of the profile Gaussian filter. Its weighting function has the formula of a rotationally symmetric Gaussian function with a cut-off wavelength, λ_c , given by equation

$$s(x, y) = \frac{1}{\alpha^2 \lambda_c^2} \exp \left[-\frac{\pi}{\alpha^2} \left(\frac{x^2 + y^2}{\lambda_c^2} \right) \right] \quad (5.34)$$

Where x is the distance from the centre (maximum) of the weighting function in X direction, y is the distance from the centre (maximum) of the weighting function in Y direction, λ_c is the cut-off wavelength, α is the constant, to provide 50% transmission characteristic at the cut-off λ_c . The Graph of the areal Gaussian filter weighting function is shown in Fig.5.12.

Fig.5.12 The weighting function of a Gaussian areal filter.

The transmission characteristic is determined from the weighting function by means of the Fourier transformation. The transmission characteristic of the long wave component is:

$$\frac{a_1}{a_0} = H(\lambda | \lambda_c) = \exp \left[-\pi \left(\alpha \frac{\lambda_c}{\lambda} \right)^2 \right] \quad (5.35)$$

Where a_0 is the amplitude of a sine wave surface before filtering, a_1 is the amplitude of the long wave component of a sine wave surface, λ is the wavelength of a sine surface in any direction. The transmission characteristic of the long wave component with λ_c for a sine wave in any direction with wave length λ is shown in Fig.5.13.

Fig.5.13 Long wave transmission function of the areal Gaussian filter for planar surfaces with λ_c .

The transmission characteristic of the short wave component is complementary to the transmission characteristic of the long wave profile component. The transmission characteristic of short wave component is given by Equation 5.36. Fig.5.14 shows the transmission characteristic of the short wave component with λ_c for a sine wave in any direction with wavelength λ .

$$\frac{a_2}{a_0} = 1 - \frac{a_1}{a_0} = 1 - H(\lambda | \lambda_c) = 1 - \exp \left[-\pi \left(\alpha \frac{\lambda_c}{\lambda} \right)^2 \right] \quad (5.36)$$

Where a_2 is the amplitude of the short wave component of a sine wave surface.

Fig.5.14 Short wave transmission function of the areal Gaussian filter for planar surfaces with λ_c

5.3 Verification with synthetic data

5.3.1 Verification of the parameterization algorithm

For the parameterization of surface roughness, the software Matlab is used to develop algorithms for the calculation of surface parameters specified in the part of Chapter 5.1. The accuracy of algorithms are validated with the synthetic data provided by National Institute of Standards and Technology (NIST) [20].

NIST was founded in 1901 and now is part of the U.S. Department of Commerce. NIST is one of the U.S. nation's oldest physical science laboratories. Congress established the agency to remove a major handicap to U.S. industrial competitiveness at the time - a second-rate measurement infrastructure that lagged behind the capabilities of the United Kingdom, Germany, and other economic rivals. Today, NIST measurements support the smallest of technologies - nanoscale devices so tiny that tens of thousands can fit on the end of a single human hair – to the largest and most complex of human-made creations, from earthquake-resistant skyscrapers to wide-body jetliners to global communication networks.

The Internet based surface Metrology Algorithm Testing System of NIST is utilized, as shown in Fig.5.15, and 3D Virtual SRM Database is chosen as the testing parameter standards.

Fig.5.15 The website of the Internet based surface Metrology Algorithm Teting System of NIST.

This testing system provides a number of data files from different creators with various ranges of parameters, as shown in Fig.5.16.

Fig.5.16 Data files provided by the Internet based surface Metrology Algorithm Tesing System of NIST.

To make the software program testing as reliable as possible, here choose three data bases with the values of areal arithmetical mean height S_a , spacing, etc. varies as much as possible. Data files SG_1-2 (Random + roughness + surface), SG_1-4 (Random + roughness + surface), SG_3-4 (Random + roughness + surface) are chosen.

a. Information about the database SG_1-2

Part Information	
Part Name:	SG_1-2
Created by:	Dr. M. Uchidate Dept. of Mechanical Engineering Iwate University, Japan
Description:	Random roughness surface
Process Information	
Process Name:	Numerically Generated Process
Measurement Information	
Instrument type:	N/A
Data file	
File Name:	SG_1-2.sdf
Units:	μm
Number Points:	256
Number of Profiles:	256
Spacing X-direction:	1 μm
Spacing Y-direction:	1 μm
Data type:	3D
Filter Information	
Filter type:	N/A
Method:	N/A
Cutoff:	0 mm
Additional Information:	Raw Data
Uncertainty Information	
Assume that Z co-ordinates have standard uncertainty of 10.0 nm (1% of S_q);	
X co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
Y co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
measurement errors on Z, X, and Y co-ordinates are Gaussian distribution and independent.	

Level of Confidence = 95 %

Areal surface parameters:

Label	Nominal Value	Mean Value	Standard Uncertainty
S_a	0.80376 μm	0.8038 μm	0.077 nm
S_q	1 μm	1.00005 μm	0.077 nm
S_{sk}	0.19232	0.19231	0.00037
S_{ku}	2.91199	2.912	0.00062
S_t	6.60403 μm	6.60477 μm	26.79 nm
S_p	3.58892 μm	3.58905 μm	17.86 nm
S_v	3.0151 μm	3.0145 μm	18.01 nm

b. Information about the database SG_1-4

Part Information	
Part Name:	SG_1-4
Created by:	Dr. M. Uchida- Dept. of Mechanical Engineering Iwate University, Japan
Description:	Random roughness surface
Process Information	
Process Name:	Numerically Generated Process
Measurement Information	
Instrument type:	N/A
Data file	
File Name:	SG_1-4.sdf
Units:	μm
Number Points:	256
Number of Profiles:	256
Spacing X-direction:	2 μm

Spacing Y-direction:	2 μm
Data type:	3D
Filter Information	
Filter type:	N/A
Method:	N/A
Cutoff:	0 mm
Additional Information:	Raw Data
Uncertainty Information	
Assume that Z co-ordinates have standard uncertainty of 50.0 nm (1% of S_q);	
X co-ordinates have standard uncertainty of 40.0 nm (2% of sampling interval);	
Y co-ordinates have standard uncertainty of 40.0 nm (2% of sampling interval);	
measurement errors on Z, X, and Y co-ordinates are Gaussian distribution and independent.	
Level of Confidence = 95 %	

Areal surface parameters:

Label	Nominal Value	Mean Value	Standard Uncertainty
S_a	3.98884 μm	3.98904 μm	0.35 nm
S_q	5 μm	5.00023 μm	0.33 nm
S_{sk}	0.07009	0.07011	0.00047
S_{ku}	2.95848	2.95846	0.00065
S_t	37.82351 μm	37.81541 μm	140.41 nm
S_p	18.71759 μm	18.71417 μm	95.59 nm
S_v	37.04346 μm	37.05147 μm	56.07 nm

c. Information about the database SG_3-4

Part Information	
Part Name:	SG_3-4
Created by:	Dr. M. Uchida-Dept. of Mechanical Engineering, Iwate University, Japan
Description:	Random roughness surface
Process Information	
Process Name:	Numerically Generated Process
Measurement Information	
Instrument type:	N/A
Data file	
File Name:	SG_3-4.sdf
Units:	μm
Number Points:	256
Number of Profiles:	256
Spacing X-direction:	1 μm
Spacing Y-direction:	1 μm
Data type:	3D
Filter Information	
Filter type:	N/A
Method:	N/A
Cutoff:	0 mm
Additional Information:	Raw Data
Uncertainty Information	
Assume that Z co-ordinates have standard uncertainty of 10.0 nm (1% of S_q);	
X co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
Y co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
measurement errors on Z, X, and Y co-ordinates are Gaussian distribution and independent.	
Level of Confidence = 95 %	

Areal surface parameters:

Label	Nominal Value	Mean Value	Standard Uncertainty
S_a	0.63279 μm	0.63286 μm	0.076 nm
S_q	1 μm	1.00005 μm	0.072 nm
S_{sk}	0.61422	0.61412	0.00088
S_{ku}	15.38937	15.38704	0.0073
S_t	25.77481 μm	25.77746 μm	26.43 nm

S_p	13.94336 μm	13.94489 μm	18.49 nm
S_v	11.83145 μm	11.83112 μm	18.81 nm

After import those data into Matlab and process them by those algorithms developed in this work, the results of the height parameters calculated by the program can be found in Tab.5.3. This table also shows the comparisons of the difference between the values given by NIST and calculated by the developed algorithms in this work. Surface height distribution can be found in Fig.5.17, histogram of these areal height parameters are shown in Fig.5.18.

Fig.5.17 Surface height distribution.

Tab.5.3 Results calculated by the program and comparison with the values given by NIST of the data base SG_1-2.

Label	NIST		Calculated		Difference between the mean values given by NIST and Calculated		Difference between the Uncertainties	
	Mean Value [μm]	Standard Uncertainty [nm]	Mean Value [μm]	Standard Uncertainty [nm]	Difference [μm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]	Difference [nm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]
S_a	0.8038	$7.7000 \cdot 10^{-2}$	0.8038	$7.7775 \cdot 10^{-2}$	$-6.5228 \cdot 10^{-7}$	$-8.1150 \cdot 10^{-5}$	$-7.7547 \cdot 10^{-4}$	-0.0101
S_q	1.0001	$7.7000 \cdot 10^{-2}$	1.0000	$7.8138 \cdot 10^{-2}$	$1.3098 \cdot 10^{-6}$	$1.3098 \cdot 10^{-4}$	$-1.1377 \cdot 10^{-3}$	-0.0148
S_p	3.5891	17.9	3.5890	20.1	$9.5266 \cdot 10^{-5}$	0.0027	$-7.7547 \cdot 10^{-4}$	-0.0101
S_v	3.0145	18.0	3.0157	18.6	-0.0012	-0.0411	-0.60749	-0.0337
S_t	6.6048	26.8	6.6047	27.5	$7.7310 \cdot 10^{-5}$	0.0012	-0.67381	-0.0252
S_{ku}	2.9120	$6.2000 \cdot 10^{-4}$	2.9120	$7.1254 \cdot 10^{-4}$	$-4.3842 \cdot 10^{-6}$	$-1.5056 \cdot 10^{-4}$	$-9.2535 \cdot 10^{-5}$	-0.1493
S_{sk}	0.1923	$3.7000 \cdot 10^{-4}$	0.1923	$3.2041 \cdot 10^{-4}$	$1.4620 \cdot 10^{-5}$	0.0076	$4.9592 \cdot 10^{-5}$	0.1340
Note: S_{ku} and S_{sk} do not have units								

The covariance of the height parameters can be found in Tab.5.4. The covariance of two parameters is calculated by the following equation:

$$C(X, Y) = \frac{1}{N-1} \sum_{i=1}^N (X_i - \bar{X})(Y_i - \bar{Y}) \quad (5.37)$$

The correlation coefficients of the height parameters are shown in Tab.5.5, and the correlation coefficient is calculated by the Equation 5.38. Correlation coefficient ranges from -1 to 1. If the correlation coefficient is one, it means that the parameters have the best correlation, means they are the same, such as the correlation of S_a and S_a is one.

$$r(X, Y) = \frac{C(X, Y)}{\sqrt{C(X, X) \cdot C(Y, Y)}} \quad (5.38)$$

Tab.5.4 The covariance of the height parameters.

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	$1.524 \cdot 10^{-9}$	$1.236 \cdot 10^{-9}$	$6.482 \cdot 10^{-10}$	$2.064 \cdot 10^{-9}$	$2.712 \cdot 10^{-9}$	$-4.718 \cdot 10^{-9}$	$-4.774 \cdot 10^{-10}$
S_q	-	$1.546 \cdot 10^{-9}$	$5.342 \cdot 10^{-9}$	$5.292 \cdot 10^{-9}$	$1.063 \cdot 10^{-8}$	$7.853 \cdot 10^{-12}$	$-6.69 \cdot 10^{-12}$
S_p	-	-	$9.915 \cdot 10^{-5}$	$-6.917 \cdot 10^{-7}$	$9.845 \cdot 10^{-5}$	$2.164 \cdot 10^{-7}$	$4.406 \cdot 10^{-8}$
S_v	-	-	-	$8.569 \cdot 10^{-5}$	$8.500 \cdot 10^{-5}$	$1.154 \cdot 10^{-7}$	$-4.427 \cdot 10^{-8}$
S_t	-	-	-	-	$1.835 \cdot 10^{-4}$	$3.318 \cdot 10^{-7}$	$-2.007 \cdot 10^{-10}$
S_{ku}	-	-	-	-	-	$1.283 \cdot 10^{-7}$	$2.151 \cdot 10^{-8}$
S_{sk}	-	-	-	-	-	-	$2.597 \cdot 10^{-8}$

Tab.5.5 The correlation coefficient of the height parameters

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	1	0.811	0.000	0.000	0.001	-0.335	-0.061
S_q		1	0.014	0.011	0.018	-0.008	0.008
S_p			1	0.002	0.734	0.006	0.037
S_v				1	0.680	0.032	0.039
S_t					1	0.071	0.000
S_{ku}						1	0.374
S_{sk}							1

Fig.5.18 Distributions of the areal height parameters of the Data base of SG_1-2.

The results of processing data base SG_1-4 can be found in Tab.5.6, and in Tab.5.6 also compares the difference between the values given by NIST and calculated by this algorithm. Surface height distribution can be found in Fig.5.19, histogram of these areal height parameters are shown in Fig.5.20.

Tab.5.6 Results Calculated by the Program and Comparison with the Values given by NIST of the data base SG_1-4.

Label	NIST		Calculated		Difference between the mean values given by NIST and Calculated		Difference between the Uncertainties	
	Mean Value [μm]	Standard Uncertainty [nm]	Mean Value [μm]	Standard Uncertainty [nm]	Difference [μm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]	Difference [nm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]
S_a	3.9890	0.3500	3.9890	0.3897	$-1.9772 \cdot 10^{-6}$	$-4.9566 \cdot 10^{-5}$	$-3.9167 \cdot 10^{-2}$	-0.1119
S_q	5.0002	0.3300	5.0002	0.3922	$-1.9876 \cdot 10^{-5}$	$-3.9450 \cdot 10^{-4}$	$-6.2178 \cdot 10^{-2}$	-0.1884
S_p	19.1043	95.9	19.1071	97.0	-0.0028	$-3.9750 \cdot 10^{-4}$	$-3.9167 \cdot 10^{-2}$	-0.1119
S_v	18.7142	92.6	18.7178	100.0	-0.0036	-0.0193	-7.1	0.3026
S_t	37.8154	140.4	37.8249	138.9	-0.0094	-0.0250	1.2	0.0088
S_{ku}	2.9585	0.6500	2.9585	0.7223	$-2.7902 \cdot 10^{-5}$	$-9.4311 \cdot 10^{-4}$	$-6.7952 \cdot 10^{-5}$	-0.1045
S_{sk}	0.0701	0.4700	0.0701	0.3283	$3.0672 \cdot 10^{-5}$	0.0437	$1.4225 \cdot 10^{-4}$	0.3026
Note: S_{ku} and S_{sk} do not have units								

The covariance of the height parameters can be found in Tab.5.7. The correlation coefficients of the height parameters are shown in Tab.5.8.

Tab.5.7 The covariance of the Height Parameters.

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	$3.739 \cdot 10^{-8}$	$3.102 \cdot 10^{-8}$	$3.643 \cdot 10^{-8}$	$-1.17 \cdot 10^{-8}$	$2.472 \cdot 10^{-8}$	$-1.183 \cdot 10^{-7}$	$-1.165 \cdot 10^{-8}$
S_q	$3.102 \cdot 10^{-8}$	$3.854 \cdot 10^{-8}$	$1.113 \cdot 10^{-7}$	$7.625 \cdot 10^{-8}$	$1.876 \cdot 10^{-7}$	$-2.401 \cdot 10^{-9}$	$-1.831 \cdot 10^{-9}$
S_p			0.0013	$3.268 \cdot 10^{-6}$	0.0013	$5.377 \cdot 10^{-6}$	$1.318 \cdot 10^{-6}$
S_v				0.0012	0.0012	$2.745 \cdot 10^{-6}$	$-9.388 \cdot 10^{-7}$
S_t					0.0025	$8.122 \cdot 10^{-6}$	$1.993 \cdot 10^{-7}$
S_{ku}						$3.172 \cdot 10^{-6}$	$5.187 \cdot 10^{-7}$
S_{sk}							$6.364 \cdot 10^{-7}$

Tab.5.8 The correlation coefficient of the height parameters

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	1	0.807	0.000	-0.005	-0.0038	-0.318	0.000
S_q		1	0.006	0.006	0.009	0.010	0.011
S_p			1	-0.018	0.692	0.069	0.028
S_v				1	0.710	0.081	-0.033
S_t					1	0.107	0.004
S_{ku}						1	0.116
S_{sk}							1

Fig.5.19 Surface height distribution.

Fig.5.20 Distributions of the areal height parameters of the Data base of SG_1-4.

Testing program for the data base SG_3-4:

The results calculated by the program can be found in Tab.5.9, and in Tab.5.9 also compares the difference between the values given by NIST and calculated by this program. Surface height distribution can be found in Fig.5.22, histogram of these areal height parameters are shown in Fig.5.23.

Tab.5.9 Results Calculated by the Program and Comparison with the Values given by NIST.

Label	NIST		Calculated		Difference between the mean values given by NIST and Calculated		Difference between the Uncertainties	
	Mean Value [μm]	Standard Uncertainty [nm]	Mean Value [μm]	Standard Uncertainty [nm]	Difference [μm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]	Difference [nm]	Ratio $\frac{NIST - Calculated}{NIST} \times 100$ [%]
S_a	0.6329	7.6000e-2	0.6329	7.7375e-2	-2.5160e-6	-3.9756e-4	-1.3746e-3	-0.0181
S_q	1.0001	7.2000e-2	1.0000	7.8592e-2	1.5230e-6	1.5229e-4	-6.5920e-3	-0.0916
S_p	13.9449	18.5	13.9433	20.0	0.0016	0.0114	-1.3746e-3	-0.0181
S_v	11.8311	0.0188	11.8341	0.0200	-2.7127e-4	-0.0023	1.2	-0.0641
S_t	25.7775	0.0264	25.7747	0.0283	0.0028	0.0107	1.9	-0.0725
S_{ku}	15.3870	0.0073	15.3868	0.0079	1.9482e-4	0.0013	-5.6584e-4	-0.0775
S_{sk}	0.6141	8.8000e-4	0.6141	8.7667e-4	-6.0048e-6	-9.7779e-4	3.3293e-6	0.0038

Note: S_{ku} and S_{sk} do not have units

The covariance of the height parameters can be found in Tab.5.10. The correlation coefficients of the height parameters are shown in Tab.5.11.

Tab.5.10 The covariance of the Height Parameters.

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	$1.511 \cdot 10^{-9}$	$9.630 \cdot 10^{-10}$	$3.266 \cdot 10^{-10}$	$3.121 \cdot 10^{-9}$	$3.448 \cdot 10^{-9}$	$-4.068 \cdot 10^{-8}$	$-1.228 \cdot 10^{-9}$
S_q		$1.532 \cdot 10^{-10}$	$2.136 \cdot 10^{-8}$	$1.753 \cdot 10^{-8}$	$3.890 \cdot 10^{-8}$	$8.786 \cdot 10^{-10}$	$3.298 \cdot 10^{-11}$
S_p			$1.012 \cdot 10^{-4}$	$-7.554 \cdot 10^{-7}$	$1.005 \cdot 10^{-4}$	$1.541 \cdot 10^{-5}$	$8.689 \cdot 10^{-7}$
S_v				$9.968 \cdot 10^{-5}$	$9.892 \cdot 10^{-5}$	$8.831 \cdot 10^{-6}$	$-6.474 \cdot 10^{-7}$
S_t					$1.994 \cdot 10^{-4}$	$2.424 \cdot 10^{-5}$	$2.215 \cdot 10^{-7}$
S_{ku}						$1.545 \cdot 10^{-5}$	$5.105 \cdot 10^{-7}$
S_{sk}							$1.921 \cdot 10^{-7}$

Tab.5.11 The correlation coefficient of the height parameters

Label	S_a	S_q	S_p	S_v	S_t	S_{ku}	S_{sk}
S_a	1	0.644	0.006	0.016	0.016	-0.259	-0.088
S_q		1	0.062	0.064	0.089	0.007	-0.001
S_p			1	0.007	0.712	0.394	0.205
S_v				1	0.707	0.232	-0.043
S_t					1	0.441	0.043
S_{ku}						1	0.301
S_{sk}							1

Fig.5.21 Surface height distribution.

Fig.5.22 Distributions of the areal height parameters of the Data base of SG_3-4.

The results calculated by the Matlab program are very similar to that given by NIST. From Tab.5.3, Tab.5.6, and Tab.5.9, we can see that the difference between the arithmetical mean height S_a and the root mean square height given by NIST and calculated range from 10^{-7} to 10^{-5} quantities with units of μm ; the difference between the maximum peak height S_p , the maximum pit height S_v , the maximum height S_t given by NIST and calculated range from 10^{-5} to 10^{-3} quantities with units of μm ; the difference between the Kurtosis S_{ku} and Skewness S_{sk} given by NIST and calculated range from 10^{-5} to 10^{-3} quantities. The difference between the uncertainties of the arithmetical mean height S_a , the root mean square height, the maximum peak height, given by NIST and calculated range from 10^{-5} to 10^{-3} quantities with units of nm; the difference between the uncertainties of the maximum pit height S_v , the maximum height S_t , given by NIST and calculated range from 10^{-3} to 10^0 quantities with units of nm; the difference between the uncertainties of the kurtosis and skewness given by NIST and calculated range from 10^{-2} to 10^{-4} quantities. The percentages of the differences are also calculated, which are around $10^{-3}\%$. The differences are very negligible, indicating that those parametrization algorithms developed in this work are reliable.

5.3.1 Verification of the filtration algorithm

The data base SG_1-2 mentioned above in part 5.3.1 is processed for verification of the filtration algorithm. SG_1-2 was first opened by the Surface Metrology Algorithm Testing System of NIST, as shown in Fig.5.24, then the cutoff wavelengths of x direction, λ_x , is set as 10 μm , and that of the y direction, λ_y is also set as 10 μm . Convolution method is applied for the filtration calculation, the Gaussian window is chosen as $[-\lambda_{cx}/2 \text{ to } \lambda_{cx}/2, -\lambda_{cy}/2 \text{ to } \lambda_{cy}/2]$. After the processing, data of the raw surface, of the roughness, and of the waviness as well as a report of the calculation are downloaded and compared with the results calculated by the algorithms developed in this work. Fig.5.25 shows the reconstruction of the raw surface, the waviness, and the roughness according to the data sets provided by NIST.

Fig.5.23 Testing system for Surface filtration provided by NIST.

Fig.5.24 Reconstruction of the Surface calculated by NIST testing system: (a) raw surface; (b) waviness; (c) roughness.

Tab.5.12 Comparison of the results provided by NIST and calculated.

Data NIST	S_a [um]	S_q [um]	S_p [um]	S_v [um]	S_t [um]	S_{ku}	S_{sk}
Raw surface NIST	0.8038	1.0000	2.9120	0.1923	3.5889	3.0151	6.6040
Roughness NIST	0.1103	0.1382	0.5646	0.5864	1.1510	2.9844	0.0163
Waviness NIST	0.7564	0.9383	3.2138	2.7587	5.9725	2.8854	0.2089
Waviness Calculated	0.7313	0.9361	3.3333	2.8787	6.2120	3.0665	0.1914
Difference	-0.0251	-0.0022	0.1195	0.1200	0.2395	0.1811	-0.0175
Percentage of Difference [%]	3.3199	0.2317	3.7178	4.3508	4.0102	6.2773	8.3929

Fig.5.25 Construction of surface of the waviness calculated by our developed algorithms. **Fig.5.26** 3D view construction of the waviness calculated by our developed algorithms.

The data set of the raw surface provided by NIST was imported into MATLAB[®] and processed by the algorithms developed in this work. As the Testing System for filtration only provide data of the waviness and roughness surface, not provide any values of height parameters as the Testing system for surface parameters, both the data sets of waviness provided by NIST and the waviness calculated by the developed algorithm in this work are processed by the same parameterization algorithms developed by this work, i.e. the algorithms developed and validated in the former part of this chapter. The results are showed and compared in Tab.5.12. Seven areal height parameters, S_a , S_q , S_p , S_v , S_t , S_{ku} , S_{sk} , are calculated and compared. The difference of the seven height parameters of the waviness are calculated by the following equations:

$$\text{Difference} = S_{\text{Waviness Calculated}} - S_{\text{Waviness NIST}} \quad (5.39)$$

$$\text{Percentage of Difference} = abs \left[\frac{S_{\text{Waviness Calculated}} - S_{\text{Waviness NIST}}}{S_{\text{Waviness NIST}}} \times 100 \right] \quad (5.40)$$

Where, $S_{\text{Waviness Calculated}}$ is the height parameters, such as S_a , S_q , etc., calculated by the waviness processed by our developed algorithms, $S_{\text{waviness NIST}}$ is the height parameters calculated by the waviness surface provided by the NIST Testing System. Fig.5.26 shows the constructed surface by the waviness data processed by the algorithms developed in this work, and Fig.5.27 shows the waviness surface construction in a 3D view. It can be found that the difference of the height parameters of the waviness provided by NIST and calculated by this

work is between $[-0.0022 \mu\text{m}, 0.2395 \mu\text{m}]$, the difference in percentage ranges from 0.2317% to 8.3929%. Comparing the constructed surface of waviness in Fig.5.26 and the waviness provided by NIST, almost no difference can be found. Considering that the difference is of nanometer magnitude, it can be concluded that the filtration algorithm developed by this work is valid and reliable.

5.4 References of Chapter 5

- [1] ISO 4287: 1998 Geometrical product specification (GPS) - Surface texture: Profile method - Terms, definitions and surface texture parameter.
- [2] B. Muralikrishnan. J. Raja, Computational Surface and Roundness Metrology, Springer, 2009.
- [3] R. Leach, Characterisation of Areal Surface Texture, Springer, 2013.
- [4] ISO 25178-3: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 3: Specification operators.
- [5] Michigan Metrology, LLC., 3D Spatial Parameters, 2016.
- [6] ISO 25178-2: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 2: Terms, definitions and surface texture parameters.
- [7] ISO 14406:2010 Geometrical product specifications (GPS) - Extraction.
- [8] ISO 16610-21: 2012 Geometrical product specifications (GPS) - Filtration - Part 21: Linear profile filters: Gaussian filters.
- [9] ISO 16610-22:2015. Geometrical product specifications (GPS) – Filtration – Part 22: Linear profile filters: Spline filters.
- [10] ISO 16610-28: 2015 Geometrical product specifications (GPS) - Filtration - Part 28: Profile filters: End effects.
- [11] ISO 16610-29:2015 Geometrical product specifications (GPS) - Filtration - Part 29: Linear profile filters: Spline wavelets.
- [12] ISO 16610-31:2015 Geometrical product specifications (GPS) - Filtration - Part 31: Robust profile filters: Gaussian regression filters.
- [13] ISO 16610-32: 2015 Geometrical product specifications (GPS) - Filtration - Part 32: Robust profile filters: Spline filters.
- [14] ISO 16610-41: 2015 Geometrical product specifications (GPS) - Filtration - Part 41: Morphological profile filters: Disk and horizontal line - segment filters.

- [15] ISO 16610-49: 2015 Geometrical product specifications (GPS) - Filtration - Part 49: Morphological profile filters: Scale space techniques.
- [16] ISO 16610-61: 2015 Geometrical product specifications (GPS) - Filtration - Part 61: Linear areal filters: Gaussian filters.
- [17] ISO 16610-71: 2015 Geometrical product specifications (GPS) - Filtration - Part 71: Robust areal filters: Gaussian regression filters.
- [18] ISO 16610-85: 2015 Geometrical product specifications (GPS) - Filtration - Part 85: Morphological areal filters: Segmentation.
- [19] ISO 11562: 1996 Geometrical product specifications (GPS) - Surface texture: Profile method - Metrological characteristics of phase correct filters.
- [20] Internet Based Surface Metrology Algorithm Testing System.
<https://physics.nist.gov/3DVSC/jsp/Database3D.jsp?state=0>. 7th Feb 2018.

Chapter 6: Comparison of statistical methods for outlier identification in surface metrology

Abstract: This chapter studies the statistical methods for outlier identification and apply those methods for surface measurement data. Ten statistical methods for outlier identification which can be implemented in the area of surface metrology are analysed and compared. Twenty-four Mat files were created based on two standard data sets provided by the National Institute of Standards and Technology for experimental study of those statistical methods. Based on processing the same series of contaminated data sets, the number of missed outliers, the difference of the height parameters, and the elapsed time by each method are compared. Algorithm efficiency, robustness, breakdown point, limitations, advantages, etc. are compared and analysed. Two of those ten methods were combined to know their potential. A type C1 spacing standard artefact was measured by 3D image confocal microscopy, and the data was processed by those algorithms. The difference of S_a and that of elapsed time are compared.

6.1 Introduction

Raw measurement data files obtained from optical instruments are often affected by local measurement defects due to local slopes, scanning speed, light intensity, material transparency, circular groove, etc. [33]. These defects mainly include unmeasured points and outliers. In the area of surface metrology, outlier is defined as local portion in a data set that is not representative for the partitioned integral feature [38]. In the statistical interpretation,

outliers are defined as member of a small subset of observations that are inconsistent with the remainder of a given sample [3].

Surface metrology characterization using image confocal microscopy frequently leaves unmeasured points and outliers together in one surface measurement. This is especially the case when measuring structured surfaces, such as hydrophobic materials, which are constructed with complicated pattern units, causing a large variation of local slopes, light reflection, etc. Treatment of these abnormal points is necessary for a high level of accuracy. There are two ways of treating unmeasured points: leaving them unmeasured, for which the calculation algorithms must be able to exclude them; or replacing them with a plausible height value, using methods of interpolation of neighbouring points, or methods of interpolation, or fitting, of the surrounding valid pixels for determination of a best fit value [25]. Some investigators prefer the first method because it does not introduce additional error [25]; some others tend to fill in small unmeasured areas to obtain a complete measured surface, but leave large unmeasured areas for which there might be holes [33]. This work tends to leave those unmeasured points without treatment so as not to introduce additional errors, and focuses on investigating methods for identification of outliers.

Surface topography can be viewed as a superposition of different scales of geometrical features and these features are usually scaled as form, waviness, and roughness [36]. Aside from these three components, an engineering surface might also have data inclination, noise, and outliers. All of these features can be separated by filters while outliers are managed as part of noise [37, 35]. The ISO 16610 series has defined three kinds of areal filters: linear areal filters, robust areal filters, and morphological areal filters [38]. The areal Gaussian filter is the default linear areal filter, and it is widely used by almost all instrument manufacturers. This filter, however, is not robust against outliers and in fact it often follows them [36, 37]. Robust areal filters are defined as Gaussian Regression Filters. As indicated in ISO 16610-30 [39] robustness is not an absolute property of a filter but a relative one. One can only say that a given filter is robust compared to an alternative filter against a particular phenomenon. In ISO 16610, Robust Areal Filters are named in reference to Linear Areal Filters, which does not mean the Robust Areal Filters defined by ISO 16610 are absolutely robust against outliers. In fact, some previous investigators have shown that those robust filters cannot completely remove those outliers from the data set either [37].

Another disadvantage of those linear areal filters is that they map each point on a surface to a weighted average of its neighbouring points [9], as shown in equation 6.1, where $z(s)$ is the unfiltered profile or surface, and $K(x,s)$ is the kernel function. $K(x,s)$ is the weighting applied to average those input data. Different choices of the kernel function will lead to different linear filters.

$$y(x) = \int_{-\infty}^{+\infty} K(x,s)z(s)ds \quad (6.1)$$

For traditional stochastic surfaces, those linear areal filters or robust areal filters might work well by mapping a point to a weighted average of its neighbouring point. For structural surfaces, however, as shown in Fig. 6.1, which is a dimpled surface where the features only fill part of the tile and are surrounded by background surface, the filters are very likely to fail as features and background on a pattern unit often vary greatly. The shift from stochastic to structured surfaces is among the three important aspects of current paradigm shifts in surface metrology, while the other two aspects are the shift from profile to areal characterization and from simple geometries to complex freeform geometries [40].

Fig. 6.1. Pattern units (blue) and individual features (red) of a structural surface.

ISO 16610-30 [39] also declared the importance of data pre-processing, indicating that pre-processing followed by a filter results in a robust filter and it has the advantage that once a

method has been found to be capable of removing unwanted phenomena, then it will work with any filter [39]. This standard defined two pre-processing methods, i.e. scale-space pre-processing and wavelet pre-processing. However, these two methods aim at removing profile discontinuities before filtration, but are not used to remove outliers.

M. F. Ismail, *et al.* [37] proposed an outlier correction procedure applied to areal surface data measured by optical instruments. Their procedure includes two stages: outlier candidate detection and outlier verification. For outlier candidate detection, they first determine the sufficient size of an outlier detection window, and make the reference of the detection by comparing the relative height between the median of the surrounding data and the observed data. The difference will be noticeable when the observed data is an outlier and the surrounding data are normal. To have the median value of the surrounding data arise from normal ones, the investigators have to enlarge the detection window. This makes their algorithm cumbersome and unreliable for various reasons. Firstly, an enlarged detection window might reach other clusters of outliers which go against the expectation of normal data. Secondly, for structured surfaces, points between background and features usually differ significantly. The median value of the surrounding background might not have any obvious difference from outliers on the feature. They also defined methods for setting threshold value, outlier verification and correction, with illustrations of application for measurement of surface of dental implants, as well as comparing their proposed method to a Gaussian filter and a median filter, and it shows that their proposed method obviously functions better than the typical filtering methods. This method works well with stochastic surfaces with simple distribution of outlier clusters, but might fail when applied to structured surfaces or to those surfaces containing adjacent outlier clusters.

Yutao Wang, *et al.* [41] investigated the formation of outliers in scanning reflective surfaces, and developed two outlier formation models based on mixed reflections and multi-path reflections. The outlier formation models they developed can be applied to sensor view and scan path planning. In addition to this, they also proposed an outlier detection method for scanned point clouds using majority voting [42]. The main feature of their method is the majority voting scheme to reliably remove connections between non-isolated outlier clusters and the scanned surface even when these outlier clusters form planar patches.

G Le Goic, *et al.* [12] proposed a method for metrological outlier filtering based on distributions of the points of the entire surface being compliant with the normality assumption. The first step is to simulate height distribution of the entire surface data. As most surface heights usually do not follow normal distribution, a method based on discrete modal decomposition (DMD) is proposed for data transformation. After the data transformation, Grubbs' Test is applied to an analysis window of variable size that slides and is recursive over the entire surface.

6.2 Statistical methods for outlier identification

Ten statistical methods for outlier identification are introduced mathematically in this part. Methodology and results of experimental study of those methods are introduced in the next part. In this section, developments of the algorithms for those methods are also introduced.

6.2.1 Interquartile range (IQR)

The interquartile range is defined as the difference between the third and first quartiles for a sorted data set [13, 14], and it is calculated as:

$$IQR = Q_3 - Q_1 \quad (6.2)$$

$$Q_1 = x_{\lfloor n/4 \rfloor} \quad (6.3)$$

$$Q_3 = x_{\lceil 3n/4 \rceil} \quad (6.4)$$

where, $\lceil \dots \rceil$ rounds up to the nearest integer and $\lfloor \dots \rfloor$ rounds down to the nearest integer.

Outliers are those data points below $Q_1 - 1.5 \times IQR$ or above $Q_3 + 1.5 \times IQR$. The breakdown value of this method is only 25%, but it has a simple interpretation and calculation. Algorithm using IQR method for outlier detection in the measurement data is shown below.

Objective: Detect outliers in the surface measurement data using the IQR method.

Algorithm. Outliers detection using IQR (set Z_{input});

- (i) Load database SG_1-4, set $Z_{input} = \{z_i\}_{i=1}^N$ and sort Z_{input} in an ascending sequence;

- (ii) Compute $IQR = Q_3 - Q_1$; $Q_1 = x_{\lceil 3n/4 \rceil}$; $Q_3 = x_{\lfloor n/4 \rfloor}$
 - (iii) Set lower boundary by $Q_1 - 1.5 \times IQR$ and upper boundary by $Q_3 + 1.5 \times IQR$;
 - (iv) Find $Z_{input} < Q_1 - 1.5 \times IQR$ or $Z_{input} > Q_3 + 1.5 \times IQR$
 - (v) Record the points that lie beyond either boundary and compare detected outliers with those generated outliers;
 - (vi) Compare height parameters calculated by original data z and those by processed contaminated data;
- end**

6.2.2 Median absolute deviation (MAD)

Median absolute deviation (MAD) calculates the median med_i of a data set and median deviation. MAD is very simple but also very useful [15]. Their robustness and quick calculation make them ideal for screening outliers by computing from equation 6.4.

$$\frac{|x_i - med_j x_j|}{MAD_N} \quad (6.5)$$

For each x_i of variable $\{x_i\}_{i=1}^N$, if its result is greater than the threshold, the corresponding x_i is termed as an outlier [16].

Let's define T as a regression estimator, which yields a simple of n data points $Z = \{(x_{11}, \dots, x_{1p}, y_1), \dots, (x_{n1}, \dots, x_{np}, y_n)\}$ with a regression coefficient $\hat{\theta}$

$$T(Z) = \hat{\theta} \quad (6.6)$$

Now consider that those data points Z are contaminated by some m arbitrary points yielding a corrupted sample Z' . The bias between the regressions of contaminated sample and original sample is defined as:

$$bias(m; T, Z) = \sup_{Z'} \|T(Z') - T(Z)\| \quad (6.7)$$

Where supremum is over all possible corrupted data Z' . If $bias(m; T, Z)$ is finite, it means that those corrupted points have affected the estimator too much, and the estimator is not reliable, which means the estimator 'break down'. The break down point of an estimator is defined as

$$\varepsilon^*(T, Z) = \min \left\{ \frac{m}{n}; bias(m; T, Z) \text{ is infinite} \right\} \quad (6.8)$$

The breakdown point of Least Median Square regression is $\left\{ \frac{\left[\frac{n}{2} \right] - p + 2}{n} \right\}_{p>1}$ near 50%, which is very high. Algorithm using MAD method for outlier detection in the measurement data is shown below.

Objective: Detect outliers in the surface measurement data using the MAD method.

Algorithm. Outlier detection using MAD (set $\mathbf{Z}_{input}$, set cutoff threshold)

- (i) Set $\mathbf{Z}_{input} = \{z_i\}_{i=1}^N$ and $threshold = sigthresh$, in this case $sigthresh = 1.2$;
- (ii) Compute $scores_{i=1}^N = \frac{|z_i - med_j z_j|}{MAD_N}$ for $\mathbf{Z}_{input}$ and detect z_i that exceeds the certain cutoff $sigthresh$;
- (iii) **while** exist scores $> sigthresh$
 - calculate median value of $\mathbf{Z}_{input}$ without nans
 - calculate MAD value of $\mathbf{Z}_{input}$
 - compute scores
 - Detect scores $> sigthresh$
 - Find the index outliers
 - if** no outliers found
 - break the loop
 - end**
- (iv) Replace outliers with NAN

end

6.2.3 The Q_n Estimator

The Q_n Estimator calculates the difference between two elements in a data set as shown in equation 6.5

$$Q_n = d\{x_i - x_j \mid i < j\}_{(k)} \quad (6.9)$$

where $k = \binom{b}{2} \approx \binom{n}{2}/4$, and $b = \lfloor \frac{n}{2} \rfloor + 1$ with $\lfloor \dots \rfloor$ rounds down to the nearest integer, d is the correction coefficient of bias as Fisher-consistent for σ [16]. This equation takes the k_{th} order statistic of the $\binom{b}{2}$ interpoint distances.

Peter J. Rousseeuw, *et al.* [13], determined the breakdown point, which indicates at which point the method fails, of the Q_n Estimator as

$$\varepsilon_n^*(Q_n, X) = \lfloor n/2 \rfloor / n \quad (6.10)$$

However, they did not define a method for screening outliers. This work established two methods for outlier detection. The first method is to compare the maximum $Q_n|_{i=1}^n$ with $Q_n|_k$ as:

$$\max_s Q_n|_{i=1}^n / Q_n|_k \quad (6.11)$$

Based on this method for screening outliers, algorithm using the Q_n Estimator method for outlier detection in the measurement data is shown below.

Objective: Detect outliers in the surface measurement data using the Q_n Estimator.

Algorithm. Outliers detection using Q_n Estimator (set $\mathbf{Z}_{\text{input}}$, set cutoff threshold)

- (i) Set $\mathbf{Z}_{\text{input}} = \{z_i\}_{i=1}^N$, and $threshold = sigthresh$;

- (ii) Compute $Q_n = d \{ |z_i - z_j|; i < j \}$ for $\{z_i\}_{i=1}^N$, sort $Q_n|_{i=1}^N$ in an ascending order,
- (iii) Calculate $k = \left(\frac{b}{2}\right)$, find $Q_n|_{\max}$ and $Q_n|_k$
- (iv) Compare $\max_s Q_n|_{i=1}^n / Q_n|_k$ with sigthresh
- (v) **if** $\max_s Q_n|_{i=1}^n / Q_n|_k > \text{sigthresh}$
 determine z_i and z_j in $Q_n|_{\max}$ as outliers
- end**

The second method is similar to the method of outlier screening with MAD, by computing:

$$\frac{Q_{n(i < j \in \{x_i\}_{i=1}^N)}}{Q_{n(k)}} \quad (6.12)$$

Based on this method for screening outliers, algorithm using the Q_n Estimator for outlier detection in the measurement data is shown below.

Objective: Detect outliers in the surface measurement data using the Q_n Estimator.

Algorithm. Outliers detection using Qn Estimator (set Zinput, set cutoff threshold)

- (i) Set $\mathbf{Z}_{\text{input}} = \{z_i\}_{i=1}^N$, and $\text{threshold} = \text{sigthresh}$;
- (ii) Compute, $\text{scores}_{i=1}^N = \frac{Q_{n(i < j \in \{x_i\}_{i=1}^N)}}{Q_{n(k)}}$ for $\{z_i\}_{i=1}^N$;
- (iii) compare $\max_s Q_n|_{i=1}^n / Q_n|_k$ with sigthresh;
- (iv) Detect scores $> \text{sigthresh}$
- (v) Find the index outliers
- (vi) Replace outliers with NAN or delete outliers
- end**

6.2.4 The Trimmed Mean method

The Trimmed Mean method unifies other estimators, such as median and mean [17]. It is the mean of a data set excluding the extreme values and its calculation equation is as shown

below [18]. This equation calculates the mean value excluding p percent of the highest and lowest observations [32].

$$T(p) = \frac{\sum_{i=r+1}^{n-r} x_i}{n - 2r} \quad (6.13)$$

$$r = \lfloor pn \rfloor \quad (6.14)$$

Where x_i is the sample values, p is the percent of trimming, and n is the size of the sample. From this equation we can find that trimmed mean can unify sample mean and median by varying p . Trimmed mean equals sample mean by setting p as zero, while it equals sample mean when p is set as $\lfloor (n-1)/2 \rfloor / n$.

6.2.5 Grubbs' Test

Grubbs' test is based on the assumption of normality. It is obligatory to verify that the data can be reasonably approximated by a normal distribution before applying the Grubbs' test. [20]. Grubbs' test detects one outlier at a time. This outlier is expunged from the dataset and the test is iterated until no outliers are detected. However, multiple iterations change the probabilities of detection, and the test should not be used for sample sizes of six or fewer since it frequently tags most of the points as outliers.

The Grubbs' Test statistic is calculated according to equation 6.11 and it is defined for the hypothesis [21]:

H_0 : There are no outliers in the data set.

H_a : There is at least one outlier in the data set.

$$G = \frac{\max_{i=1, \dots, N} |x_i - \bar{x}|}{s} \quad (6.15)$$

Where x_i is the value of this sample, $\bar{x}$ is the sample mean, and s denotes the standard deviation. This is the two-sided test but it can also identify one side. Equation 6.17 is to test whether the minimum value is the outlier and equation 6.18 is to detect whether the maximum value is an outlier, with $x_{\min}$ and $x_{\max}$ denoting minimum and maximum values respectively.

$$G = \frac{\bar{x} - x_{\min}}{s} \quad (6.16)$$

$$G = \frac{x_{\max} - \bar{x}}{s} \quad (6.17)$$

For the two-sided test, the hypothesis H_0 is rejected when

$$G > \frac{N-1}{\sqrt{N}} \sqrt{\frac{t_{\alpha/(2N), N-2}^2}{N-2 + t_{\alpha/(2N), N-2}^2}} \quad (6.18)$$

where $t_{\frac{\alpha}{2N}, N-2}$ represents the upper critical value of the t-distribution with $N-2$ degrees of freedom and a significance level of $\frac{\alpha}{2N}$ while for the one-sided tests, replace $\frac{\alpha}{2N}$ with $\frac{\alpha}{N}$. This method has an advantage of not necessarily set a threshold.

6.2.6 The Extreme Studentized Deviate method (*ESD*)

The Extreme Studentized Deviate (*ESD*) test is quite good at identifying one or more outliers in a univariate dataset that is approximately normal sample. The generalized ESD method requires an upper bound for the suspected number of outliers. Given the upper bound and suspected number r , the ESD method performs r separate tests based on hypothesis: a test for an outlier until the r_{th} outlier.

The Extreme Studentized Deviate method defines the hypothesis as [22]:

H_0 : No outliers in the data set.

H_a : Existing r outliers in the data set.

The outlier factor is computed by equation 6.20:

$$R_i = \frac{\max_i |x_i - \bar{x}|}{s} \quad (6.19)$$

Where $\bar{x}$ denotes mean value and s denotes standard deviation. Critical value λ_i is calculated according to equation 6.21:

$$\lambda_i \approx \frac{(n-i)t_{p,n-i-1}}{(n-i-1+t_{p,n-i-1}^2)(n-i+1)} \quad (6.20)$$

where $i = 1, 2, \dots, r$, $p = 1 - \frac{\alpha}{2(n-i+1)}$, $t_{p,n-i-1}$ is the $100p$ percentage point from the t distribution with $n-i-1$ degrees of freedom. H_0 is rejected when $R_i > \lambda_i$. Critical Value λ_i for suspected number of 1 to 3 and significance level α of 1% and 5% is shown in Tab. 6.1. Simulation studies by Rosner [32] indicate that this critical value approximation is very accurate for sample size $n \geq 25$ and reasonably accurate for $n \geq 15$.

Tab. 6.1 Critical value λ_i for $r = 1, 2$, or 3 and significance levels of $\alpha = 1\%$, 5% .

n	Number of suspected outliers					
	1		2		3	
	α		α		α	
	1%	5%	1%	5%	1%	5%
5	1.764	1.715	1.496	1.481	1.155	1.154
10	2.482	2.290	2.387	2.215	2.274	2.127
15	2.806	2.548	2.755	2.507	2.699	2.462
20	3.001	2.708	2.968	2.681	2.932	2.652
25	3.135	2.822	3.112	2.802	3.087	2.780
30	3.236	2.908	3.218	2.893	3.199	2.876
35	3.316	2.978	3.301	2.965	3.286	2.952
40	3.381	3.036	3.369	3.025	3.356	3.014
50	3.482	3.128	3.474	3.120	3.464	3.112
60	3.560	3.200	3.553	3.193	3.546	3.187
70	3.622	3.258	3.616	3.252	3.610	3.247
80	3.673	3.306	3.668	3.302	3.663	3.297
90	3.716	3.348	3.712	3.344	3.708	3.340
100	3.754	3.384	3.750	3.381	3.747	3.377

Although the generalized ESD is essentially the Grubbs' Test applied sequentially, there are a few important distinctions: The generalized ESD test makes appropriate adjustments for the critical values based on the number of outliers being tested for that the sequential application of Grubbs' Test does not; if there is significant masking, applying Grubbs' Test sequentially may stop too soon.

6.2.7 Dixon-type tests

Dixon-type tests are based on the ratios of ranges and ordered statistics [23, 25]. They can identify whether the largest and the smallest observations are outliers and can as well test the largest observation as an outlier avoiding the smallest observation and test the smallest observation as an outlier avoiding the largest observation according to equations 6.21-6.24, respectively.

$$r_{10} = \frac{x_n - x_{n-1}}{x_n - x_1} \quad (6.21)$$

$$r_{10} = \frac{x_2 - x_1}{x_n - x_1} \quad (6.22)$$

$$r_{11} = \frac{x_n - x_{n-1}}{x_n - x_2} \quad (6.23)$$

$$r_{11} = \frac{x_2 - x_1}{x_{n-1} - x_1} \quad (6.24)$$

The first class of ratios, r_{10} , is used when the suspected outlier is the largest or smallest observation while the second set of ratios, r_{11} is used when the potential observation is the second smallest or second largest. Dixon-type tests have many advantages: they are flexible enough to allow for specific observations to be tested; they perform well with small sample sizes, with no need to assume the normality of the data. Critical values Q_{crit} of Dixon-type tests are shown in Tab. 6.2.

Tab. 6.2 Critical values of Q_{crit}

N	Q_{crit} (with confidence level of)		
	90%	95%	99%
3	0.941	0.970	0.994
4	0.765	0.829	0.926
5	0.642	0.710	0.821
6	0.560	0.625	0.740
7	0.507	0.568	0.680
8	0.468	0.526	0.634
9	0.437	0.493	0.598
10	0.412	0.466	0.568

6.2.8 Chauvenet's Criterion

The idea of Chauvenet's Criterion [23, 24] is to find a probability band centred on the mean and distributed by normal distribution, as shown in Fig. 6.2. This probability band contains all the normal samples and those data points lying outside this band are outliers. This method is calculated by the following equation:

$$D_{\max} \geq |x - u| / \sigma \quad (6.25)$$

Where x represents suspected value, u is sample mean, σ is sample standard deviation, $D_{\max}$ represents the maximum allowable deviation.

Fig. 6.2. Probability band for identification of outliers as Chauvenet's Criterion.

Algorithm for outlier identification using Chauvenet's Criterion is:

Objective: Detect outliers in the surface measurement data using Chauvenet's Criterion.

Algorithm. Outliers detection using Chauvenet's criterion

- (i) Set $\mathbf{Z}_{\text{input}} = \{z_i\}_{i=1}^N$, and Chauvenet's criterion;
- (ii) Compute $T_i = |x_i - \bar{x}| / s$ for $\mathbf{Z}_{\text{input}}$ and detect T_i that exceeds the certain criterion;
- (iii) Record the points that lie beyond either boundary and compare detected outliers with those generated outliers;
- (iv) Compare height parameters calculated by original data z and those by processed contaminated data.

end

Tab. 6.3 Chauvenet's Criterion Table

N	T	N	T	N	T
3	1.383	17	2.178	31	2.406
4	1.534	18	2.200	32	2.418
5	1.645	19	2.222	33	2.429
6	1.732	20	2.241	34	2.440
7	1.803	21	2.260	35	2.450
8	1.863	22	2.278	36	2.460
9	1.915	23	2.295	37	2.470
10	1.960	24	2.311	38	2.479
11	2.000	25	2.326	39	2.489
12	2.037	26	2.341	40	2.498

13	2.070	27	2.355	50	2.576
14	2.100	28	2.369	100	2.807
15	2.128	29	2.382	500	3.291
16	2.154	30	2.394	1000	3.481

6.2.9 The Pauta Criterion (also named 3σ criterion)

The Pauta Criterion is also named 3σ criterion, this name comes from its outlier identification method [25] [26]. If $|v_k| > 3\sigma$, then v_k is considered an outlier, where v_k and σ are calculated respectively by equations 6.26 and 6.27.

$$v_k = X_k - \bar{X} \quad (6.26)$$

$$\begin{aligned} \sigma &= \sqrt{\frac{1}{(n-1)} \sum_i (v_i^2)} \\ &= \sqrt{\frac{1}{(n-1)} \left(\sum_i (x_i)^2 - (\sum_i \bar{x}_i)^2 / n \right)} \end{aligned} \quad (6.27)$$

where X_k is the k_{th} element, $\bar{X}$ is the sample mean, n is the size of the sample.

As the standard deviation σ is usually replaced with the experimental standard deviation $s(X_k)$ since σ is usually not known and this criterion can be iterated. This method did not detect any outliers for the 24 data sets.

Objective: Detect outliers in the surface measurement data using Pauta Criterion.

Algorithm. Outliers detection using Pauta criterion

- (i) Set $\mathbf{Z}_{\text{input}} = \{z_i\}_{i=1}^N$;
- (ii) Compute v_k and $s(x_k)$ for $\mathbf{Z}_{\text{input}}$ and detect v_k that exceeds $3 \times s(x_k)$;
- (iii) Record the points that lie beyond either boundary and compare detected outliers with those generated outliers;
- (iv) Compare height parameters calculated by original data z and those by processed contaminated data.

end

6.2.10 Tukey's test

Tukey's test is based on measures such as the interquartile range. For example, if Q_1 and Q_3 are the lower and upper quartiles respectively, then one could define an outlier to be any observation outside the range:

$$[Q_1 - k(Q_3 - Q_1), Q_3 + k(Q_3 - Q_1)] \quad (6.28)$$

John Tukey proposed this test, where $k = 1.5$ indicates an "outlier", and $k = 3$ indicates data that is "far out" [27]. This method is the same with IQR method.

6.3 Methodology of the experimental study

To compare the efficiency of various statistical methods for outlier detection implemented in surface metrology, the algorithms of each method are developed and processed with a same series of data sets. Twenty-four data sets were created by four factors with two to three levels. Two standard databases provided by the National Institute of Standards and Technology (NIST) [20], SG_1-2 and SG_1-4, were implemented. Information of their areal surface parameters is shown in Tab. 6.5 and Tab. 6.6. Outliers of amount of 1%, 5% and 10% of the entire amount of areal points are added to each data set. The variations in amplitude of the outliers are three and five times of the height of their corresponding points individually. The uncertainties of surface height are respectively 10 nm and 100 nm following a normal distribution model employing the Monte Carlo method. The arrangement of the data sets can be found in Tab. 6.7. This arrangement is to simulate the possible cases of most measurement instrumentations, considering that different instruments generate different percentages and amplitudes of outliers, different uncertainties of surface heights, etc. The choice of two standard databases was based on the idea of surface height parameters S_a , S_q , etc., varying as much as possible. The surface patterns of these two databases are shown in Fig. 6.3.

This arrangement of data sets takes into consideration the surface-dependency and instrument limitations for surface characterization. Properties such as local slopes, material transparency, circular grooves, smoothness, etc., are surface-dependent and will render different amplitudes

and quantities of uncertainties and outliers [33, 29]. The numerical aperture determines the greatest slope angle on the surface that can be measured and affects the optical resolution [29]. One limitation of the interferometric microscope is that its measurement accuracy depends on the smoothness of its reference surface [5]. Although there are other instruments that do not require a nearly perfect reference, they are limited by the size of the probe beam and the width of the reference beam, etc.

All the algorithms are processed on the same laptop with an Intel(R) Core(TM) i5-4210U CPU and memory of 8 GB RAM. The number of missed outliers and the difference in height parameters between certified results and those calculated after outlier detection of the 24 data sets, are compared within every method, in order to know whether the method performs well for various kinds of measurement data, or is limited to some specific type of data. In addition to this, those results and the time consumed by each method is compared mutually for comparison of the accuracy, efficiency, preference of data types, etc.

Fig. 6.3 Images of surfaces from the standard databases: (a) SG_1-2; (b) SG_1-4.

Tab. 6.4 Areal surface parameters from the standard database SG_1-2.

Parameter	Nominal Value (NV)	Mean Value (MV)	Standard Uncertainty
S_a	0.80376 μm	0.8038 μm	0.077 nm
S_q	1 μm	1.00005 μm	0.077 nm
S_{ku}	2.91199	2.912	0.00062
S_{sk}	0.19232	0.19231	0.00037
S_p	3.58892 μm	3.58905 μm	17.86 nm
S_v	3.0151 μm	3.0145 μm	18.01 nm

S_t	6.60403 μm	6.60477 μm	26.79 nm
-------	-----------------------	-----------------------	----------

Tab. 6.5 Areal surface parameters from the standard database SG_1-4.

Parameter	Nominal Value (NV)	Mean Value (MV)	Standard Uncertainty
S_a	3.98884 μm	3.98904 μm	0.35 nm
S_q	5 μm	5.00023 μm	0.33 nm
S_{ku}	2.95848	2.95846	0.00065
S_{sk}	0.07009	0.07011	0.00047
S_p	18.71759 μm	18.71417 μm	95.59 nm
S_v	37.04346 μm	37.05147 μm	56.07 nm
S_t	37.82351 μm	37.81541 μm	140.41 nm

Tab. 6.6 Arrangement of data sets.

Experiment	Data	Outlier	Variation	Uncertainty	Experiment	Data	Outlier	Variation	Uncertainty
1	SG 1-4	1%	5	100	13	SG 1-2	1%	5	100
2	SG 1-4	1%	5	10	14	SG 1-2	1%	5	10
3	SG 1-4	1%	3	100	15	SG 1-2	1%	3	100
4	SG 1-4	1%	3	10	16	SG 1-2	1%	3	10
5	SG 1-4	5%	5	100	17	SG 1-2	5%	5	100
6	SG 1-4	5%	5	10	18	SG 1-2	5%	5	10
7	SG 1-4	5%	3	100	19	SG 1-2	5%	3	100
8	SG 1-4	5%	3	10	20	SG 1-2	5%	3	10
9	SG 1-4	10%	5	100	21	SG 1-2	10%	5	100
10	SG 1-4	10%	5	10	22	SG 1-2	10%	5	10
11	SG 1-4	10%	3	100	23	SG 1-2	10%	3	100
12	SG 1-4	10%	3	10	24	SG 1-2	10%	3	10

Part Information

Part Name: SG_1-4

Created by: Dr. M. Uchida-Dept. of Mechanical Engineering, Iwate University,

Experiment	Data	Outlier	Variation	Uncertainty	Experiment	Data	Outlier	Variation	Uncertainty
------------	------	---------	-----------	-------------	------------	------	---------	-----------	-------------

Description: Japan
Random roughness surface

Process Information

Process Name: Numerically Generated Process

Measurement Information

Instrument type: N/A

Data file

File Name: SG_1-4.sdf
Units: μm
Number Points: 256
Number of Profiles: 256
Spacing X-direction: $2\ \mu\text{m}$
Spacing Y-direction: $2\ \mu\text{m}$
Data type: 3D

Filter Information

Filter type: N/A
Method: N/A
Cutoff: 0 mm
Additional Information: Raw Data

Uncertainty Information

Assume that Z co-ordinates have standard uncertainty of 50.0 nm (1% of S_q);
X co-ordinates have standard uncertainty of 40.0 nm (2% of sampling interval);
Y co-ordinates have standard uncertainty of 40.0 nm (2% of sampling interval);
measurement errors on Z, X, and Y co-ordinates are Gaussian distribution and independent.
Level of Confidence = 95 %

Areal surface parameters:

Label	Nominal Value	Mean Value	Standard Uncertainty
S_a	$3.98884\ \mu\text{m}$	$3.98904\ \mu\text{m}$	0.35 nm
S_q	$5\ \mu\text{m}$	$5.00023\ \mu\text{m}$	0.33 nm
S_{sk}	0.07009	0.07011	0.00047
S_{ku}	2.95848	2.95846	0.00065
S_l	$37.82351\ \mu\text{m}$	$37.81541\ \mu\text{m}$	140.41 nm
S_p	$18.71759\ \mu\text{m}$	$18.71417\ \mu\text{m}$	95.59 nm
S_v	$37.04346\ \mu\text{m}$	$37.05147\ \mu\text{m}$	56.07 nm

The algorithm for generating the MAT file is:

Objective: Produce a data for experimental study.

Algorithm.

- (i) Import the database SG1-4;
- (ii) Generate 5 surfaces according to SG1-4 and distribute uncertainties of 50.0 nm (1% of S_q) to each surface;
- (iii) Define values of outliers as $\pm k \times z_i$, in our case $k = \pm 3$;
- (iv) Determine the number of outliers for adding, 1% of the total number of SG1-4
- (v) Generate the random points of those 5 surfaces and add outliers to them
- (vi) Generate the expected MAT file with information of 5 contaminated surfaces and with recording of the position of outliers.

end

To use this data, we just need to type 'load name.mat', name represents the name of the MAT file. After loading our generated data, there is information including matrix of outliers, surface of original data, and those contaminated surfaces. Matrix of outliers indicates the position of contaminated points, i.e. which row, column, and surface those outliers belong to.

6.4 Experimental study and comparison of those methods for surface measurement

6.4.1 Experimental study of IQR

All the algorithms were developed in Matlab® and those 24 data sets were processed and compared. Experimental study and results are introduced in this section. Analysis and comparisons are introduced in section 6.5. As there are 24 data sets, after the processing 24 results are obtained. Three typical results of each method are selected for demonstration.

The height parameters processed are shown in Tab. 6.8. These three results are chosen as the least, the middle, and the largest difference of height parameters. The difference is calculated as $(OD-MV)/MV \times 100$, where OD represents the value calculated by data with outliers deleted, MV represents the value calculated by mean value. This calculation of difference is applied for all the other methods. As can be observed in Tab. 6.8, the difference between the height parameters is high, because this algorithm has missed a big amount of outliers.

Tab. 6.7 Results of the height parameters processed by IQR.

Parameter (mean value)	Experiment 1			Experiment 12			Experiment 22		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.1517	4.0698	2.0305	4.7917	4.3995	10.2960	1.1254	0.9688	20.5326
S_q [μm]	5.2834	5.1378	2.7564	6.0943	5.5517	11.0343	1.4579	1.227	22.6973
S_{ku}	3.6049	3.2731	10.6347	3.2864	3.1698	7.1429	3.7744	3.3616	15.4402
S_{sk}	0.0829	-0.0637	-190.9204	0.07	-0.2257	-422.0398	0.2284	-0.4036	-309.8801
S_p [μm]	32.3274	19.2492	0.7497	25.7517	19.5086	2.1076	6.4601	3.7461	4.3803
S_v [μm]	28.6483	28.5639	52.6047	26.2091	25.809	37.8861	5.3482	5.1864	72.0156
S_t [μm]	60.9757	47.8131	26.4110	51.9607	45.3175	19.8132	11.8083	8.9326	35.2595

6.4.2 MAD

To choose the best threshold (k), the range of outlier factor is calculated first, which is between $[0, 3.3219]$. The difference between S_a , the number of identified outliers, and the number of missed outliers processed by different thresholds are indicated in Tab. 6.9 and compared in Fig. 6.4. This is an example of threshold confirmation with data from Experiment 2. The other 23 data sets use the same threshold selection method.

Tab. 6.8 Comparison of results processed by different thresholds.

Threshold (k)	0.9	1.5	2.0	2.5	2.6	2.7
Difference between S_a [%]	NaN	0.0065	0.1912	0.1905	0.1905	0.1905
Number of identified outliers	65536	64219	42955	19250	15918	12839
Number of missed outliers	99	93	95	181	182	184
Threshold (k)	2.8	2.9	3.0	3.1	3.2	3.3
Difference between S_a [%]	0.1904	0.1904	0.1908	0.1988	3.9727	3.9727
Number of identified outliers	9977	7366	5303	3774	154	3
Number of missed outliers	186	194	197	290	3275	3275

Fig. 6.4. Comparison of results processed by different thresholds

Taking into account the difference of arithmetic mean value S_a , the number of identified outliers, and the number of missed outliers, the threshold $k = 3.1$ was reached. It detected 3774 points as outliers, while the data set has 3275 outliers. This algorithm has missed 290 outliers. The difference between S_a is 0.1988, etc., as shown in Tab. 6.9. The same method for the threshold reached is applied to the other method that needs threshold designation. To indicate the importance of the threshold, results processed as $k = 3.0$ are shown in Tab. 6.9. It detected 5303 points as outliers, while missing 197 outliers. The difference between S_a is 0.1908%, the difference between S_{ku} is 2.9627%, etc. The above two results indicate that the threshold is crucial for the MAD method. The reconstruction of the contaminated surface and the surface with outlier deletion can be found in Fig. 6.5.

(a)

(b)

Fig. 6.5 Reconstruction of surface: (a) before deletion of outliers; (b) after deletion of outliers

After processing, 24 data sets were obtained and three of them are shown in this work. These three series of height parameters and the difference between the mean value provided by NIST and that calculated by the data after outlier deletion can be found in Tab. 6.10. The differences between the height parameters (with outliers and after deletion of outliers) are very small when compared with those obtained by the IQR method.

Tab. 6.9 Results of the height parameters processed by MAD.

Parameter (mean value)	Experiment 10			Experiment 19			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	5.5831	3.9889	0.0011	0.8853	0.8148	1.3789	0.9667	0.8246	2.5980
S_q [μm]	7.2729	5.0000	0.0006	1.1147	1.0078	0.7820	1.2202	1.0143	1.4307
S_{ku}	3.7711	2.9584	-0.0016	3.2425	2.8593	-1.8103	3.2421	2.8124	-3.4208
S_{sk}	0.0777	0.0701	0.0120	0.1985	0.1880	-2.2699	0.2049	0.1848	-3.9167
S_p [μm]	34.4187	19.1059	-0.0002	3.5879	3.5889	-0.0289	5.0055	3.5450	-1.2228
S_v [μm]	33.6758	18.7070	-0.0568	4.2767	3.1093	3.1227	4.2701	3.0140	-0.0381
S_t [μm]	68.0946	37.8128	-0.0282	9.0817	6.6791	1.4100	9.2756	6.5590	-0.6819

6.4.3 The Q_n estimator

For the method of Q_n estimator, there is no defined method for screening outliers. This work established two methods for outlier screening. The first method is to compare the maximum

$Q_n|_{i=1}^n$ with $Q_n|_k$ as:

$$\max_{\hat{s}} Q_n|_{i=1}^n / Q_n|_k \quad (6.29)$$

By this method, experiment 2 elapsed 24.238 seconds. This algorithm detected 9280 points as outliers while the database has 3275 outliers. This algorithm has missed 128 outliers. Results processed by Q_n estimator can be found in Tab. 6.11.

Tab. 6.10 Results of Experiment 2 processed by Q_n Estimator with threshold = 18.

Parameter (mean value)	Reference value	Original data	With outliers	Outlier deleted	Difference [%]
---------------------------	--------------------	------------------	------------------	--------------------	-------------------

S_a [μm]	3.98904	3.9888	4.1473	3.9956	0.1705
S_q [μm]	5.00023	5.000	5.2784	5.0128	0.2566
S_{ku}	2.95846	2.9585	3.6710	3.0097	1.7326
S_{sk}	0.07009	0.0701	0.0873	0.0713	1.7230
S_p [μm]	18.71759	19.1059	34.3881	25.7150	34.5918
S_v [μm]	37.05147	18.7176	32.0533	28.7722	53.7174
S_t [μm]	37.81541	37.8235	66.4434	54.4872	44.0564

The second method is similar to the method of outlier screening with MAD, by computing:

$$\frac{Q_{n(i < j \in \{x_i\}_{i=1}^N)}}{Q_{n(k)}} \quad (6.30)$$

The first method deletes the maximum and minimum values simultaneously. The second method fails easily, especially when outliers scatter far away from the bulk points. The three typical results of the 24 data sets processed by the first outlier screening method can be found in Tab. 6.12. As can be observed, the difference between the height parameters is small when the roughness of the surface is high. On the contrary, this method is unable to eliminate the outliers when the roughness is small.

Tab. 6.11 Results of the height parameters processed by the Qn Estimator.

Parameter (mean value)	Experiment 2			Experiment 9			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.1499	3.9890	0.0034	5.5954	4.0101	0.5336	0.9667	0.8522	6.0272
S_q [μm]	5.2791	5.0001	0.0023	7.3079	5.0147	0.2942	1.2202	1.0419	4.1930
S_{ku}	3.5757	2.9584	-0.0022	3.8168	2.9475	-0.3712	3.2421	2.7112	-6.8964
S_{sk}	0.0890	0.0701	-0.0048	0.0746	0.0700	-0.1047	0.2049	0.1703	-11.4348
S_p [μm]	29.3459	19.1150	0.0474	34.3134	19.1166	0.0558	5.0055	3.5983	0.2608
S_v [μm]	29.2815	18.7176	-0.0002	33.5071	18.7362	0.0996	4.2701	3.0818	2.2128
S_t [μm]	58.6273	37.8325	0.0239	67.8204	37.8528	0.0775	9.2756	6.6801	1.1520

6.4.4 The Trimmed Mean

The three typical results of the 24 data sets processed by the Fast Trimmed Mean method can be found in Tab. 6.13. This method presents the same behaviour as the Q_n Estimator method.

Tab. 6.12 Results of the height parameters processed by Fast Trimmed Mean with $p = 0.2$.

Parameter (mean value)	Experiment 10			Experiment 19			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	5.5831	3.9906	0.0034	0.8853	0.8129	1.1044	0.9667	0.8207	2.1074
S_g [μm]	7.2729	5.0014	0.0024	1.1147	1.0084	0.8271	1.2202	1.0155	1.5477
S_{ku}	3.7711	2.9574	-0.0023	3.2425	2.8854	-0.8360	3.2421	2.8640	-1.6482
S_{sk}	0.0777	0.0701	-0.0110	0.1985	0.1896	-0.9173	0.2049	0.1875	-2.5019
S_p [μm]	34.4187	19.1094	0.0269	4.8051	3.5917	1.0636	5.0055	3.5975	0.2376
S_v [μm]	33.6758	18.7109	-0.0045	4.2767	3.1046	1.1619	4.2701	3.0827	2.2404
S_t [μm]	68.0946	37.8203	0.0113	9.0817	6.6963	1.1085	9.2756	6.6801	1.1520

6.4.5 Grubbs' test

The three typical results of the 24 data processed by Grubbs' Test can be found in Tab. 6.14. This method presents good behaviour, since the differences between the height parameters, in general, are small.

Tab. 6.13 Results of the height parameters processed by the Grubbs' Test with $t = 2.3530$.

Parameter (mean value)	Experiment 4			Experiment 21			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.0675	3.9888	-0.0001	1.1273	0.8052	0.1737	0.9667	0.8060	0.2750
S_g [μm]	5.1169	5.0000	-0.0001	1.4587	1.0015	0.1481	1.2202	1.0018	0.1766
S_{ku}	3.0861	2.9585	0.0009	3.7240	2.9123	0.0110	3.2421	2.9101	-0.0662
S_{sk}	0.0806	0.0701	-0.0235	0.2180	0.1918	-0.2654	0.2049	0.1922	-0.0689
S_p [μm]	26.1714	19.1031	-0.0147	6.5547	3.6825	2.6349	5.0055	3.5445	-1.2389
S_v [μm]	24.5160	18.7000	-0.0937	5.5239	2.9915	-0.7819	4.2701	3.0322	0.5665

S_r [μm]	50.6874	37.8032	-0.0538	12.0786	6.6750	1.0749	9.2756	6.5766	-0.4147
-------------------------	---------	---------	---------	---------	--------	--------	--------	--------	---------

There are other implementations for this algorithm, as proposed by Beliakov [31], that could be used to reduce computation times (the method of equation 10 takes about 40s of calculation), but it is only effective when the number of repetitions of the measurement is high ($n > 100$).

6.4.6 The extreme studentized deviate

As here are only 5 variables, the suspected number r is set as 1 and significance level chosen as 95%. Therefore, the critical value λ_i is 1.175. The three typical results of the 24 data processed by *ESD* method can be found in Tab. 6.14. As can be seen, this method presents the same behaviour as the Grubbs' Test method.

Tab. 6.14 Results of the height parameters processed by *ESD* method with $\lambda_i = 1.175$.

Parameter (mean value)	Experiment 8			Experiment 17			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.3873	3.9888	0.0001	0.9642	0.8053	0.1877	0.9667	0.8061	0.2926
S_q [μm]	5.5679	5.0000	-0.0005	1.2473	1.0019	0.1892	1.2202	1.0021	0.2066
S_{ku}	3.3000	2.9584	-0.0015	3.9875	2.9132	0.0418	3.2421	2.9106	-0.0477
S_{sk}	0.0803	0.0701	0.0286	0.2099	0.1926	0.1438	0.2049	0.1924	0.0425
S_p [μm]	26.7434	19.1060	0.0002	6.3295	3.6447	1.5535	5.0055	3.5444	-1.2398
S_v [μm]	22.1855	18.7173	-0.0016	5.3365	3.0663	1.6969	4.2701	3.0322	0.5675
S_r [μm]	48.9289	37.8232	-0.0007	11.6660	6.7109	1.6189	9.2756	6.5766	-0.4147

6.4.7 Dixon-type test

The three typical results of the 24 data sets processed by the Dixon-type method can be found in Tab. 6.15. This method presents the same behaviour as the *ESD* method.

Tab. 6.15 Results of the height parameters processed by Dixon-type method with $Q = 0.7100$.

Parameter (mean value)	Experiment 6			Experiment 17			Experiment 19		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.7851	3.9888	0.0002	0.9642	0.8061	0.2860	0.8853	0.8084	0.5835
S_q [μm]	6.2371	5.0000	0.0000	1.2473	1.0016	0.1607	1.1147	1.0027	0.2687

S_{ku}	4.0614	2.9585	0.0008	3.9875	2.9102	-0.0625	3.2425	2.8959	-0.5517
S_{sk}	0.0774	0.0701	-0.0256	0.2099	0.1929	0.3040	0.1985	0.1911	-0.6387
S_p [μm]	34.3851	19.1015	-0.0230	6.3295	3.6196	0.8540	4.8051	3.5875	-0.0399
S_v [μm]	33.3805	18.7123	-0.0283	5.3365	3.0326	0.5815	4.2767	3.1097	3.1358
S_t [μm]	67.7656	37.8138	-0.0256	11.6660	6.6522	0.7296	9.0817	6.6971	1.4100

6.4.8 Chauvenet's criterion

The three typical results of the 24 data sets processed by Chauvenet's Criterion can be found in Tab. 6.17. This method presents good behaviour as the previous methods.

Tab. 6.16 Results of the height parameters processed by Chauvenet's Criterion.

Parameter (mean value)	Experiment 2			Experiment 11			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]
S_a [μm]	4.1499	3.9888	-0.0009	4.7887	3.9893	0.0104	0.9667	0.8079	0.5135
S_g [μm]	5.2791	5	-0.0004	6.0837	5.0001	0.0012	1.2202	1.0023	0.2351
S_{ku}	3.5757	2.9585	0.0012	3.2601	2.9591	0.0225	3.2421	2.9032	-0.3000
S_{sk}	0.089	0.0701	-0.0096	0.0731	0.0701	0.0234	0.2049	0.1918	-0.2729
S_p [μm]	29.3459	1.1097	0.0198	26.7259	19.0802	-0.1346	5.0055	3.5446	-1.2363
S_v [μm]	29.2815	18.7176	-0.0002	25.7182	18.7473	0.1588	4.2701	3.0321	0.5633
S_t [μm]	58.6273	37.8273	0.0099	52.4441	37.8275	0.0106	9.2756	6.5766	-0.4147

6.4.9 The Pauta criterion

As the standard deviation σ is usually replaced with the experimental standard deviation $s(X_k)$ since σ is usually not known and this criterion can be iterated. This method did not detect any outliers for the 24 data sets.

6.4.10 Turkey's test

This method is the same as the IQR method and gives the same results.

6.4.11 Combination of IQR and Dixon-type Test

The possibilities of combining two methods for outlier identification are evaluated. The IQR and Dixon-type test methods were programmed to process the 24 data sets. The representative three series of results are shown in Tab. 6.18. It can be seen that the difference between the height parameters are smaller than that processed by the individual methods.

Tab. 6.17 Results of the height parameters processed by the combination of the IQR and the Dixon-type test.

Parameter (mean value)	Experiment 6			Experiment 21			Experiment 23		
	With outliers (WO)	Outlier deleted (OD)	Difference[%]	With outliers (WO)	Outlier deleted (OD)	Difference [%]	With outliers (WO)	Outlier deleted (OD)	Difference[%]
S_a [μm]	4.7851	3.9888	0.0001	1.1273	0.8066	0.3540	0.9667	0.8098	0.7551
S_q [μm]	6.2371	5.0000	0.0000	1.4587	1.0017	0.1724	1.2202	1.0032	0.3238
S_{ku}	4.0614	2.9585	0.0009	3.7240	2.9085	-0.1207	3.2421	2.8954	-0.5700
S_{sk}	0.0774	0.0701	-0.0289	0.2180	0.1945	1.1486	0.2049	0.1967	2.2569
S_p [μm]	34.3851	19.1017	-0.0223	6.5547	3.6354	1.2939	5.0055	3.5476	-1.1508
S_v [μm]	33.3805	18.7122	-0.0290	5.5239	3.0176	0.0820	4.2701	3.0114	-0.1238
S_t [μm]	67.7656	37.8138	-0.0256	12.0786	6.6529	0.7406	9.2756	6.5590	-0.6819

6.5 Analysis and comparison of the ten methods

The breakdown value of the IQR method is only 25%, but it has a simple interpretation and calculation. From Fig. 6.6 it can be observed that this method is among those with the shortest elapsed time. The advantage of this method is that it is not necessary to reach a threshold. However, in fact, in the equations $Z_{\text{input}} < Q_1 - 1.5 \times IQR$ and $Z_{\text{input}} > Q_3 + 1.5 \times IQR$, 1.5 and quartiles is a threshold to some extent.

Fig. 6.6 Comparison of the elapsed time by each method.

To calculate the breakdown point for the MAD method, the first step is to define T as a regression estimator, which yields a simple n data points $Z = \{(x_{11}, \dots, x_{1p}, y_1), \dots, (x_{n1}, \dots, x_{np}, y_n)\}$ with a regression coefficient $\hat{\theta}$ [32]

$$T(Z) = \hat{\theta} \quad (6.31)$$

Considering that those data points Z are contaminated by some m arbitrary points yielding a corrupted sample Z' , the bias between the regressions of contaminated sample and original sample is defined as [33]:

$$\text{bias}(m; T, Z) = \sup_{Z'} T(Z') - T(Z) \quad (6.32)$$

where supremum is over all possible corrupted data Z' . If $\text{bias}(m; T, Z)$ is finite, it means that those corrupted points have affected the estimator too much, and the estimator is not reliable, which means the estimator 'breaks down'. The breakdown point of an estimator is defined as the lowest number of outliers identified. Meanwhile, the number of missed outliers is also

among one of the lowest, which means this method is very efficient at identifying outliers and confuses the normal points with fake points very little.

$$\varepsilon^*(T, Z) = \min \left\{ \frac{m}{n}; \text{bias}(m; T, Z) \text{ is infinite} \right\} \quad (6.33)$$

The robustness of the MAD comes at a cost: it is less efficient than the mean with the normal model. From Fig. 6.6 it can be found that MAD method consumed the third-longest time for calculation. But when all the factors are taken into account, this method displays the best work efficiency.

Fig. 6.7 Comparison of the difference between S_a processed by the ten methods and the combination method with a logarithmic scale on the y axis.

Fig. 6.8 Comparison of the number of missed outliers by each method.

The Q_n estimator is the first quartile of all pairwise differences between two data points. The breakdown value of the Q_n estimator is $\varepsilon_n^*(Q_n, X) = \lfloor n/2 \rfloor / n$, which is about 50%. The disadvantage of this algorithm is that it deletes two values at the same time, i.e. the maximum value and the minimum value, without detecting in advance which one is the outlier. In addition, the threshold significantly affects the results obtained by this method. Attention must be paid to the threshold reached when utilizing this method for outlier identification. Results will vary a lot for different threshold values.

The Trimmed Mean can unify the sample mean and median by varying p . The Trimmed Mean equals the sample mean by setting p as zero, while it equals the sample median when p is set as $\lfloor (n-1)/2 \rfloor / n$.

The Grubbs' Test is based on the normal distribution, i.e. the data set must be verified as normal distribution before applying this method [38]. This method detects one outlier at a time

and iterates until no outliers are left. After expunging outliers, the probabilities of outlier identification change and this method should not be used for sample sizes of fewer than 6 as it often tags most of the points as outliers.

The Extreme Studentized Deviate (*ESD*) method is quite good at identifying one or various outliers in a univariate data set that is of normal distribution. By giving the number n of suspected outliers and an upper bound, this method will identify one outlier at a time and iterate n times until it finds all the suspected outliers.

Dixon-type tests and Chauvenet's criterion consumed a similar amount of time for calculation and results in similar height parameters as shown in Fig. 6.7 and Fig. 6.8. Their calculation equations are very different, but the number of missed outliers is almost the same. As shown in Fig. 6.8, only experiments 19, 21 and 23 indicate some small differences. The data from experiment 19, 21 and 23 have a small value of S_a , but a high uncertainty as 100 nm, and a high percent of outliers in the data. Dixon-type tests are based on the ratios of ranges and ordered statistics while Chauvenet's criterion is to find a probability band centred on the mean. Tukey's test is intrinsically the same as the Interquartile Range method. Both of them define a range based on the lower and upper quartiles.

The Pauta Criterion identifies outliers based on the difference between v_k and 3σ , as for any residual v_k , exists:

$$v_k^2 < \sum_{k=1}^n v_k^2 \quad (6.34)$$

Therefore,

$$|v_k| \leq \sqrt{\sum_{k=1}^n v_k^2} = \sqrt{n-1} \sqrt{\frac{\sum_{k=1}^n v_k^2}{n-1}} = \sqrt{n-1} s(X_k) \quad (6.35)$$

It is obvious that the Pauta Criterion is not fit for $n \leq 10$. This criterion is based on normal distribution. When n is infinite, the confidence level is larger than 99%. However, as n is finite, and $s(X_k)$ is used instead of σ , this method is an approximation criterion. The

possibility that the Pauta Criterion will delete the normal value is shown in Tab. 6.18. The possibility of the Pauta Criterion deleting the normal values decreases with the increasing number of observations and finally will be stable at 0.3%. This mathematical analysis is consistent with the experimental analysis in this work. From Fig. 6.8 it can be found that the Pauta Criterion displays the worst efficiency in outlier identification as the number of missed outliers is the highest. This method has missed all of the outliers. The possible reason may be that the data sample is too small, which leads to the experimental standard deviation $s(X_k)$ lying far away from the residual v_k .

Tab. 6.18 The possibility of deletion of normal values by the Pauta Criterion.

Observations n	11	16	61	121	333
Possibility p	0.019	0.011	0.006	0.004	0.003

Fig. 6.9 Comparison of filtered surfaces of Experiment 2 by methods of: (a) IQR; (b) MAD; (c) Q_n Estimator; (d) Trimmed Mean; (e) Grubbs' Test; (f) *ESD*; (g) Dixon-type tests; (h) Chauvenet's criterion; (i) Pauta criterion; (j) Tukey's test.

Fig. 6.9 shows the surfaces filtered by each statistical method of Experiment 2. When comparing Fig. 6.8 and Fig. 6.9, it can be found that the smoothness of surfaces is related with the number of missed outliers while the number of identified outliers has no impact on the surfaces. This is logical because the mean value of the filtered data contains five contaminated surfaces for surface reconstruction. Even though normal points are identified as outliers and are deleted, when the mean value of the remaining points is calculated, the results would not be influenced or biased. If the outliers are missed they will be calculated as normal points, therefore the results will be skewed.

6.6 Comparison of the 10 methods by a standard artefact

A Type C1 spacing standard with grooves having a sine wave profile, as shown in Fig. 6.10, with a certified value of S_a equal to $1.003 \mu\text{m}$ and expanded uncertainty of $0.03 \mu\text{m}$ ($k = 2$), was measured using the Leica DCM-3D Confocal Microscopy at the Metrology Laboratory of the Technical University of Madrid. A magnification objective of 50X was used, with a numerical aperture of 0.90. The measurement was performed under a controlled temperature at $20 \pm 1^\circ\text{C}$.

Fig. 6.10 The Type C1 spacing standard: (a) photograph of the standard; (b) surface processed by MAD method.

After the measurement and the process of algorithms, two parameters are compared. One is the difference between the certified and the calculated values of S_a . The other is the elapsed time measuring the physical standard artefact as shown in Fig. 6.11. The difference is calculated as $(S_{a_calculated} - S_{a_standard})/S_{a_standard} \times 100$.

Fig. 6.11 Comparison of the difference of S_a and the elapsed time measuring the physical standard artefact.

These algorithms detected and deleted those outliers and calculated those height parameters, without recording which data are deleted. The elapsed time for the MAD, Chauvenets' criterion, and Q_n methods was the greatest, i.e. 35.03, 32.44, and 27.22 seconds individually, while the differences between S_a processed by these three methods are also among the smallest. The Dixon-type test and IQR methods consumed the least time, i.e. 7.98 and 9.47 seconds respectively, and the Dixon-type resulted in the smallest S_a difference. The combination of these two methods took 11.99 seconds for calculation. The differences between S_a vary from 2.764% to 2.780% for the ten statistical methods and the combination methods of IQR and Dixon-type test. The surface of this standard artefact is very similar to Experiment 16, as the surface roughness, the percentage, the amplitude of the outliers, and the uncertainties are all very small. Fig. 6.10 shows a surface processed by MAD method.

6.7 Summary

Ten statistical methods for outlier detection which can be implemented in the area of surface metrology for surface evaluation are analysed and compared. The mathematical model, the method for screening out outliers, and the calculations of outlier factors of those ten methods are introduced. Algorithms are developed for data processing in Matlab®. Twenty-four Mat files were created based on two standard databases provided by the National Institute of Standards and Technology. These data were assigned four factors with two to three levels for simulating the most common types of surfaces in a mechanical field. The four factors are surface roughness, percentage of outliers, amplitude of outliers, and uncertainties, with roughness of 0.8038 μm and 3.9890 μm , outliers of 1%, 5% or 10%, three and five times larger than the value of the point, uncertainties of 10 nm or 100 nm. These files were processed by the ten methods individually. The IQR and Dixon-type test methods are combined for data processing and the combination results in less difference between height parameters than the individual methods. The experiments show that the combination can decrease the difference of the value of S_a . The elapsed time for the combination of the algorithm was a little more than the individual algorithm but far less than the summation of the two elapsed times. Results of the number of missed outliers, the difference of the height parameters defined by ISO 25178 between certified and calculated after outlier detection are presented and the elapsed time by each method is compared. Algorithm efficiency, robustness, advantages, disadvantages, etc. of those 10 outlier identification methods are compared and analysed. IQR has a breakdown value of 25% but has an advantage of simple interpretation and no need to choose threshold values. MAD method has a breakdown value of about 50% but it is less efficient than the mean when the data follows a normal model; MAD consumes a relatively long time but its missed number of outliers is among the lowest. The Trimmed Mean method can unify sample mean and median by varying p . The Pauta Criterion does not fit for $n \leq 10$. A Type C1 spacing standard with grooves having a sine wave was measured and processed by the ten methods and the combination of the IQR and Dixon-type methods, the difference between S_a ranges from 2.764% to 2.780% and the elapsed times vary from 7.98 seconds to 35.03 seconds. Due to the paradigm shifts in surface metrology from stochastic to structured surfaces, the importance of data pre-processing before the application of filters is increasing. This work will make the implementation of statistical

methods for identification of measurement outliers easier. The developed algorithms can be applied to other types of instruments and ranges of measurements.

6.8 References of Chapter 6

- [1] Richard Leach, Optical measurement of surface topography, Springer, 2011.
- [2] ISO 16610-1:2015. Geometrical product specifications (GPS) – Filtration – Part 1: Overview and basic concepts.
- [3] ISO 16269-4: Statistical interpretation of data - Part 4: Detection and treatment of outliers.
- [4] Gavin MacAulay, Characterization of structured surfaces and assessment of associated measurement uncertainty, NPL, 2015.
- [5] R. Leach, Characterisation of Areal Surface Texture, National Physical Laboratory, Springer Heidelberg New York Dordrecht London, 2013.
- [6] M. F. Ismail, K. Yanagi, A. Fujii, An outlier correction procedure and its application to areal surface data measured by optical instruments, Measurement science and technology 21 (10) (2010) 105105(11pp).
- [7] ISO 16610-60: 2015. Geometrical Product Specimen (GPS) - Filtration - Part 60: Linear areal filters: Basic concepts.
- [8] ISO 16610-30: 2015(en). Geometrical product specifications (GPS)-Filtration-Part 30: Robust profile filters: Basic concepts.
- [9] X. Jiang, P. J. Scott, D. J. Whitehouse, and L. Blunt, Paradigm shifts in surface metrology. Part II. The current shift, Proceedings of the Royal Society, 2007.
- [10] Y. Wang, H. Y. Feng, Modeling outlier formation in scanning reflective surfaces using a laser stripe scanner, Measurement 57 (2014) 108–121.
- [11] Y. Wang, H. Y. Feng, Outlier detection for scanned point clouds using majority voting, Computer-Aided Design 62 (2015) 31 – 43.
- [12] G. L. Goic, C. A. Brown, H. Favreliere, S. Samper, F. Formosa, Outlier filtering: a new method for improving the quality of surface measurements, Measurement science and technology 24 (2013) 015001(13pp).
- [13] P. J. Rousseeuw, M. Hubert, Robust statistics for outlier detection, WIREs Data Mining and Knowledge Discovery 1 (2011) 73–79.
- [14] A. Ullrich, Detecting measurement outliers - Remeasure efficiently, in: Montgomery, MW and Maurer, W (Ed.), PHOTOMASK TECHNOLOGY 2010, Vol. 7823 of Proceedings of SPIE, BACUS; SPIE, SPIE-INT SOC OPTICAL ENGINEERING, 1000 20TH ST, PO BOX 10, BELLINGHAM, WA 98227-0010 USA, 2010, Conference on Photomask Technology 2010, Monterey, CA, SEP 13-16, 2010.

- [15] C. Park, M. Leeds, A highly efficient robust design under data contamination, *COMPUTERS & INDUSTRIAL ENGINEERING* 93 (2016) 131–142.
- [16] P. J. Rousseeuw, C. Croux, Alternatives to the median absolute deviation, *Journal of the American Statistical Association* 88 (424) (1993) 1273–1283.
- [17] M. R. Sindhumol, M. R. Srinivasan, M. Gallo, A robust dispersion control chart based on modified trimmed standard deviation, *ELECTRONIC JOURNAL OF APPLIED STATISTICAL ANALYSIS* 9 (1) (2016) 111–121.
- [18] T. Hu, S. Y. Sung, A trimmed mean approach to finding spatial outliers, *Intelligent Data Analysis* 8 (1) (2004) 79–95.
- [19] Steven Walfish, A review of statistical outlier methods, *Pharmaceutical Technology* 30 (2006) 1–5.
- [20] Asad Ali, Muhammad F. Qadir, A Modified M-Estimator for the Detection of Outliers, *PJSOR* 1 (2005) 49–64.
- [21] F. Velasco, S. Verma, M. Guevara, Comparison of the performance of fourteen statistical tests for detection of outlying values in geochemical reference material databases, *MATHEMATICAL GEOLOGY* 32 (4) (2000) 439–464.
- [22] J.-P. Stauffert, F. Niebling, M. E. Latoschik, Towards Comparable Evaluation Methods and Measures for Timing Behavior of Virtual Reality Systems, in: Spencer, SN (Ed.), *22ND ACM CONFERENCE ON VIRTUAL REALITY SOFTWARE AND TECHNOLOGY (VRST 2016)*, ACM; ACM SIGCHI; ACM SIGGRAPH, ASSOC COMPUTING MACHINERY, 1515 BROADWAY, NEW YORK, NY 10036-9998 USA, 2016, pp. 47–50, 22nd ACM Conference on Virtual Reality Software and Technology (VRST), Munich, GERMANY, NOV 02-04, 2016.
- [23] J. Gawlowski, J. Bartulewicz, T. Gierczak, J. Niedzielski, Tests for outliers. A Monte Carlo evaluation of the error of first type, *CHEMIA ANALITYCZNA* 43 (4) (1998) 743–753.
- [24] R. D' Amato, J. Caja, P. Maresca, E. G 贸 mez, Use of coordinate measuring machine to measure angles by geometric characterization of perpendicular planes. Estimating uncertainty, *Measurement* 47 (2014) 598–606.
- [25] S.S.Qian, *Measurement Uncertainty: Process and Representation of Experimental Data*, 2002.
- [26] Z. Bi-Ming, J. Qi-Yun, M. Dan, X. Long-Ying, A novel method for handling gross errors in electromagnetic prospecting data, *CHINESE JOURNAL OF GEOPHYSICS-CHINESE EDITION* 58 (6) (2015) 2087–2102.
- [27] H. Elsaied, R. Fried, Tukey's M-estimator of the Poisson parameter with a special focus on small means, *STATISTICAL METHODS AND APPLICATIONS* 25 (2) (2016) 191–209.
- [28] Internet Based Surface Metrology Algorithm Testing System.
<https://physics.nist.gov/3DVSC/jsp/Database3D.jsp?state=0>. 7th Feb 2018.

- [29] R. Leach, Fundamental principles of engineering nanometrology 2nd Edition, William Andrew, 2014.
- [30] T. V. Vorburger, Tutorial in optics: Chapter 8 Methods for characterizing surface topography, Optical society of America, 2010.
- [31] G. Beliakov, Fast computation of trimmed means, Journal of statistical software 39 (2) (2011) 1–6.
- [32] R. Andersen, Modern Methods for Robust Regression, SAGE Publications, 2008.
- [33] A. M. L. Peter J. Rousseeuw, Robust Regression and Outlier Detection, John Wiley & Sons, New York, 1987.

Chapter 7: Confidence Distance Matrix for surface outlier identification

Abstract: This chapter proposes a new statistical method for outlier identification for surface measurement data obtained by confocal microscopy. The implemented statistical method is Confidence Distance Matrix (CDM) which were widely used in statistics and many engineering areas, such as signal processing, sensor data fusion, information problems, etc. However, **no investigations on identifying outliers in measured surface data using CDM have been found**. This chapter introduces and simplifies the mathematical model of CDM method. Algorithms for identifying random outliers using Monte Carlo method for uncertainty evaluation and for identifying outliers in a unique measured surface are developed and validated. Two experiments are carried out, respectively on a Type C1 spacing standard and on a steel surface.

7.1 Introduction

The surface quality is one of the most important factors that influence the final performances of a product [1]. Quality control in the manufacturing sectors has been an area of intense investigations. In fact, in the case of the aerospace and automotive industries, the inability to identify certain defects in the production process can lead to downtime in the production line generating economic losses in terms of costs [2]. For this reason, in recent years, several authors have focused their studies on research problems related to surface quality. For example, Krolczyk *et al.* have presented a study to determine the effect of manufacturing process conditions as a key factor in generation of the surface morphology [3, 4]. All of these studies were conducted by using optical measurement techniques that allow the characterization of the areal surface topography. This characterization allows the manufacturer to control and to radically change the functionality of a part. Naturally, in order to control such manufacturing methods requires appropriate measurement strategies. These measurement strategies include a wide range of new optical techniques on the market, or under study in the academic world, capable of measuring the topography of the surface area. Each measurement method has its advantages and its limitations. For example, in the case of confocal microscopies, local defects, scanning speed, light intensity, material transparency, etc., often affect surfaces measured, leading to measurement outliers [33]. Filtering and outlier detection, which are part of the data pre-processing, are crucial as the outlying points

affect the visual appearance on the one hand and distort geometric measures on the other [6]. The outlier, that are characterized by scale and magnitude, is defined, according to the specification of ISO 16610-1 as local portion in a data set that is not typical or not representative for the partitioned integral feature [38]. By the statistical interpretation, outlier is member of a small subset of observations, which appears to be inconsistent with the remainder of a given sample data [3]. Previous investigations on outlier treatment of measured surface data mainly studied methods of filtrations and methods of detection and correction of outliers. For example, G. L. Goic, *et al.* in 2012 presented a study on the new method in order to improve the quality of the surface measurement. In their study the authors introduced a new filtering technique by removing measurement artefacts (Spikes and batwing) that affect the analysis. The proposed method is based on discrete modal decomposition (DMD). Outliers are identified using a criterion based on Grubbs' test. Finally, the Authors developed a user interface in order to facilitate the use of the filter. This interface allows the results and indicators to be visualized at different stages of the process and allows to save the resulting surfaces in the desired format, after identifying and excluding outliers. [12]. Y. Wang, *et al.*, in 2015 presented a study on the numerous measurement outliers that could contaminate the 3D laser scanning of any artifact. The proposed method was based on the principle of majority voting. The authors presented a comparison study with several existing methods used in the process of 3D scanner and respectively cloud points. The results of their research demonstrate that the proposed method is able to achieve superior results in detecting all types of outliers and preserving distinct geometric features such as sharp edges in a scanned point cloud. [42]. X. J. Jiang, *et al.*, in 2012 presented a study on the surface classification system in association with the filtration, numeric parametric techniques, fractals associated with function and standardization [6]. Filtration methods map each point on a surface to a weighted average of its neighbors with some filters by convolution or Fourier transformation. This is the reason that many filters follow outliers [36]. For example, M. F. Ismail, *et al.*, in 2010 presented a new procedure for areal surface topography taking in account of the median relative height of the surrounding data. The presented method was tested by dental implant surface topography data measured by a confocal laser scanning microscope. The results demonstrated that their proposed method was excellent on outlier removal comparing to typical filtering methods [37]. Robust filters do not mean absolutely robust against outliers but only behave robust comparing to some linear filters [39, 35, 16]. Outlier detection and correction plays a crucial role in the quality control of surface characterizations [16]. H. Huang, *et al.*, in 2009 indicated that the presented point cloud consolidation surface reconstruction schemes could better suggest the topology and geometry of the shape from raw input data in challenging situations [17]. A. Nurunnabi, *et al.*, in 2015

presented two different statistical techniques for outlier detection in point cloud data. The first method was based on a robust z-score and the other used a Mahalanobis type robust distance. Both presented methods couple the ideas of point to plane orthogonal distance and local surface point consistency to get Maximum Consistency with Minimum Distance (MCMD). The results of their research show that the proposed algorithms are significantly faster, more accurate and robust [18].

The concept of distance measure is widely used in statistics and is applied to many engineering areas[19], such as signal processing [20], sensor data fusion [21, 22], information problems [23, 24], image processing [25], etc. However, there are no researches using this statistical method for surface metrology found until now. For this reason, the aim of this study is to propose.

7.2. Methodology for identifying outliers in surface measurement data

The method of outlier identification for measured surface data proposed contains two parts. The first part is to identify and remove the random noise such as instability in the instrument electronics, ground vibrations, ventilation, sound, short and long-term temperature fluctuations, etc. [20]. This part is in accordance with the Monte Carlo method defined in GUM-S1 [62] and GUM-S2 [63] for evaluation of measurement uncertainty. To obtain a surface measurement with uncertainty evaluation as precision as possible, measures are usually repeated n times for acquisition of mean values and standard deviations. Assuming that outliers happen randomly and only exist in a very small portion of the overall database, repeats of surface measurement can be organized as arrays in unit of points and calculate the distance matrix inside every unit. In combination with the determination of threshold, outliers can be distinguished from normal points.

The second part treats outliers in measurement in surface metrology. Outliers may be caused by different disturbing effects, such as steep edges and high gradients on the technical surface, residual caused by lubricant, oil, dirt or dust on the surface, physical principles of the optical instruments, such as numerical aperture, underexposure or overexposure [29]. A detection window is introduced for simplification of data processing, which was also implemented by previous researchers [37].

Both parts share the same outlier screening method, i.e. confidence distance measures, which is introduced in section 3. The predetermined condition for method of confidence distance measures is threshold value, but there is no concrete method for its determination. Threshold value is very crucial for obtaining the correct values. If the higher boundary is too large, some outliers might be missed; if the lower boundary is too small, many normal points might be

identified as outliers. This work focuses on optimizing mathematical algorithms of the CDM method, developing a method for confirmation of threshold values, applying this method for treatment of areal topography data.

This method is first applied to the processing of a synthetic data provided by NIST with height parameters already known, aiming at the validation of the algorithm. Then it is implemented for processing an artificial stochastic surface generated by our own algorithms, of which its height parameters are also already known. By comparing the differences of height parameters of the original data and the data after processing outliers with reference to the certified values, as well as comparisons of histogram of height distributions, surface reconstructions, slopes and curvatures, the validation of our algorithms can be observed.

Finally, two experiments are carried out. The first experiment measures a Type C1 spacing standard artefact using our imaging confocal microscopy. The second experiment measures an iron surface. Surface reconstruction, histogram, and parameterization of the measured data and the data after processing outliers are compared.

7.3 Mathematical model of the Confidence Distance Matrix

Statistical distance measures, for some types of distance measures are referred to as statistical divergences [30, 31], include, among others, the J-divergence, Matsusita, Bhattacharyya distances, etc [21]. In this work, the mathematical model proposed in the paper of R. C. Luo, *et al* [21] is introduced in this work, simplified and adapted for outlier detection in surface measurement.

The procedure of distance matrix calculation begins with the definition of error function [21]:

$$erf(\theta) = \frac{1}{\sqrt{\pi}} \int_{-\theta}^{\theta} e^{-t^2} dt = \frac{2}{\sqrt{\pi}} \int_0^{\theta} e^{-t^2} dt \quad (7.1)$$

where, $t(x; u, \sigma) = \frac{x-u}{\sqrt{2}\sigma}$, and therefore:

$$dt = \frac{1}{\sqrt{2}\sigma} dx \quad (7.2)$$

Equation 7.1 transforms to:

$$erf(\theta) = \frac{\sqrt{2}}{\sqrt{\pi}\sigma} \int_0^{\theta} e^{-\frac{1}{2}(\frac{x-u}{\sigma})^2} dx \quad (7.3)$$

Therefore,

$$\operatorname{erf}\left(\frac{x_j - x_i}{\sqrt{2}\sigma}\right) = 2 \int_{x_i}^{x_j} P_i(x/x_i) dx \quad (7.4)$$

Where $P_i(x/x_i)$ is the conditional probability that x is accurate.

Fig. 7.1 Confidence distance measures: (a) d_{ij} ; (b) d_{ji} [21].

The confidence distance measures are shown in Fig. 7.1, the equations are:

$$d_{ij} = 2 \int_{x_i}^{x_j} P_i(x/x_i) P_i(x_i) dx = 2 P_i(x_i) \int_{x_i}^{x_j} P_i(x/x_i) dx = \frac{1}{\sqrt{2\pi}\sigma(s)} \operatorname{erf}\left(\frac{x_j - x_i}{\sqrt{2}\sigma}\right) \quad (7.5)$$

$$d_{ji} = 2 \int_{x_j}^{x_i} P_j(x/x_j) P_j(x_j) dx = 2 P_j(x_j) \int_{x_j}^{x_i} P_j(x/x_j) dx = \frac{1}{\sqrt{2\pi}\sigma(s)} \operatorname{erf}\left(\frac{x_i - x_j}{\sqrt{2}\sigma}\right) \quad (7.6)$$

Where d_{ij} and d_{ji} represents the confidence distance between x_i and x_j . For evaluation of measurement uncertainty by means of MCM method, usually measure the surface specimen repeating n times, each point of the surface will have n values. The first part of this proposed algorithm intends to identify outliers generated by random noises as specified above. It is assumed that outliers are those that are not representative for its partitioned integral features and are characterized by scale or magnitude criteria [39]. As x_i and x_j belong to the same set array, it can be found:

$$P_i(x/x_i) = P_j(x/x_j) \quad (7.7)$$

Therefore,

$$\operatorname{erf}\left(\frac{x_j - x_i}{\sqrt{2}\sigma}\right) = \operatorname{erf}\left(\frac{x_i - x_j}{\sqrt{2}\sigma}\right) \quad (7.8)$$

So that,

$$d_{ij} = d_{ji} \quad (7.9)$$

For points of data within a surface, the distance among its n measures is:

$$\mathbf{D} = \begin{bmatrix} \mathbf{d}_{11} & \mathbf{d}_{12} & \cdots & \mathbf{d}_{1n} \\ \mathbf{d}_{21} & \mathbf{d}_{22} & \cdots & \mathbf{d}_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{d}_{n1} & \mathbf{d}_{n2} & \cdots & \mathbf{d}_{nn} \end{bmatrix} \quad (7.10)$$

Where, $d_{ij} = e^{-\frac{1}{2} \frac{(X_j - X_i)^2}{(2u_i)^2}}$, X_i and X_j is the value of this set, u_i is the standard deviation of this set.

Relationships between those points can be determined as $\mathbf{R}$ after having obtained the distance matrix $\mathbf{D}$,

$$\mathbf{R} = \begin{bmatrix} \mathbf{r}_{11} & \mathbf{r}_{12} & \cdots & \mathbf{r}_{1m} \\ \mathbf{r}_{21} & \mathbf{r}_{22} & \cdots & \mathbf{r}_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{r}_{m1} & \mathbf{r}_{m2} & \cdots & \mathbf{r}_{mm} \end{bmatrix} \quad (7.11)$$

Where r_{ij} is the value of d_{ij} filtered by threshold and it is:

$$r_{ij} = \begin{cases} 1, & \text{if } d_{ij} > \text{threshold value} \\ 0, & \text{if } d_{ij} \leq \text{threshold value} \end{cases} \quad (7.12)$$

The raw data are filtered to obtain $r_{ij} = 1$ ($i, j = l, m, s \in \{1, 2, \dots, n\}$).

7.4 Methods and algorithms for outlier detection in surface measurement data

This section is divided into two parts. The first part introduces the methods and algorithms for random outlier identification consistent with the MCM method, implementing a synthetic data SG_3-3 provided by NIST [20] for validation. Values of the seven height parameters are compared between the original data of NIST, contaminated data, and the processed data using our proposed method. The second part introduces the method and algorithm for identifying outliers in a unique surface. An artificial stochastic surface data generated by our own algorithm is processed for the validation of this algorithm.

7.4.1 Proposal and validation of method and algorithms for random outlier identification, threshold determination

Relationship values r_{ij} vary from zero to one. One means x_i and x_j is consistent while zero means x_i and x_j has nothing in common. Threshold can be chosen between 0 and 1. This work selects the threshold value based on the height parameter Sa does not change obviously. Gap between thresholds is first set as 0.1 and if necessary, the second iteration can be carried out by gap 0.01 after minimize the range of thresholds in the first calculations.

A mat file created based on a standard dataset provided by National Institute of Standards and Technology (NIST) [20] is processed for validation of this method. The processed dataset is a MAT file which contains 1% outliers. SG_3-3 was chosen and the surface reconstruction of this data is shown in Fig. 7.2, information of its areal surface parameters is shown in Tab. 7.1. After adding outliers, the reconstruction of its surface is shown in Fig. 7.3, including a 2D contour and a 3D surf plot. Surface height distributions of the original surface and of the contaminated surface are shown in Fig. 7.4. The distribution of the original surface data follows a U-shaped distribution. After adding outliers, the major points also follow a U-shaped distribution, but exist some points lies outside the shape in the two-extreme side.

Fig. 7.2 Surface reconstruction of the data set SG_3-3 provided by NIST: (a) 2D contour plot; (b) 3D surf plot.

Tab. 7.1 areal surface parameters of the specimen provided by NIST [20].

Label	Nominal Value	Mean Value	Standard Uncertainty
Sa	0.89928 μm	0.8993 μm	0.077 nm
Sq	1 μm	1.00004 μm	0.075 nm
Ssk	0.01957	0.01956	0.00027
Sku	1.51103	1.51136	0.00016
St	2.91342 μm	2.96455 μm	10.55 nm
Sp	1.46487 μm	1.49284 μm	7.34 nm
Sv	1.44855 μm	1.47266 μm	6.8 nm

Fig. 7.3 Surface reconstruction of the data set SG_3-3 after adding outliers: (a) 2D contour plot; (b) 3D surf plot.

(a) (b)
Fig. 7.4 Histogram of the surface heights: (a) original data set SG_3-3; (b) SG_3-3 with outliers.

The algorithm for generating the MAT file is shown below, which is in accordance with the Monte Carlo method for evaluation of uncertainty:

Algorithm. Generating the MAT file of surface data with outliers.

- (i) Import the database SG_3-3;
- (ii) Generate 5 surfaces according to SG_3-3 and distribute uncertainties of 10.0 nm (1% of Sq) to each surface;
- (iii) Define values of outliers as $k \times z_i$, in this work $k = 3$;
- (iv) Determine the number of outliers for adding, 1% of the total number of SG_3-3;
- (v) Generate the random points of those 5 surfaces and add outliers to them;
- (vi) Generate the expected MAT file with information of 5 contaminated surfaces and with recording of the position of outliers.

end

Results of arithmetical mean height Sa by different values of threshold with gap of 0.1 is shown in Tab. 7.2. The trending plot of values of Sa can be found in Fig. 7.5. When threshold is selected as 1, none of those points will be deleted. Arithmetic mean height Sa is 0.9173 μm when threshold equals zero, which is the arithmetic mean height with all outliers. As the threshold increases, the number of deleted points increases. Sa first decreases logically as outliers are deleted. When the threshold decreases to an extent, the value of Sa becomes stable, this might be due to most or all the outliers are deleted. The threshold 0.8 can be selected as the threshold due to the height parameter Sa are stable in a logical position. The corresponding value of Sa is 0.8993 μm . This result is the same with the mean value of Sa provided by NIST [20].

Tab. 7.2 Arithmetic mean height value Sa according to different threshold value.

Threshold	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
Sa	0.9173	0.9176	0.9174	0.9171	0.9171	0.9169	0.9001	0.8993	0.8993	0.8993	0.8993

Fig. 7.5 Variation of S_a according to different threshold value.

Fig. 7.6 manifests both the 2D and 3D reconstruction of the surface of the contaminated data set after detection and deletion of outliers with threshold value of 0.8. Comparing it to the surface reconstruction of the original data set shown in Fig. 7.2, it can be found that the distributions of peaks and valleys are very similar, although the 3D view of the surface seems smoother after deletion of the outliers. This is because that each height of this surface is mean value of five surfaces after deletion of outliers. In the original surface, 1% of normal points were modified to be outliers. Those outliers are deleted after implementation of our proposed method for random outlier identification. In the surface after deletion of the outliers, there are less points than the original data due to outliers' deletion. Fig. 7.7 shows the histogram of the height distribution of the surface point of the processed data set. Comparing this to the histogram of the surface heights of the original data set and the contaminated data set shown in Fig. 7.4, it is obvious that the outliers are seemed all detected. The data after deletion of outliers manifests a very similar distribution with the original data.

Fig. 7.6 Surface reconstruction of the data set after deleting outliers: (a) 2D contour plot; (b) 3D surf plot.

Fig. 7.7 Histogram of the height distribution of the data set after deletion of outliers.

Tab. 7.3 compares the seven height parameters between the original data, the contaminated data, and the processed data using our proposed method for outlier detection. It can be found that the values of the seven height parameters are much improved after the implementation of our proposed method for outlier identification. The certified value of the arithmetic mean height Sa , specified by NIST, is 0.8993 μm ; When the data is added 1% of outliers, its arithmetic mean height Sa is 0.9169 μm ; After processing the data by deleting outliers, its Sa is 0.8993 μm . Although the certified value and the calculated value are the same when shown in short format, i.e. 4 digits after the decimal point, they are different in fact in the computing software Matlab®. The difference between the calculated Sa of the data after deletion of

outliers and the certified value of Sa specified by NIST is 0.0017%. The difference is calculated as:

$$Dif = abs\left(\frac{V_{cal} - V_{cert}}{V_{cert}}\right) \times 100 \quad (7.13)$$

Where, V_{cal} represents the calculated values of the height parameters, such as the arithmetic mean height Sa of the data after processing outliers, V_{cert} represents the certified value, which is terminated as a reference, such as the certified value of the arithmetic mean height Sa provided by NIST. All this chapter applies the same method for calculations of difference between values.

The difference of the root mean square height Sq of the data with outliers is 2.3342% and after deletion of outliers is 0.0037%. The difference between heights of peaks and valleys decreased from 77.9937% and 78.0719% to 1.7550% and 1.9094%.

Tab. 7.3 Comparison of height parameters of the original data, data with outliers, and data after deletion of outliers.

Label	Certified Value by NIST	Parameterization with outliers		Parameterization after deletion of outliers	
		Values	Difference [%]	Values	Difference [%]
Sa [μm]	0.8993	0.9169	1.9626	0.8993	0.0017
Sq [μm]	1.00004	1.0234	2.3342	1.0000	0.0037
Ssk	0.01956	0.0206	5.4015	0.0196	0.0866
Sku	1.51136	1.5739	4.1381	1.5110	0.0215
St [μm]	2.96455	5.2368	77.9937	2.9134	1.7550
Sp [μm]	1.49284	2.6365	78.0719	1.4649	1.9094
Sv [μm]	1.47266	2.6003	77.8490	1.4486	1.6644

The mathematical models for mean profile slope $\frac{\partial z}{\partial x}$ and mean profile curvature $-\frac{\partial^2 z}{\partial x^2}$ of digitized profile were presented by B. Bhushan [33]. For any point on a surface, its surface slope is obtained by calculating the square roots of the sum of the squares of the slopes in both x- and y- directions. Its surface curvature is calculated as the average of the curvatures in both x- and y- coordinate [33]. Based on this definition and some other references [34, 28], the mathematical models for surface slope and curvature are developed, as indicated by Equation 7.14 and Equation 7.15.

$$Sda = \tan^{-1} \sqrt{\left(\frac{z_{(i+1,j)} - z_{(i,j)}}{\Delta x}\right)^2 + \left(\frac{z_{(i,j+1)} - z_{(i,j)}}{\Delta y}\right)^2} \quad (7.14)$$

$$Spc = \frac{2z_{(i,j)} - z_{(i-1,j)} - z_{(i+1,j)}}{\Delta x^2} + \frac{2z_{(i,j)} - z_{(i,j-1)} - z_{(i,j+1)}}{\Delta y^2} \quad (7.15)$$

Where, Sda represents the surface slope for any point in unit of radian, Spc represents the surface curvature in unit of $1/\mu m$. Mean slope and mean curvature for all the points on a surface are indicated in Equations 7.16 and 7.17.

$$Sda_{mean} = \frac{1}{(N-1)(M-1)} \sum_{i=1}^{N-1} \sum_{j=1}^{M-1} \tan^{-1} \sqrt{\left(\frac{z_{(i+1,j)} - z_{(i,j)}}{\Delta x} \right)^2 + \left(\frac{z_{(i,j+1)} - z_{(i,j)}}{\Delta y} \right)^2} \quad (7.16)$$

$$Spc_{mean} = \frac{1}{2(N-2)(M-2)} \sum_{i=2}^{N-1} \sum_{j=2}^{M-1} \left(\frac{2z_{(i,j)} - z_{(i-1,j)} - z_{(i+1,j)}}{\Delta x^2} + \frac{2z_{(i,j)} - z_{(i,j-1)} - z_{(i,j+1)}}{\Delta y^2} \right) \quad (7.17)$$

Tab. 7.4 compares the parameters of slopes and curvatures of the original data, data with outliers, and data after deletion of outliers. The minimum curvature of the original data is -1.62 $1/\mu m$. After adding outliers, the minimum curvature is -5.79 $1/\mu m$. After processing the outliers, the minimum curvature returns back to -1.62 $1/\mu m$. This parameter indicates the high efficiency of our proposed method for outlier identification.

Tab. 7.4 Surface slopes and curvatures of the original data, data with outliers, and data after deletion of outliers.

Data Parameters	Original Data	Data with outliers	Data After Deletion of Outliers
Minimum Slope Sda_{min} [rad]	0	0	0
Maximum Slope Sda_{max} [rad]	1.16	1.35	1.30
Mean Slope Sda_{mean} [rad]	0.35	0.37	0.34
Minimum Curvature Spc_{min} [$1/\mu m$]	-1.62	-5.79	-1.62
Maximum Curvature Spc_{max} [$1/\mu m$]	1.41	5.87	5.02
Mean Curvature Spc_{mean} [$1/\mu m$]	-1.32×10^{-4}	-1.37×10^{-4}	-1.32×10^{-4}

From the results and the analysis above, it can be concluded that the outliers are detected correctly. Moreover, all the results of the seven height parameters, Sa , Sq , Ssk , Sku , St , Sp , Sv are much improved after processing outliers using our proposed method. The results of the seven height parameters of the processed data is very similar to the certified values provided by NIST [20]. The difference between the calculated heights and the certified heights are

neglectable. The difference between the parameterization and the certified values decreased almost 1000 times for all seven height parameters after processing outliers with our proposed method. Parameters of surface slopes and curvatures of the data after deletion of outliers are much closer to the parameters of the original data than the data with outliers. These give an indication that our proposed method for random outlier deletion is consistent with MCM method is valid and reliable.

7.4.2 Proposal and validation of method and algorithms for identifying outliers in a stochastic surface

The same mathematical model as introduced in Section 3 is implemented for screening outliers in a data set. Besides this, a detection window is introduced for simplification of computation. The concept of detection window was previously proposed by M. F. Ismail, *et al.* [37], as shown in Fig. 7.8. Assuming that the outlier clusters are square and the largest outlier cluster in the surface data covering an area of $w \times w$, which consists of w^2 data points, the side length of the detection window is defined as l_{wd} and specified as:

$$l_{wd} = 2n+1 > \sqrt{2}w \quad (7.18)$$

This equation indicates that the total number of points within a detection window must be more than $2w^2$, assuring the normal data points within the detection window must be more than w^2 . This is because that the normal data must be more than outliers in the science of statistics, otherwise the roles of normal data and outliers are interchanged [16].

Fig. 7.8 Detection window for screening outliers [37].

The heights of the points within the detection window are put into the mathematical model proposed in Section 3 for calculating their Confidence Distance Matrix, Equation 7.10, and their relationship matrix, Equation 7.11. After thresholding, the normal data and outliers will be detected and separated.

For validation of our proposed mathematical model and algorithms, a synthetic data of an artificial stochastic surface is generated and added with outliers. The artificial surface is produced by our own algorithm for data generation, by defining the standard deviation of the areal heights, Hurst exponent (roughness exponent, $0 \leq H \leq 1$), side length of the topography in X-coordinate, number of pixels in both X- and Y- directions. Reconstruction of the generated artificial surface is shown in Fig. 7.9. This stochastic surface has heights distributed stochastically, showing no features, which is contrary to structured surface. Tab. 7.5 gives an indication of the parameters of this artificial surface. Tab. 7.6 presents the values of the uncertainty matrix of the seven height parameters, also named covariance matrix [16], with elements equal to the variances and covariances of the variables. The diagonal elements, $v(x_i, x_i) \equiv \sigma^2(x_i)$, are the variances. The off-diagonal elements, $v(x_i, x_j)$ are the covariances. The uncertainty is evaluated by the Type A evaluations defined in GUM [16, 37], with implementation of MCM simulation method defined in GUM-S1 [62] and GUM-S2 [63]. Tab. 7.7 indicates the matrix of the correlation coefficients of the 7 height parameters of our produced artificial stochastic surface. The correlation coefficient measures the relative mutual dependence of two variables. It is calculated as the ratio of their covariances to the positive square root of the product of their variances. The formula proposed in GUM [16] is defined as:

$$\rho(y, z) = \rho(z, y) = \frac{v(y, z)}{\sqrt{v(y, y)v(z, z)}} = \frac{v(y, z)}{\sigma(y)\sigma(z)} \quad (7.19)$$

With estimate in surface height parameters is:

$$r(x_i, x_i) = \frac{u(x_i, x_i)}{u(x_i)u(x_i)} \quad (7.20)$$

The correlation coefficient is a scalar value in a range of $[-1, 1]$, i.e. $-1 \leq \rho(y, z) \leq +1$ or $-1 \leq r(x_i, x_i) \leq +1$. If the estimates x_i and x_j are independent, $r(x_i, x_i) = 0$.

Fig. 7.9 Reconstruction of our generated artificial stochastic surface: (a) 2D contour plot; (b) 3D surf plot.

Fig. 7.10 Surface reconstruction of our generated artificial surface after adding random outliers: (a) 2D contour plot; (b) 3D surf plot.

Tab. 7.5 Areal height parameters of our generated artificial surface data.

Label	Mean Value	Minimum Value	Maximum Value	Standard Uncertainty
<i>Sa</i>	1.1294 μm	1.1249 μm	1.1336 μm	2.2 nm
<i>Sq</i>	1.4142 μm	1.4093 μm	1.4193 μm	2.6 nm
<i>Ssk</i>	0.0272	0.0138	0.0402	0.0068
<i>Sku</i>	2.9787	2.9520	3.0058	0.0137
<i>St</i>	12.2769 μm	11.3851 μm	13.3359 μm	0.5 nm
<i>Sp</i>	6.2595 μm	5.5689 μm	7.0018 μm	0.4 nm
<i>Sv</i>	6.0174 μm	5.4111 μm	6.7026 μm	0.3 nm

Tab. 7.6 Covariance matrix of the height parameters of our produced artificial surface.

	<i>Sa</i>	<i>Sq</i>	<i>Sp</i>	<i>Sv</i>	<i>St</i>	<i>Sku</i>	<i>Ssk</i>
<i>Sa</i>	4.9821×10^{-6}	5.2796×10^{-6}	-8.3524×10^{-6}	1.2127×10^{-5}	3.7745×10^{-6}	-9.1081×10^{-6}	-8.9933×10^{-10}
<i>Sq</i>	5.2796×10^{-6}	6.6240×10^{-6}	1.3916×10^{-6}	3.0193×10^{-5}	3.1585×10^{-5}	2.0856×10^{-8}	2.1514×10^{-7}
<i>Sp</i>	-8.3524×10^{-6}	1.3916×10^{-6}	0.1466	-0.0011	0.1455	8.2642×10^{-4}	1.8163×10^{-4}
<i>Sv</i>	1.2127×10^{-5}	3.0193×10^{-5}	-0.0011	0.1181	0.1170	6.2350×10^{-4}	-1.7264×10^{-4}
<i>St</i>	3.7745×10^{-6}	3.1585×10^{-5}	0.1455	0.1170	0.2625	0.0014	8.9961×10^{-6}
<i>Sku</i>	-9.1081×10^{-6}	2.0856×10^{-8}	8.2642×10^{-4}	6.2350×10^{-4}	0.0014	1.8709×10^{-4}	6.0111×10^{-6}
<i>Ssk</i>	-8.9933×10^{-10}	2.1514×10^{-7}	1.8163×10^{-4}	-1.7264×10^{-4}	8.9961×10^{-6}	6.0111×10^{-6}	4.5761×10^{-5}

Tab. 7.7 Correlation matrix of the height parameters of our produced artificial surface.

	<i>Sa</i>	<i>Sq</i>	<i>Sp</i>	<i>Sv</i>	<i>St</i>	<i>Sku</i>	<i>Ssk</i>
<i>Sa</i>	1	0.9190	-0.0098	0.0158	0.0033	-0.2983	-5.9561×10^{-5}
<i>Sq</i>	0.9190	1	0.0014	0.0341	0.0240	5.9244×10^{-4}	0.0124
<i>Sp</i>	-0.0098	0.0014	1	-0.0082	0.7418	0.1587	0.0701
<i>Sv</i>	0.0158	0.0341	-0.0082	1	0.6646	0.1327	-0.0743
<i>St</i>	0.0033	0.0240	0.7418	0.6646	1	0.2069	0.0026
<i>Sku</i>	-0.2983	5.9244×10^{-4}	0.1578	0.1327	0.2069	1	0.0650
<i>Ssk</i>	-5.9561×10^{-5}	0.0124	0.0701	-0.0743	0.0026	0.0650	1

According to Tab. 7.7, the height parameter *Sa* and *Sq* of our produced artificial stochastic surface is highly dependent, while *Ssk* is almost dependent from all other 6 parameters. A surface data with outliers is produced by adding 1% outliers to the artificial surface randomly. Fig. 7.11 compares the height distributions of our produced artificial surface and this surface after adding 1% outliers. It can be found that the mean value of the artificial surface does not change after adding outliers, while they span a bigger interval after adding outliers, from a range of -4 to 4 to a bigger range of -10 to 10. Both two surfaces follow normal distributions. Tab. 7.8 presents the areal height parameters of the artificial surface after adding outliers.

Covariance matrix of this surface with data is presented in Tab. 7.9. Matrix of the correlation coefficients of the areal height parameters is manifested in Tab. 7.10.

Fig. 7.11 Histogram of our produced artificial surface heights: (a) original data; (b) Data with outliers.

Tab. 7.8 Areal height parameters of the artificial surface data with outliers.

Label	Mean Value	Minimum Value	Maximum Value	Standard Uncertainty
<i>Sa</i>	1.1643 μm	1.1598 μm	1.1688 μm	2.3 nm
<i>Sq</i>	1.4685 μm	1.4634 μm	1.4740 μm	2.7 nm
<i>Ssk</i>	-0.0323	-0.0472	-0.0166	0.0078
<i>Sku</i>	3.3915	3.3339	3.4504	0.0296
<i>St</i>	20.7056 μm	18.6939 μm	22.7503 μm	1047.4 nm
<i>Sp</i>	10.2653 μm	8.9120 μm	11.8274 μm	754.8 nm
<i>Sv</i>	10.4412 μm	9.0925 μm	11.8862 μm	727.6 nm

Tab. 7.9 Covariance matrix of the height parameters of the artificial surface data with outliers.

	<i>Sa</i>	<i>Sq</i>	<i>Sp</i>	<i>Sv</i>	<i>St</i>	<i>Sku</i>	<i>Ssk</i>
<i>Sa</i>	5.2959×10^{-6}	5.5748×10^{-6}	-1.8227×10^{-5}	2.4947×10^{-6}	-1.5732×10^{-5}	-1.5931×10^{-5}	4.0981×10^{-7}
<i>Sq</i>	5.5748×10^{-6}	7.0555×10^{-6}	2.2386×10^{-5}	5.3114×10^{-5}	7.5500×10^{-5}	2.8172×10^{-7}	5.3362×10^{-8}
<i>Sp</i>	-1.8227×10^{-5}	2.2386×10^{-5}	0.5698	-0.0011	0.5687	0.0070	8.3329×10^{-4}
<i>Sv</i>	2.4947×10^{-6}	5.3114×10^{-5}	-0.0011	0.5294	0.5283	0.0075	-8.3339×10^{-4}
<i>St</i>	-1.5732×10^{-5}	7.5500×10^{-5}	0.5687	0.5283	1.0969	0.0145	-1.0795×10^{-7}
<i>Sku</i>	-1.5931×10^{-5}	2.8172×10^{-7}	0.0070	0.0075	0.0145	8.7830×10^{-4}	-1.4763×10^{-5}
<i>Ssk</i>	4.0981×10^{-7}	5.3362×10^{-8}	8.3329×10^{-4}	-8.3339×10^{-4}	-1.0795×10^{-7}	-1.4763×10^{-5}	6.1098×10^{-5}

Tab. 7.10 Matrix of the correlation coefficients of the height parameters of the artificial surface data with outliers.

	Sa	Sq	Sp	Sv	St	Sku	Ssk
Sa	1	0.9120	-0.0105	0.0015	-0.0065	-0.2336	0.0228
Sq	0.9120	1	0.0112	0.0275	0.0271	0.0036	0.0026
Sp	-0.0105	0.0112	1	-0.0020	0.7193	0.3107	0.1412
Sv	0.0015	0.0275	-0.0020	1	0.6932	0.3494	-0.1465
St	-0.0065	0.0271	0.7193	0.6932	1	0.4667	-1.3186×10^{-5}
Sku	-0.2336	0.0036	0.3107	0.3494	0.4667	1	-0.0637
Ssk	0.0228	0.0026	0.1412	-0.1465	-1.3186×10^{-5}	-0.0637	1

After implementation of our proposed method for outlier deletion using statistical method CDM, the outliers are mostly detected and deleted. Fig. 7.12 shows the surface reconstruction of our artificial stochastic surface data after deletion of outliers, both in 2D and 3D view. When comparing it to the surface reconstruction of the original data shown in Fig. 7.9, it can be found that they are very similar. The distribution of the heights of the surface data after applying our method for outlier detection is shown in Fig. 7.13. This distribution is also very similar to that of the original data shown in Fig. 7.11 (a).

Fig. 7.12 Reconstruction of the artificial stochastic surface after deletion of outliers: (a) 2D contour plot; (b) 3D surf plot.

Fig. 7.13 Histogram of the heights of the artificial surface after deletion of outliers.

The height parameters of the data of the artificial surface after deletion of outliers is shown in Tab. 7.11. It can be found that it is very similar to the height parameters calculated from the original artificial surface data shown in Tab. 7.5. The covariance matrix of the height parameters of the artificial surface after deletion of outliers is shown in Tab. 7.12. The matrix of the correlation coefficients of the height parameters is shown in Tab. 7.13.

Tab. 7.11 Areal height parameters of the artificial surface after deletion of outliers.

Label	Mean Value	Minimum Value	Maximum Value	Standard Uncertainty
<i>Sa</i>	1.1169 μm	1.1126 μm	1.1213 μm	2.2 nm
<i>Sq</i>	1.4073 μm	1.4021 μm	1.4121 μm	2.6 nm
<i>Ssk</i>	-0.0110	-0.0246	0.0028	0.0070
<i>Sku</i>	3.0358	3.0095	3.0677	0.0148
<i>St</i>	12.4852 μm	11.4544 μm	13.4789 μm	527.3 nm
<i>Sp</i>	6.1738 μm	5.5572 μm	6.9279 μm	361.8 nm
<i>Sv</i>	6.3115 μm	5.6492 μm	7.0871 μm	379.4 nm

Tab. 7.12 Covariance matrix of the height parameters of the artificial surface after deletion of outliers.

	<i>Sa</i>	<i>Sq</i>	<i>Sp</i>	<i>Sv</i>	<i>St</i>	<i>Sku</i>	<i>Ssk</i>
<i>Sa</i>	4.9485×10^{-6}	5.2456×10^{-6}	2.4155×10^{-5}	-1.4233×10^{-6}	2.2732×10^{-5}	-9.9537×10^{-6}	-7.6828×10^{-8}
<i>Sq</i>	5.2456×10^{-6}	6.6310×10^{-6}	5.3292×10^{-5}	2.0212×10^{-5}	7.3504×10^{-5}	1.7745×10^{-7}	-1.2249×10^{-7}
<i>Sp</i>	2.4155×10^{-5}	5.3292×10^{-5}	0.1309	0.0016	0.1325	8.5170×10^{-4}	2.2293×10^{-4}
<i>Sv</i>	-1.4233×10^{-6}	2.0212×10^{-5}	0.0016	0.1439	0.1456	0.0010	-2.1560×10^{-4}
<i>St</i>	2.2732×10^{-5}	7.3504×10^{-5}	0.1325	0.1456	0.2781	0.0019	7.3306×10^{-6}
<i>Sku</i>	-9.9537×10^{-6}	1.7745×10^{-7}	8.5170×10^{-4}	0.0010	0.0019	2.1910×10^{-4}	-3.2831×10^{-6}
<i>Ssk</i>	-7.6828×10^{-8}	-1.2249×10^{-7}	2.2293×10^{-4}	-2.1560×10^{-4}	7.3306×10^{-6}	-3.2831×10^{-6}	4.8588×10^{-5}

Tab. 7.13 Matrix of the correlation coefficients of the height parameters of the artificial surface after deletion of outliers.

	Sa	Sq	Sp	Sv	St	Sku	Ssk
Sa	1	0.9157	0.0300	-0.0017	0.0194	-0.3023	-0.0050
Sq	0.9157	1	0.0572	0.0207	0.0541	0.0047	-0.0068
Sp	0.0300	0.0572	1	0.0118	0.6946	0.1590	0.0884
Sv	-0.0017	0.0207	0.0118	1	0.7276	0.1782	-0.0815
St	0.0194	0.0541	0.6946	0.7276	1	0.2373	0.0020
Sku	-0.3023	0.0047	0.1590	0.1782	0.2373	1	-0.0318
Ssk	-0.0050	-0.0068	0.0884	-0.0815	0.0020	-0.0318	1

Fig. 7.14 manifests the comparison of the seven areal height parameters between the three data, i.e. the original artificial stochastic surface, the artificial surface with outliers, and the artificial surface after deletion of outliers using our proposed method. It can be found that the height parameters of the data after processing outliers are very similar to those of the original data and are much smaller than the data with outliers, especially for the maximum peak height Sp , the maximum pit height Sv , and the maximum height St .

Fig. 7.14 Comparison of areal height parameters calculated from the original data, with outliers, and after deletion of outliers of the artificial stochastic surface.

Tab. 7.14 compares the parameters of the slopes and curvatures of the original artificial data, the data after adding outliers, and the data after deletion of outliers with implementation of our proposed algorithms. It can be found that there are obvious differences of the minimum, maximum and mean slopes and curvatures between the data with outliers and after deletion of outliers. The results of the data after deletion of outliers are much closer to the original data.

Tab. 7.14 Comparison of the surface slopes and curvatures

Data Parameters	Original Data	Data with outliers	Data After Deletion of Outliers
Minimum Slope Sda_{min} [rad]	1.67×10^{-4}	1.80×10^{-3}	1.70×10^{-3}
Maximum Slope Sda_{max} [rad]	1.06	1.47	1.06
Mean Slope Sda_{mean} [rad]	0.40	0.42	0.39
Minimum Curvature Spc_{min} [$1/\mu m$]	-1.46	-14.88	-1.59
Maximum Curvature Spc_{max} [$1/\mu m$]	1.55	13.43	1.98
Mean Curvature Spc_{mean} [$1/\mu m$]	1.63×10^{-5}	-1.43×10^{-5}	5.08×10^{-5}

According to the result and the analysis indicated above, i.e. the seven height parameters, slopes and curvatures of the three data, the original data, the data with outliers, and the data after processing outliers with implementation of our proposed method, the surface reconstruction of each of the three data, the histograms of the distributions of the heights of the three data, etc., it can be concluded that our proposed method for identifying outliers in a stochastic surface is valid and reliable.

7.5. Experimental study

Two experiments are carried out. The first one studies a Type C1 spacing standard. The second one studies a steel surface with grooves produced by Advanced Laser Based Manufacturing of the Laser Centre of Technical University of Madrid (UPM, Spain).

7.5.1 Experiment 1: measurement and data processing of a Type C1 spacing standard.

A Type C1 spacing standard with grooves having a sine wave profile, as shown in Fig. 7.15, with a certified value of Ra equal to $1.003 \mu m$ and expanded uncertainty of $0.03 \mu m$ ($k = 2$), was measured using the Leica DCM-3D Confocal Microscopy at the Metrology Laboratory of the Technical University of Madrid. A magnification objective of 50X was used, with a numerical aperture of 0.90. The measurement was performed under a controlled temperature at 20 ± 1 °C.

Fig. 7.15 The Type C1 spacing standard: (a) photograph of the standard; (b) Image by Dino-Lite Digital Microscope.

This standard artefact is very suitable for confocal microscopy, as almost no defects can be observed if it is measured in a standard way, i.e. cleaning before measurement. To meet the objective of our study, some dusts are dropped onto its surface before measuring it. Fig. 7.16 manifests the surface reconstruction of the original data and the data after removing its form. The measured surface is tilted. After removing its form, the surface is parallel with the XY plane. This reconstruction implemented the function of ‘plot3’ in Matlab®. Fig. 7.17 shows the reconstructed surface of the data after removing its form by 2D contour plot and 3D surf plot. It can be found that this surface contains both large outliers and small ones.

Fig. 7.16 Reconstruction of the measured surface: (a) original measurement data; (b) after removal of the form.

Fig. 7.17 Surface reconstruction of the data after removing from: (a) 2D contour; (b) 3D surf.

After implementation of our proposed method, i.e. using statistical Confidence Distance Measures for outlier detection, the surface reconstruction of the data after deletion of outliers is shown in Fig. 7.18. It can be found that the outliers are detected correctly. From the 2D contour, it can be found that the positions having had outliers are left blank. From the 3D surf plot, it can be observed that the surface is much smoother when comparing to the reconstructed surface of the data before processing outliers shown in Fig. 7.17.

Fig. 7.18 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.

Fig. 7.19 compares the height distributions of the data before processing outliers and after deletion of outliers. The range of the distribution of the heights is much smaller after deletion of the outliers.

Fig. 7.19 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.

The values of the height parameters Sa and St of the measured data and the data after processing outliers using our proposed CDM method are shown in Tab. 7.15. The difference of the arithmetic mean height Sa between the certified value and the calculated value of the measured data is 29.65%. After the deletion of outliers, the difference decreases to 3.52%. The difference of the maximum height value St decreases from 813.94% to 18.07%.

Tab. 7.15 Comparison of height parameters of the original data, data with outliers, and data after deletion of outliers.

Label	Certified Value of the standard	Parameterization of the measured surface		Parameterization after deletion of outliers	
		Values	Difference [%]	Values	Difference [%]
Sa [μm]	1.003	1.3004	29.65	0.9677	3.52
St [μm]	3.36	30.7085	813.94	3.9670	18.07

Tab. 7.16 compares the parameters of the slopes and curvatures of the raw measurement data and the data after processing outliers. The minimum curvature of the measured data is -139.20 $1/\mu\text{m}$, after deletion of the outliers the result is -10.42 $1/\mu\text{m}$. The maximum surface curvature decreased from 103.69 $1/\mu\text{m}$ to 1.39 $1/\mu\text{m}$ after deletion of outliers.

Tab. 7.16 Comparison of the surface slopes and curvatures

Data Parameters	Measured Data	Data After processing outliers
Minimum Slope $Sda_{\min}$ [rad]	1.97×10^{-4}	0
Maximum Slope $Sda_{\max}$ [rad]	1.54	1.39
Mean Slope Sda_{mean} [rad]	0.15	0.13
Minimum Curvature $Spc_{\min}$ [$1/\mu\text{m}$]	-139.20	-10.42
Maximum Curvature $Spc_{\max}$ [$1/\mu\text{m}$]	103.69	1.39
Mean Curvature Spc_{mean} [$1/\mu\text{m}$]	9.39×10^{-5}	2.79×10^{-4}

According to the results shown above, i.e., comparisons of the surface construction between measured data and data after processing outliers, histogram of the distribution of the heights of the two data, the height parameters, surface slopes and curvatures, it can be concluded that our proposed method for outlier detection in areal surface measured data works well.

7.5.2 Experiment 2: measurement and data processing of a steel plate.

The surface of the steel plate, type S235JR, is measured and processed by our proposed method using CDM for outlier identification. Photograph of this specimen is shown in Fig. 7.20. It is produced by Advanced Laser Based Manufacturing of the Laser Centre of Technical University of Madrid (UPM, Spain).

Fig. 7.20 Image of the specimen: (a) Photograph; (b) Image by Dino-Lite Digital Microscope.

Fig. 7.21 shows the surface reconstruction of the measured data both in 2D contour and 3D surf plot. Many outliers can be observed both in 2D and 3D view. Fig. 7.22 manifests the surface reconstruction of the data after deletion of outliers. It can be found that the outliers are detected correctly.

Fig. 7.21 Surface reconstruction of the measured data: (a) 2D contour; (b) 3D surf.

Fig. 7.22 Surface reconstruction of the data after processing outliers: (a) 2D contour; (b) 3D surf.

Fig. 7.23 makes a comparison of the distributions of the heights between the measured surface data and the data after deletion of outliers, using histogram. Fig. 7.24 compares the height distributions of the two data using Quantile-Quantile plot. Both figures indicate a big difference between the two distributions. After deletion of outliers, the range of the distribution of the heights decreases from -30 to 15 to a range of -6 to 6.

Fig. 7.23 Histogram of the distribution of the areal heights: (a) The measured data; (b) Data after deletion of outliers

Fig. 7.24 QQ plot of the measured surface data versus the data after deletion of outliers.

Tab. 7.17 compares the parameters of the slopes and curvatures of the raw measurement data of the steel plate and the data after processing outliers. The minimum curvature of the measured data is $-139.20 \text{ 1/}\mu\text{m}$, after deletion of the outliers the result is $-32.47 \text{ 1/}\mu\text{m}$. The maximum surface curvature decreased from $157.08 \text{ 1/}\mu\text{m}$ to $28.44 \text{ 1/}\mu\text{m}$ after deletion of outliers.

Tab. 7.17. Comparison of the surface slopes and curvatures of the data of the steel plate

Data Parameters	Measured Data	Data After processing outliers
Minimum Slope $Sda_{\min}$ [rad]	2.42×10^{-4}	2.42×10^{-4}
Maximum Slope $Sda_{\max}$ [rad]	1.55	1.49
Mean Slope Sda_{mean} [rad]	0.18	0.18
Minimum Curvature $Spc_{\min}$ [$1/\mu\text{m}$]	-139.20	-32.47
Maximum Curvature $Spc_{\max}$ [$1/\mu\text{m}$]	157.08	28.44
Mean Curvature Spc_{mean} [$1/\mu\text{m}$]	-2.22×10^{-5}	-2.32×10^{-4}

By comparing Fig. 7.21 and Fig. 7.22, it can be observed that outliers are deleted very well. As indicated by Fig. 7.23 and Fig. 7.24, after deletion of outliers using our proposed method the range of the distributions of the surface heights are much smaller. According to Tab. 7.17, there are obvious differences of the slopes and curvatures between measurement data and processed data. It can be concluded that our proposed method for detecting outliers in measured surface data using the statistical method of Confidence Distance Measures works well.

7.6 Summary

This chapter proposed a method for identifying outliers in areal surfaces measured by confocal microscopy. The statistical method Confidence Distance Matrix (CDM) is introduced and simplified. This method has been widely applied in statistics and engineering areas, such as sensor data fusion, signal processing, information problems, image processing, etc. However, no investigations have been found on using CDM for identifying outliers in surface measurement data. This chapter mainly includes the following points:

First, proposal of using CDM for outlier identification in surface metrology. This method contains two parts. The first part treats the outliers in consistent with the Monte Carlo method (MCM). The second part treats outliers existed in a single measured surface.

Second, two validations of our proposed method. The algorithm for the first part was validated by processing a synthetic data SG_3-3 provided by National Institute of Standards and Technology (NIST). A method for threshold selection was also introduced. Histogram of the distribution of the heights of the original data, the data with outliers, and the data after deletion of outliers are compared. The seven height parameters, slopes and curvatures between the original data, the contaminated data, and the processed data using CDM method are compared. The surface parameters are much closer to the certified values after deletion of outliers. For example, the difference of the root mean square height Sq of the data with

outliers was 2.3342% and after deletion of outliers was 0.0037%. The difference between heights of peaks and valleys decreased from 77.9937% and 78.0719% to 1.7550% and 1.9094%. The second algorithms are validated using an artificial stochastic surface data generated by our own algorithm, with its areal height parameters already known. A detection window with side length l_{wd} was also introduced. The arithmetic mean height of the original data, the data with outliers, and the data after deletion of outliers are respectively 1.1294 μm , 1.1643 μm , and 1.1169 μm .

Third, two experiments were carried out. The first experiment measured a Type C1 spacing standard. Its certified arithmetic mean height Ra is 1.003 μm . Before measuring it, some dust was dropped onto its surface. Surface reconstruction of the measured data shows obvious outliers. Parameterization of Sa of the measured data was 1.3004 μm , with 29.65% difference to the certified value. The arithmetic mean height Sa of the data after deletion of outliers was 0.9677 μm . Its difference from the certified value is 3.52%. The second experiment measured an iron surface. The surface reconstructions of the measured data and the data after processing outliers using our proposed CDM method indicated that outliers were detected effectively. Both the QQ plot and the histogram of the heights distribution of the surface data show obvious differences before and after outlier deletion.

In conclusion, the new proposed method in this thesis using CDM method for detecting outliers in surface data measured by confocal microscopy is valid and reliable, as validated by processing two synthetic data and two experiments.

7.7 References of Chapter 7

- [1] D. Huang, S. Du, G. Li, C. Zhao, Y. Deng, Detection and monitoring of defects on three-dimensional curved surfaces based on high-density point cloud data, *Precision Engineering* 53 (2018) 79–95.
- [2] H. Jia, Y. L. Murphey, J. Shi, T. S. Chang, An Intelligent Real-time Vision System for Surface Defect Detection, in: *Proceedings of the Pattern Recognition, 17th International Conference on (ICPR'04) Volume 3, ICPR '04*, IEEE Computer Society, Washington, DC, USA, 2004, pp. 239 – 242.
- [3] G. M. Krolczyk, R. W. Maruda, P. Nieslony, M. Wieczorowski, Surface morphology analysis of Duplex Stainless Steel (DSS) in Clean Production using the Power Spectral Density, *Measurement* (94) (2016) 464–470.

- [4] G. M. Krolczyk, J. B. Krolczyk, R. W. Maruda, S. Legutko, M. Tomaszewski, Metrological changes in surface morphology of high-strength steels in manufacturing processes, *Measurement* 88 (2016) 176–185.
- [5] Richard Leach, *Optical measurement of surface topography*, Springer, 2011.
- [6] C. Teutsch, E. Trostmann, D. Berndt, A parallel point cloud clustering algorithm for subset segmentation and outlier detection, *Proceedings SPIE Optical Metrology* 8085.
- [7] ISO 16610-1:2015. Geometrical product specifications (GPS) – Filtration – Part 1: Overview and basic concepts.
- [8] ISO 16269-4: Statistical interpretation of data - Part 4: Detection and treatment of outliers.
- [9] G. L. Goic, C. A. Brown, H. Favreliere, S. Samper, F. Formosa, Outlier filtering: a new method for improving the quality of surface measurements, *Measurement science and technology* 24 (2013) 015001(13pp).
- [10] Y. Wang, H. Y. Feng, Outlier detection for scanned point clouds using majority voting, *Computer-Aided Design* 62 (2015) 31 – 43.
- [11] X. J. Jiang, D. J. Whitehouse, Technological shifts in surface metrology, *CIRP Annals - Manufacturing Technology* 61 (2012) 815–836.
- [12] R. Leach, *Characterisation of Areal Surface Texture*, Springer, 2013.
- [13] M. F. Ismail, K. Yanagi, A. Fujii, An outlier correction procedure and its application to areal surface data measured by optical instruments, *Measurement science and technology* 21 (10) (2010) 105105(11pp).
- [14] ISO 16610-30: 2015(en). Geometrical product specifications (GPS)-Filtration-Part 30: Robust profile filters: Basic concepts.
- [15] ISO 16610-60: 2015. Geometrical Product Specimen (GPS) - Filtration - Part 60: Linear areal filters: Basic concepts.
- [16] C. Wang, J. Caja, E. Gomez, Comparison of methods for outlier identification in surface characterization, *Measurement* 117 (2018) 312 – 325.

- [17] H. Huang, D. Li, H. Zhang, U. Ascher, D. Cohen-Or, Consolidation of Unorganized Point Clouds for Surface Reconstruction, *ACM Transactions on Graphics* 28 (5) (2009) 176:1–176:7.
- [18] A. Nurunnabi, G. West, D. Belton, Outlier detection and robust normal-curvature estimation in mobile laser scanning 3D point cloud data, *Pattern Recognition* 48 (4) (2015) 1404 – 1419.
- [19] A. Bhattacharyya, On a measure of divergence between two statistical populations defined by their probability distributions, *Bulletin of the Calcutta Mathematical Society* 35 (1943) 99–109.
- [20] T. Kailath, The Divergence and Bhattacharyya Distance Measures in Signal Selection, *IEEE Transactions on Communication Technology* 15 (1967) 52–60.
- [21] R. C. Luo, M. H. Lin, R. S. Scherp, Dynamic multi-sensor data fusion system for intelligent robots, *IEEE Journal on Robotics and Automation* 4 (4) (1988) 386–396.
- [22] R. C. Luo, M. G. Kay, Multisensor integration and fusion in intelligent systems, *IEEE Transactions on Systems, Man, and Cybernetics* 19 (5) (1989) 901–931.
- [23] Z. Xu, M. Xia, Distance and similarity measures for hesitant fuzzy sets, *Information Sciences* 181 (11) (2011) 2128 – 2138.
- [24] F. Wessel, R. Schluter, K. Macherey, H. Ney, Confidence measures for large vocabulary continuous speech recognition, *IEEE Transactions on Speech and Audio Processing* 9 (3) (2001) 288–298.
- [25] S. Chen, D. Zhang, Robust Image Segmentation Using FCM With Spatial Constraints Based on New Kernel-Induced Distance Measure, *IEEE Transactions on Systems, Man, and Cybernetics - Part B: Cybernetics* 34 (4) (2004) 1907–1916.
- [26] C. L. Giusca, R. Leach, Good Practice Guide No.128: Calibration of the metrological characteristics of Imaging Confocal Microscopy (ICMs), 2012.
- [27] JCGM 101: 2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method.

- [28] JCGM 102: 2011 Evaluation of measurement data - Supplement 2 to the "Guide to the expression of uncertainty in measurement" - Extension to any number of output quantities.
- [29] I. Raid, T. Kusnezowa, J. Seewig, Application of ordinary kriging for interpolation of micro-structured technical surfaces, *Measurement Science and Technology* 24 (9) (2013) 095201.
- [30] A. Basu, H. Shioya, C. Park, *Statistical Inference: The Minimum Distance Approach*, New York: Chapman and Hall/CRC., 2011.
- [31] P. J. Huber, *Robust Statistics*, Springer Berlin Heidelberg, 2011, pp. 1248–1251.
- [32] Internet Based Surface Metrology Algorithm Testing System. <https://physics.nist.gov/3DVSC/jsp/Database3D.jsp?state=0>. 7th Feb 2018.
- [33] B. Bhushan, *Modern Tribology Handbook*, CRC Press LLC, 2001, Ch. Chapter 2 Surface Roughness Analysis and Measurement Techniques.
- [34] R. Deltombe, K. Kubiak, M. Bigerelle, How to select the most relevant 3D roughness parameters of a surface, *Scanning* 36 (1) (2014) 150–160.
- [35] E.S. Gadelmawla, M.M. Koura, T.M.A. Maksoud, I.M.Elewa, H.H. Soliman, Roughness parameters, *Journal of Materials Processing Technology* 123 (2002) 133–145.
- [36] *Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement (GUM)*.
- [37] JCGM 104: 2009 Evaluation of measurement data - An introduction to the "Guide to the expression of uncertainty in measurement" and related documents.

Chapter 8: Calibration of the lateral stage of confocal microscopy

Abstract: This chapter presents a method for characterizing and correcting the geometric errors of the movement of the lateral stage of Imaging Confocal Microscope in extended topography measurement. For an extended topography measurement, a defined number of 2D images are taken and stitched by correlation methods. Inaccuracies due to linear displacement, vertical and horizontal straightness errors, angular errors, and squareness errors based on the assumption of the rigid body kinematics are described. A mathematical model for the scale calibration of the X- and Y- coordinates is derived according to the system kinematics, the axis chain vector of confocal microscope, and the geometric error functions and their approximations by Legendre polynomials. The correction coefficients of the kinematic modelling are determined by the measured and certified data of a dot grid target standard artefact. To process the measurement data, algorithms for data partitions, fittings of cylinder centres, and determinations of coefficients are developed and validated. During which methods such as form removal, K-means clustering, linear and non-linear Least Squares are implemented.

8.1 Introduction to the X- and Y- axis scale calibration

The calibration of measuring machines is both important for test acceptance and error compensation [1]. Use of software techniques started from the very beginning for the correction of the systematic errors of measurement instruments, as the mechanical accuracy is expensive while repeatability cost little [2]. Over the last several decades, the measurement accuracy and error compensation have been an area of intensive investigation [3, 4, 56].

Lateral calibration of the X- and Y- coordinate serves as a calibration of the magnification of the X- and Y- axis scale [6]. Lateral calibration/correction of Confocal Microscope can be classified mainly into two groups: Imaging system calibration and machine system calibration

[7]. Calibrations of the imaging system studies aberrations of refractive systems of objective lenses [8, 9, 10], axial distortion by point spread function or refractive-index mismatches [50, 12], etc. The machine system calibrations investigate geometric errors generated by the movement of probes [2, 13, 14]. The first study of using kinematic geometric errors for error compensation of coordinate measurement traces back to the work of G Zhang, *et al.* [15]. From then on, characterization and correction of kinematic geometric errors mainly focused on coordinate measuring machines (CMM) [16, 17], seldom applied for optical measurement instruments.

Individuals can observe huge advancement in positioning and measuring accuracy [2]. Lateral calibration of the X- and Y- coordinate serves as a calibration of the magnification of the X- and Y- axis scale [6]. This calibration is done for each objective and field of view lens. Calibration of the lateral performance of the measurement instruments includes the determination of the characteristics of amplification, linearity, perpendicularity, etc. [18]. For the X- and Y- axis scale calibration, a calibrated pattern on the material measures is required, matching its lateral scale to the lateral size of the features of the pattern through a magnification value. There are several kinds of areal material measures better suited for calibration of the lateral scales of areal topography measuring instruments [33], such as cross gratings [20], pyramidal structures [21], as shown in Fig. 8.1 and Fig. 8.2.

Fig. 8.1 Image of the cross gratings: (a) glass substrate carrying three chrome grid patterns; (b) white light interferometer image of one of the grid pattern. Source: Recent advances in traceable nanoscale dimension and force metrology in the UK [20].

Fig. 8.2 One dimensional reference structure for lateral scale calibration of scanning microscopes. Source: A landmark-based 3D calibration strategy for SPM [21].

Characterization of the amplification, linearity, and the squareness of the X- and Y- axis can be achieved through a calibrated cross grating artefact. Measuring the positions of the centre of the cross gratings' squareness with a traceable areal surface topography measuring instrument allows for traceable and stable measurements along the X- and Y- directions [33], such as the work presented by R. K. Leach, *et al* [22]. There are two ways to account for the contribution of the amplification of the scales to the measurement uncertainty. The first way is to propagate uncertainty using the equation of the line fit. The second way is to take into account the combined effect of the amplification coefficient and the scale linearity [33].

However, areal 3D measurement by Confocal Microscopes is realized by both imaging systems and machine systems. Confocal Microscopes scan in the lateral and vertical directions using different physical mechanisms [23]. To obtain a 3D topography, Confocal Microscopes capture a series of two-dimensional images by stepping either the specimen holding base or the objectives along the Z-stage [55]. For a single topography measurement, the 2D images are acquired in lateral directions either all at once by a CCD array (Imaging Confocal Microscope) or by a raster scan (Laser Scanning Confocal Microscope) [25, 26]. For an extended topography measurement, a defined number of 2D images are taken and stitched by correlation methods. Accordingly, calibrating the imaging system only is not sufficient for a Confocal Microscope as its measurement is realized by both imaging and machine systems. Lateral calibration or machine system calibration is necessary and important. It is worth mention that some works have been carried out on characterization of metrological characteristics defined in ISO 25178-600 [27], such as amplification coefficient, linearity deviation, x-y perpendicularity deviation, etc. [28, 18, 33, 29]. These metrological characteristics imply the whole instrumentation system's characteristics to some extent.

8.2 Mathematical models for X- and Y- scale calibrations

The Dual Core 3D Image Confocal Microscopy utilized in this work is a multi-axis measurement instrument consisting of a chain of translational and/or rotational kinematic components. Applying the disciplinary of machine design [16, 30] and considering the immense investigations on geometric error compensations of coordinate measuring machines [31], the kinematic behavior and the corresponding errors of our image confocal microscopy in the measurement can be an analogy to one of the coordinate systems of the coordinate measuring machines.

Generally coordinate measuring machines can be classified into four configurations according to their motions of probes and workpieces, i.e. FXYZ, XFYZ, XYFZ, and XYZF [1, 32, 33], as shown in Fig. 8.3. In this representation, F means the fixed machine foundation. The axis before F means the available movement of the workpiece along the direction in this axis with respect to the base. The axis after F means the available movement of the probe along the direction in this axis with respect to the base.

Fig. 8.3 Schematic of the 4 coordinate measuring machine configurations.

The measuring loop of the image confocal microscopy is shown in Fig. 8.4. All the measuring motions are performed by the optical probe, or by the table, or divided between the two. Fig. 8.5 shows the architecture of our image confocal microscopy. Artefacts or measurand are placed in the X- and Y- stage. Their available movements are along the X- and Y- direction with respect to the base. The optical probes are held by the Z-stage, with available movements along Z-direction with respect to the base. This demonstrate that the areal topography measurement instrument used in this work, i.e. the Dual Core 3D Image Confocal Microscopy, belongs to the configuration of XYFZ.

Fig. 8.4 Schema of the metrology loop of the Confocal Optical Microscopy.

Fig. 8.5 Architecture of the 3D Image Confocal Microscopy.

Geometric errors might come from different causes, such as position, direction, speed, acceleration. Temperature distribution, load distribution, time, measurement strategy, software programs, etc. Those error sources are studied separately by the former investigators with the implicit assumption that they are independent [30]. Tab.8.1 makes a list of the geometrical errors as well as references and devices used to measure those errors.

Tab.8.1 References and devices used to measure geometric error in machines. Source:

Geometric error measurement and compensation of machines [30].

Type of geometrical error	References and devices
Positioning errors ($\delta_i(j)$ when $i = j$; 3 error functions)	<ul style="list-style-type: none"> • Laser interferometers • Set of gauge blocks/end bars • Step gauges • Ball arrays
Straightness error motions ($\delta_i(j)$ when $i \neq j$; 6 error functions)	Straightness references
	<ul style="list-style-type: none"> • Taut wire • Mechanical and optical straightedge • Wing reflector • Laser beam
Angular error motions ($\varepsilon_i(j)$; 3 roll components when $i = j$; 3 yaw components and 3 pitch components when $i \neq j$)	Displacement indicator
	<ul style="list-style-type: none"> • Capacitance gage • Electronic gage and LVDT • Plane mirror laser interferometer • photodiode
Squareness	<ul style="list-style-type: none"> • Autocollimator • Angular laser interferometer • Mechanical level • Electronic level • Straightness measuring devices separated
Parallelism	<ul style="list-style-type: none"> • Mechanical square with collimator • Diagonal measurements • Collimator with optical square • Laser interferometer with optical square

For a three-axis machine, there is now a general consensus that using 21 parametric errors to develop a function for calculating machine volumetric errors, which contains 18 geometric errors and three squareness errors. They can be classified further into three positioning errors, six straightness errors, nine angular errors [1, 15, 33]. This is based on the assumption of the rigid body kinematics. A more detailed classification of those rigid body errors are linear displacement errors, vertical straightness errors, horizontal straightness errors, roll angular errors, pitch angular errors, yaw angular errors, and squareness errors [33]. Tab.8.2 makes a conclusion of those 21 rigid body errors. For the linear displacement errors, the representation

$\delta_x(x)$ means the position error generated by the movement along the X-axis, the same for the $\delta_y(y)$, $\delta_z(z)$; the vertical straightness error $\delta_y(x)$ means the straightness error in Y-axis generated by the movement along the X-axis, the same for the other 5 straightness errors; the roll angular error $\sigma_x(x)$ means the angular error rotating X-axis for the movement along X-axis, the pitch angular error $\sigma_x(y)$ means the angular error rotating X-axis for the movement along Y-axis, the same for the other seven angular errors; Squareness error is the error between two kinematic directions, which might come from the assembly. Due to the error in assembling the system, the angles between every two axis might not be exactly 90° . This leads to the squareness error of the axis. This error is different from the other 18 errors, as it is not a function but three constants. Fig. 8.6 manifests those rigid body errors, classifying those 21 errors into four subsets by four colors.

Tab.8.2 Classification and representation of the 21 rigid body errors.

Classification of errors		Error types	Representations
Geometric errors	Position errors	Linear displacement errors:	$\delta_x(x), \delta_y(y), \delta_z(z)$
	Straightness errors	Vertical straightness errors:	$\delta_y(x), \delta_x(y), \delta_x(z)$
		Horizontal straightness errors:	$\delta_z(x), \delta_z(y), \delta_y(z)$
	Angular errors	Roll angular errors:	$\sigma_x(x), \sigma_y(y), \sigma_z(z)$
		Pitch angular errors:	$\sigma_x(y), \sigma_y(x), \sigma_x(z)$
		Yaw angular errors:	$\sigma_z(x), \sigma_y(z), \sigma_z(y)$
Squareness errors		Squareness/orthogonality errors:	S_{xy}, S_{yz}, S_{zx}

Fig. 8.6 Illustration of the 21 rigid body errors.

For the measurement of a workpiece using the 3D image confocal microscopy, the workpiece is placed on the X- and Y- stage above the granite supporting base. As shown in Fig. 8.7, to focus laser beam onto the measurand surface, two movements are operated, i.e. movement along the X- and Y- axis controlled by the lateral stage and movement along the Z-axis controlled by the vertical stage. For example, to measure the point P on the measurand surface, its position can be denoted as $\vec{P}(P_x, P_y, P_z)$ with respect to its coordinate origin $\vec{O}(0,0,0)$. For the focus of the probe and the point of workpiece, the first movement include translation of X carriage followed by the translation of Y carriage; the second movement is the translation of Z carriage. It can be suggested that vectors $\vec{X}$, $\vec{Y}$ and $\vec{Z}$ represents the translations of X, Y and Z carriages, the rotation matrices $\mathbf{R}(\mathbf{X})$, $\mathbf{R}(\mathbf{Y})$ and $\mathbf{R}(\mathbf{Z})$ denotes the angular motion errors caused by the translations of X, Y and Z carriages, the vector $\vec{T}$ represents the X, Y and Z abbe offsets of the probe with respect to the carriage to which the probe is attached. For our image confocal microscopy, the probe is attached to the Z-stage. Therefore, it is obvious that the translation of the X and Y carriage, with an offset of the position $\vec{P}$ stop at the same

point reached by the translation of Z carriage with a probe offset $\bar{T}$, which can be understood as the focus of the probe with the measurand. According to this conclusion, a diagram of the axis chain vector of the 3D image microscopy is plotted and showed in Fig. 8.8.

Fig. 8.7 Manifestation of the vectors on the 3D image confocal microscopy.

Fig. 8.8 Diagram of the axis chain vector of the 3D image confocal microscopy.

As shown in Fig. 8.8, there are two kinematical paths from the coordinate origin O to the laser beam focus, i.e. $\bar{Z} \rightarrow \bar{T}$ and $\bar{X} \rightarrow \bar{Y} \rightarrow \bar{P}$. In each kinematical path, the actual movement of that axis is affected by the rotational error of its predecessors. The movement of $\bar{T}$ is affected by the rotational error of the movement of $\bar{Z}$. $\bar{Y}$ is affected by the rotational error of $\bar{X}$. $\bar{P}$ is affected by the rotational errors of $\bar{X}$ and $\bar{Y}$. Therefore, the chain vector shown in Fig. 8.8

for the two kinematical paths, from the same origin reaching the same laser beam focus can be expressed by Equation 8.1:

$$\bar{\mathbf{Z}} + \mathbf{R}^{-1}(\mathbf{Z})\bar{\mathbf{T}} = \bar{\mathbf{X}} + \mathbf{R}^{-1}(\mathbf{X})\bar{\mathbf{Y}} + \mathbf{R}^{-1}(\mathbf{X})\mathbf{R}^{-1}(\mathbf{Y})\bar{\mathbf{P}} \quad (8.1)$$

After rearrangement of the above equation, vector $\bar{\mathbf{P}}$ can be expressed by all the other vectors and matrices, as indicated by Equation 8.2. This result is the same with that in the work presented by G. Zhang, *et al* [1].

$$\bar{\mathbf{P}} = -\mathbf{R}(\mathbf{Y})\mathbf{R}(\mathbf{X})\bar{\mathbf{X}} - \mathbf{R}(\mathbf{Y})\bar{\mathbf{Y}} + \mathbf{R}(\mathbf{Y})\mathbf{R}(\mathbf{X})\bar{\mathbf{Z}} + \mathbf{R}(\mathbf{Y})\mathbf{R}(\mathbf{X})\mathbf{R}^{-1}(\mathbf{Z})\bar{\mathbf{T}} \quad (8.2)$$

The Equation 8.2 can also be written as:

$$\bar{\mathbf{P}} = \mathbf{R}^{-1}(\mathbf{Y})\mathbf{R}^{-1}(\mathbf{X})\bar{\mathbf{X}} + \mathbf{R}^{-1}(\mathbf{Y})\bar{\mathbf{Y}} - \mathbf{R}^{-1}(\mathbf{Y})\mathbf{R}^{-1}(\mathbf{X})\bar{\mathbf{Z}} + \mathbf{R}(\mathbf{Y})^{-1}\mathbf{R}(\mathbf{X})^{-1}\mathbf{R}(\mathbf{Z})\bar{\mathbf{T}} \quad (8.3)$$

The rotation can be expressed by the infinitesimal rotation matrix, as shown in Equation 8.4, which was widely accepted and used by many former investigators [15, 1, 33, 32]. Its inverse matrix is shown in Equation 8.5.

$$\mathbf{R}(U) = \begin{bmatrix} 1 & \sigma_z(U) & -\sigma_y(U) \\ -\sigma_z(U) & 1 & \sigma_x(U) \\ \sigma_y(U) & -\sigma_x(U) & 1 \end{bmatrix} \quad (8.4)$$

$$\mathbf{R}^{-1}(U) = \begin{bmatrix} 1 & -\sigma_z(U) & \sigma_y(U) \\ \sigma_z(U) & 1 & -\sigma_x(U) \\ -\sigma_y(U) & \sigma_x(U) & 1 \end{bmatrix} \quad (8.5)$$

According to the previous investigations on error compensation of coordinate measuring machines, the vectors $\bar{\mathbf{X}}$, $\bar{\mathbf{Y}}$, $\bar{\mathbf{Z}}$ and $\bar{\mathbf{T}}$ can be expressed as [1, 32, 33, 15]:

$$\bar{\mathbf{X}} = \begin{bmatrix} x + \delta_x(x) \\ \delta_y(x) \\ \delta_z(x) \end{bmatrix} \quad (8.6)$$

$$\bar{\mathbf{Y}} = \begin{bmatrix} \delta_x(y) - S_{xy}y \\ y + \delta_y(y) \\ \delta_z(y) \end{bmatrix} \quad (8.7)$$

$$\bar{\mathbf{Z}} = \begin{bmatrix} \delta_x(z) - S_{zx}z \\ \delta_y(z) - S_{yz}z \\ z + \delta_z(z) \end{bmatrix} \quad (8.8)$$

$$\bar{\mathbf{T}} = \begin{bmatrix} x_t \\ y_t \\ z_t \end{bmatrix} \quad (8.9)$$

Where x , y and z are nominal values of the carriage positions, x_t , y_t and z_t are the abbe offsets of the confocal probe respectively in X-, Y- and Z- directions. S_{xy} , S_{yz} , S_{zx} are out-of-squareness in the XY, YZ and ZX planes respectively.

The position vector $\bar{\mathbf{P}}$ is:

$$\bar{\mathbf{P}} = \begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} \quad (8.10)$$

Substituting Equations 8.4-8.10 into Equation 8.2, the expressions for the actual coordinates of the beam focus in the workpiece, x_p , y_p and z_p , can be acquired. Moreover, in the 3D image confocal microscopy, there is no real X- and Y- carriages, the workpiece is carried by a lateral stage mounted on a fixed base [33, 13], the Z-stage is mounted on another fixed base. Besides that, the beam focus is considered as the probe. As the focus is always on the workpiece surface and the information is acquired exactly in that point, there is no Abbe offset on x , y and z , neither angular term. This means $\bar{\mathbf{T}} = 0$ and $\mathbf{R}(Z) = 0$.

After dropping $\bar{\mathbf{T}}$ and $\mathbf{R}(Z)$, Equation 8.2 will be:

$$\bar{\mathbf{P}} = -\mathbf{R}(Y)\mathbf{R}(X)\bar{\mathbf{X}} - \mathbf{R}(Y)\bar{\mathbf{Y}} + \mathbf{R}(Y)\mathbf{R}(X)\bar{\mathbf{Z}} \quad (8.11)$$

As in this part, only geometrical errors along X- and Y- directions are studied, Equations 8.4-8.10 can be simplified as:

$$\mathbf{R}(U) = \begin{bmatrix} 1 & 0 & -\sigma_y(U) \\ 0 & 1 & \sigma_x(U) \\ \sigma_y(U) & -\sigma_x(U) & 0 \end{bmatrix} \quad (8.12)$$

$$\mathbf{R}^{-1}(U) = \begin{bmatrix} 1 & 0 & \sigma_y(U) \\ 0 & 1 & -\sigma_x(U) \\ -\sigma_y(U) & \sigma_x(U) & 0 \end{bmatrix} \quad (8.13)$$

$$\bar{\mathbf{X}} = \begin{bmatrix} x + \delta_x(x) \\ \delta_y(x) \\ 0 \end{bmatrix} \quad (8.14)$$

$$\bar{\mathbf{Y}} = \begin{bmatrix} \delta_x(y) - S_{xy}y \\ y + \delta_y(y) \\ 0 \end{bmatrix} \quad (8.15)$$

$$\bar{\mathbf{Z}} = 0 \quad (8.16)$$

$$\bar{\mathbf{P}} = \begin{bmatrix} P_x \\ P_y \\ 0 \end{bmatrix} \quad (8.17)$$

After substituting 8.4-8.10 into 8.2, the actual position of the laser beam focus is obtained as:

$$P_x = x + \delta_x(x) + z \cdot \sigma_y(x) + \delta_x(y) - y \cdot \sigma_z(y) + z \cdot \sigma_y(y) + \delta_x(z) \quad (8.18)$$

$$P_y = y + \delta_y(x) + x \cdot \sigma_z(x) - z \cdot \sigma_x(x) + \delta_y(y) + x \cdot \sigma_z(y) - z \cdot \sigma_x(y) + \delta_y(z) \quad (8.19)$$

$$P_z = z + \delta_z(x) - x \cdot \sigma_y(x) + \delta_z(y) - x \cdot \sigma_y(y) + y \cdot \sigma_x(y) + \delta_x(z) \quad (8.20)$$

After substituting 8.12-8.17, dropping out the z-stage variables, the geometrical error function for X- and Y- stage is:

$$P_x = x + \delta_x(x) + \delta_x(y) - y \cdot \sigma_z(y) \quad (8.21)$$

$$P_y = y + \delta_y(x) + x \cdot \sigma_z(x) + \delta_y(y) + x \cdot \sigma_z(y) \quad (8.22)$$

Those errors in Equation 8.21 and 8.22 are functions, which can be simulated by Legendre polynomials. The uniformly convergent Legendre series expansion is [34]:

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x) \quad (8.23)$$

For each translational or rotational error, it can be approximated by a linear combination of Legendre polynomials [33], such as:

$$\delta_x(x) = \sum_{i=0}^n a_i P^i(x) \quad (8.24)$$

Where a_i is the approximation coefficients, $P^i(x)$ is the Legendre polynomial of the i_{th} order.

The first few Legendre polynomials are [35]:

$$P^0(x) = 1 \quad (8.25)$$

$$P^1(x) = x \quad (8.26)$$

$$P^2(x) = \frac{1}{2}(3x^2 - 1) \quad (8.27)$$

$$P^3(x) = \frac{1}{2}(5x^3 - 3x) \quad (8.28)$$

$$P^4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) \quad (8.29)$$

$$P^5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x) \quad (8.30)$$

$$P^6(x) = \frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5) \quad (8.31)$$

To use the Legendre polynomials for the approximation of function errors, the order of the polynomials should be determined first. It is widely shared that the higher the order the smaller the sum of the squares of the residuals. However, the high-order error functions will

also cause the random error. Third order polynomial is the optimal choice for the approximation of the error functions [33, 36].

Therefore, the Equation 8.24 can be written as:

$$\begin{aligned}\delta_x(x) &= \sum_{i=0}^3 a_i P^i(x) \\ &= a_0 P^0(x) + a_1 P^1(x) + a_2 P^2(x) + a_3 P^3(x) \\ &= a_0 + a_1 x + \frac{1}{2} a_2 (3x^2 - 1) + \frac{3}{2} a_3 (5x^3 - 3x)\end{aligned}\tag{8.32}$$

Where a_0 , a_1 , a_2 and a_3 are 4 unknown coefficients. They can be reduced to three. Harbour the idea that all errors vanish at the starting point of the axis [33], i.e.

$$\delta_i(0) = 0\tag{8.33}$$

$$\sigma_i(0) = 0\tag{8.34}$$

Let the Equation 8.32 be [33]:

$$\delta_x(0) = 0\tag{8.35}$$

Then it can be reached:

$$0 = a_0 - \frac{1}{2} a_2\tag{8.36}$$

Hence, a_0 can be represented by a_2 as:

$$a_0 = \frac{1}{2} a_2\tag{8.37}$$

Therefore, Equation 8.32 can be simplified to:

$$\delta_x(x) = a_1 x + \frac{3}{2} a_2 x^2 + \frac{3}{2} a_3 (5x^3 - 3x)\tag{8.38}$$

The same for the other error functions in Equations 8.21 and 8.22. It is worth attention that in the work of K. Tong, *et al* [33], they clarified that the three linear terms of straightness errors $\delta_x(y)$, $\delta_x(z)$, $\delta_y(z)$ are the same with the three squareness errors S_{xy} , S_{yz} , S_{xz} , and it is

incorrect to model the same error two times. In the Equation 8.21 and 8.22, there are no errors calculated two times. Therefore, all the error functions can be approximated using the same method as $\delta_x(x)$, therefore,

$$\delta_x(y) = b_1 y + \frac{3}{2} b_2 y^2 + \frac{3}{2} b_3 (5y^3 - 3y) \quad (8.39)$$

$$\sigma_z(y) = c_1 y + \frac{3}{2} c_2 y^2 + \frac{3}{2} c_3 (5y^3 - 3y) \quad (8.40)$$

$$\delta_y(x) = d_1 x + \frac{3}{2} d_2 x^2 + \frac{3}{2} d_3 (5x^3 - 3x) \quad (8.41)$$

$$\sigma_z(x) = e_1 x + \frac{3}{2} e_2 x^2 + \frac{3}{2} e_3 (5x^3 - 3x) \quad (8.42)$$

$$\delta_y(y) = f_1 y + \frac{3}{2} f_2 y^2 + \frac{3}{2} f_3 (5y^3 - 3y) \quad (8.43)$$

Substituting Equations 8.38-8.43 into Equations 8.21 and 8.22, the final mathematical models for the beam focus point $\vec{\mathbf{P}}(P_x, P_y, 0)$ with error corrections are:

$$\begin{aligned} P_x = & x + a_1 x + \frac{3}{2} a_2 x^2 + \frac{3}{2} a_3 (5x^3 - 3x) + \\ & + b_1 y + \frac{3}{2} b_2 y^2 + \frac{3}{2} b_3 (5y^3 - 3y) - \\ & - y \cdot (c_1 y + \frac{3}{2} c_2 y^2 + \frac{3}{2} c_3 (5y^3 - 3y)) \end{aligned} \quad (8.44)$$

$$\begin{aligned} P_y = & y + d_1 x + \frac{3}{2} d_2 x^2 + \frac{3}{2} d_3 (5x^3 - 3x) + \\ & + x \cdot (e_1 x + \frac{3}{2} e_2 x^2 + \frac{3}{2} e_3 (5x^3 - 3x)) + \\ & + f_1 y + \frac{3}{2} f_2 y^2 + \frac{3}{2} f_3 (5y^3 - 3y) + \\ & + x \cdot (c_1 y + \frac{3}{2} c_2 y^2 + \frac{3}{2} c_3 (5y^3 - 3y)) \end{aligned} \quad (8.45)$$

8.3 Methodology and experimental procedures

To calibrate the kinematic geometric errors in the X- and Y- direction, a standard artefact with dot grid targets on glass is measured and a series of algorithms are developed for the process

of raw data, calculations of displacement, determination of coefficients, etc. Fig. 8.9 illustrates the standard. Those dots are scratched on the substrate, which is glass with thickness of 1.5 mm. Tab.8.3 gives an indication of the size, the dot spacing, the diameter, the accuracy, etc., of the dot pattern,

Fig. 8.9 Illustration of the standard artefact of dot grid targets.

Tab.8.3 Detailed information about the dot grid targets standard artefact.

Width [mm]	Dot diameter [mm]	Dot spacing [mm]	X and Y axis accuracy [mm]	Dot Array		
				X	Y	Total
25	0.0625	0.125	± 0.001	201	201	40401

This artefact was measured using the Leica DCM-3D Confocal Microscopy at the Metrology Laboratory of the Technical University of Madrid. A magnification objective of 50X was used, with a numerical aperture of 0.90. The acquisition parameter, measurement area, was defined as the topography stitching measurement, with a 8×8 extended topographies, covering an area of $1.78 \times 1.33 \text{ mm}^2$. The parameter of overlapping area is 15% and the correlation takes XYZ option. The level of resolution is 2, and the measured extended topographies contain 2673×2003 pixels. The environment of the experiments was controlled under a stable temperature at $20 \pm 1 \text{ }^\circ\text{C}$. Under the individual topography measurement mode, the confocal optical probe only acquire one topography, which covers only two dots and provides the 3D point cloud for only two dots too, as shown in Fig. 8.10. Moreover, under this mode, the X- and Y-stage does not move. Under the stitching measurement mode, the optical probe acquires the indicated number of topographies, i.e. 8×8 in this case, first saving them in a temporary fold and then stitching them together by one of the three correlation methods

defined by the confocal system. The three correlation methods are: ‘None’, ‘Z’ and ‘XYZ’. The option ‘None’ means the extended measurements is stitched without adjustment. This is useful for samples like rings in which the centre of the sample is empty or for flat surfaces measured by VSI or PSI. The option ‘Z’ means stitching the topographies by calculating the Z correlations. This option is recommended for general applications. The option ‘XYZ’ means the contiguous topographies are stitched not only considering the correlations in Z but also the correlations in X and Y directions. Fig. 8.11 shows an extended measurement using the ‘XYZ’ correlation method. For extended measurement, the X- and Y-stage moves. Its movement might generate kinematic geometrical errors. To correct those errors, mathematical models and algorithms are developed. Twenty-one coefficients defined in Equations 8.44 and 8.45 are finally determined by our mathematical models and algorithms. The following part makes deep explanations on algorithms for kinematic geometric error corrections.

Fig. 8.10 Indication of the measurement range for individual topography by Objective Magnification of 50X: (a) 2D image; (b) 3D image.

Fig. 8.11 Indication of the measurement range for stitching topography by Objective Magnification of 50X.

For the correction of geometrical errors produced by the movement of the X- and Y-stage, there is a necessity for the development of mathematical models and three main algorithms. The data files with suffix ‘.dat’, which is produced by the image confocal microscopy system for the measurement, is taken as the raw measurement result. These data files are read by our developed algorithms. Fig. 8.12 gives an indication of the flowchart of the total algorithm for geometrical errors correction. The algorithm can be divided into three main parts and are explained in details in the following part. The first algorithm aims at separate the point cloud of the raw data into two parts, i.e. the flats and cylinders, taking into consideration of elimination of outliers. The second algorithm aims at fitting those cylinders, determining their centre coordinates, calculating dots distances, etc. The third algorithm applies those dots distances into the mathematical model developed in part 8.8, to obtain the numerical results of the coefficients of Equations 8.44 and 8.45.

Fig. 8.12 Flowchart of the algorithm for geometric errors correction.

8.4 Algorithms for data processing

8.4.1 Algorithm for separation of flat and cylinders

The raw measurement data contains lots of outliers and inclines a lot, as shown in Fig. 8.12. The first step is to choose an area of this raw surface with appropriate size and location,

assuring at least outliers and least measured defects as possible. This can be realized in Matlab® by manipulating arrays. Fig. 8.13 shows a surface reconstruction by trimming the raw data with 10% edges along X- and Y-direction trimmed. As there are too much measurement defects when $y > 800 \mu\text{m}$, this part is also abandoned.

Fig. 8.13 Reconstruction of the measured surface by its raw measurement data: (a) 2D contour; (b) 3D surf.

Fig. 8.14 Reconstruction of the surface with trimmed raw data.

After obtaining an appropriate area for analysis, it is necessary to eliminate its form. There are two methods for the form elimination, one is using the Gaussian filter, and the other is to

rotate the plane using Singular Value Decomposition (SVD) and Space Analytic Geometry method. The latter one is applied in this work.

SVD is very efficient for finding the normal vector of the initial surface. SVD is an eigenvalues decomposition of Matrix that is not square. It provides a convenient way for breaking a matrix into simpler, meaningful pieces. The least square solution of the homogeneous linear Equation is the least eigenvectors that corresponded with the least eigenvalues.

For a matrix M ,

$$M^T M = V \Sigma^T U^T U \Sigma V^T = V (\Sigma^T \Sigma) V^T \quad (8.46)$$

$$M M^T = U \Sigma V^T V \Sigma^T U^T = U (\Sigma \Sigma^T) U^T \quad (8.47)$$

Where, symbol T means Conjugate transpose. From these equations, it can be found that eigenvectors of $M^T M$ is the column vector of V .

In Matlab, there are two methods to solve it. First, $[V \ D] = \text{eig}(A' \times A)$, $[V \ D] = \text{eig}(A \times A')$, D is the eigenvalues of the diagonal matrix, V is the corresponding eigenvectors. The eigenvector in V corresponded by the least eigenvalue is the least square solution. Second, use the function of SVD, $[U \ S \ V] = \text{svd}(A)$, U is consisted by the eigenvectors of AA' , V is consisted by the eigenvectors of $A'A$. Therefore, the singular vector in V that corresponded by the least singular value in singular value matrix S is the least square solution, i.e. the normal vector of the plane. After finding the normal vector, the angular between the normal vector and the vector of Z-axis, i.e. $[0 \ 0 \ 1]$, could be determined. The axis of rotation is determined by the cross product of the normal vector and the Z-axis. Rotating the plane along the axis of rotation by the calculated angular will eliminate the inclination of the plane. Fig. 8.14 gives an example of the rotated surface, which is rotated from the surface shown in Fig. 8.13. Fig. 8.14 (a) was plotted by the Matlab® function 'plot3' while the Fig. 8.14 (b) was plotted by the function 'surf'. It can be found from the figure that

after the rotation the range of Z-axis is much smaller and much details of the surface can be observed. It is obvious that this surface is constructed by point clouds, which form a flat plane and many cylinders perpendicular to this flat.

Fig. 8.15 Reconstruction of the rotated surface: (a) 3D line plot; (b) 3D surface plot uses Z for the colour data.

This rotated surface now is ready for the separation of flat and cylinders. Fig. 8.15 gives an indication of the distribution of the heights of the surface. Fig. 8.16 and Fig. 8.17 gives examples of the separations of the rotated surface shown in Fig. 8.14.

Fig. 8.16 Histogram of the Z values of the rotated surface.

Fig. 8.17 The separated flat plane of the rotated surface: (a) 3D view (b) view from top down.

Fig. 8.18 The separated cylinders of the rotated surface: (a) 3D view (b) View from top down

Fig. 8.19 Separation of cylinders into individuals.

After separating the cylinders from the flat, the next step is to obtain the three coordinates of each cylinder point cloud. Fig. 8.19 gives an example of the separation of cylinders into individual clusters, characterizing the cylinders with different colours. Here applies the squared Euclidean distance metric for distance calculation, as shown in Equation 8.49. Moreover, each centroid of the point cloud is the mean of the coordinates' values of the points.

$$d(x, c) = (x - c)(x - c)^T \quad (8.48)$$

Where x is the initial observations, c is the centroid.

According to the previous investigations, there are several efficient algorithms for data partitions, such as K-means clustering algorithm [37, 38] and Lloyd's algorithm [39]. These two algorithms are iterative and data-partitioning algorithms, which assigns the initial observations into k clusters according to the squared Euclidean distance metric and the centroids. The number of clusters k is defined before data partition. In our work, the Lloyd's algorithm is used for finding the centroids of k clusters while the K-means clustering algorithm is used for partitioning the initial observations into k clusters according to the squared Euclidean distance metric with respect to the centroid of each cluster. The K-means clustering algorithm requires the input as a matrix of M points in N dimensions as well as a matrix of K initial cluster centres in N dimensions. Denoting the number of points in cluster L is $NC(L)$ and the Euclidean distance between point I and cluster L is $D(I, L)$, the

general procedure of the K-means clustering algorithm is to find a K-partition of clusters with locally optimal within-cluster sum of squares by changing the initial observations from one cluster to another [37], as indicated by Equation 8.50.

$$\min_{D^2} \sum_{i=1}^K \sum_{j=1}^{NC(L)} D^2(I, L) \quad (8.49)$$

Fig. 8.20 Flowchart of the algorithm for data partition

The procedures of the algorithm for partitioning the filtered cylinders into individuals are shown in Fig. 8.20, which is consisted of 6 steps. It is worth mention that the data are made dimensionality reduction before data partition. Those cylinders are point cloud of 3D dimensions. The aim of dimensionality reduction is to produce a compact low-dimensional encoding of a given high-dimensional data set [40]. The dimensionality can be reduced by two ways [41]. The first way is by only keeping the most relevant variables from the original dataset, which is called feature selection. The second way is to exploit the redundancy of the input data and to find a smaller set of new variables, each being a combination of the input variables, containing basically the same information as the input variables. In this work, the dimensionality of the data is reduced to 2D from 3D by projection along Z-axis.

This algorithm is explained in details in the following table:

Objective: Partition the filtered cylinders into individuals by K-means and Lloyd's cluster algorithm.

Algorithm. Data partitioning using K-means and Lloyd's algorithm;

- (i) Import matrix **M** which contains the X-, Y- and Z- coordinates of all the points of cylinders, define a constant k which is the number of clusters;
- (ii) Dimensionality reduction;
- (iii) Choose k centroids randomly;
- (iv) Compute the squared Euclidean distance metric $d(x,c) = (x-c)(x-c)^T$ of all the points to k centroids;
- (v) Assign each point to one cluster by the minimum Euclidean distance, i.e. $\min_D D(I,L)$;
- (vi) Compute the new centroids of all the clusters determined;
- (vii) Iterate steps (iv) to (vi) until the cluster assignments do not change or the maximum number of iterations is reached;

end

8.4.2 Algorithm for determination of dots center and distance

The data is first made dimensionality reduction before processing, from 3D to 2D. The principle variable of each individual cylinder is the X- and Y-coordinates. The circles are fitted by those X- and Y- coordinates and the initial circle centers are calculated. There are many investigations on circle fitting by both direct and indirect methods [42, 43, 44]. The equation for fitting a circle by X- and Y- coordinates is:

$$\mathbf{X}^2 + \mathbf{Y}^2 + a\mathbf{X} + b\mathbf{Y} + c = 0 \quad (8.50)$$

Where, a , b and c are constants to be determined by the known vectors **X** and **Y**, which are measured coordinates values of X- and Y- axis. To solve this equation, it can be rewritten as:

$$[\mathbf{X} \quad \mathbf{Y} \quad 1] \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} = -[\mathbf{X}^2 \quad \mathbf{Y}^2] \quad (8.51)$$

This equation can be solved by the least squares method as:

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = ([\mathbf{X} \quad \mathbf{Y} \quad 1]^T \cdot [\mathbf{X} \quad \mathbf{Y} \quad 1])^{-1} \cdot [\mathbf{X} \quad \mathbf{Y} \quad 1]^T \cdot (-[\mathbf{X}^2 \quad \mathbf{Y}^2]) \quad (8.52)$$

The position of the fitted circle centre is:

$$C_x = -0.5 \times a \quad (8.53)$$

$$C_y = -0.5 \times b \quad (8.54)$$

The radius of the fitted circle is:

$$R = \sqrt{(a^2 + b^2) / 4 - c} \quad (8.55)$$

In this work, the circle centres are fitted initially by those equations. After obtaining those initial centres, little increment are calculated iteratively for the optimization of those centres. Dots distances are determined by the Euclidean norm of the circle centres.

$$|d_{ij}| = \|C_i - C_j\|_2 \quad (8.56)$$

Where, d_{ij} is the distance between dot i and dot j , C_i is the coordinate of the centre of dot i , C_j is the coordinate of the centre of dot j .

Fig. 8.21 Flowchart of the algorithm for circle fitting

The flowchart of this algorithm is shown in Fig. 8.21. The input data is first made dimensionality reduction for fewer variables to be processed. The X- and Y- coordinates are fitted to individual circles by the mathematical models introduced. Finally the fitting is optimized by small increments. Finally the dots' distances are determined by the Euclidean norm of the circle centres.

8.4.3 Algorithm for determination of coefficients

This part aims at determination of the 18 parameters of coefficients, $a_1, a_2, a_3, b_1, \dots, f_3$, defined in Equations 8.44 and 8.45. The objective is to fit the 18 parameters to obtain the least squared residuals between the corrected X- and Y- coordinate point and the nominal position. That is:

$$\sum_{i=1}^n \|P_{nom}^i(x, y) - P_{corr}^i(x, y)\|_2^2 = \min \quad (8.57)$$

Where, $P_{nom}^i(x, y)$ represents the i_{th} nominal position defined by the X- and Y- coordinates, $P_{corr}^i(x, y)$ denotes the i_{th} corrected position obtained from the measured data and Equations 8.44 and 8.45.

Therefore, the objective function is

$$\begin{aligned}
 \min F(x, y) \Big|_{a_1, a_2, \dots, f_3} &= \min \sum_{i=1}^n \|P_{nom}^i(x, y) - P_{corr}^i(x, y)\|_2^2 \\
 &= \min \left(\left(x_{nom}^i - x_{corr}^i \right)^2 + \left(y_{nom}^i - y_{corr}^i \right)^2 \right) \\
 &= \min \left(\left(\begin{aligned} &x_{nom}^i - x_{meas}^i + a_1 x_{meas}^i + \frac{3}{2} a_2 (x_{meas}^i)^2 + \frac{3}{2} a_3 (5(x_{meas}^i)^3 - 3x_{meas}^i) + \\ &+ b_1 y_{meas}^i + \frac{3}{2} b_2 (y_{meas}^i)^2 + \frac{3}{2} b_3 (5(y_{meas}^i)^3 - 3y_{meas}^i) - \\ &- y_{meas}^i \cdot (c_1 y_{meas}^i + \frac{3}{2} c_2 (y_{meas}^i)^2 + \frac{3}{2} c_3 (5(y_{meas}^i)^3 - 3y_{meas}^i)) \end{aligned} \right)^2 + \right. \\
 &\quad \left. + \left(\begin{aligned} &y_{nom}^i - y_{meas}^i + d_1 x_{meas}^i + \frac{3}{2} d_2 (x_{meas}^i)^2 + \frac{3}{2} d_3 (5(x_{meas}^i)^3 - 3x_{meas}^i) + \\ &+ x_{meas}^i \cdot (e_1 x_{meas}^i + \frac{3}{2} e_2 (x_{meas}^i)^2 + \frac{3}{2} e_3 (5(x_{meas}^i)^3 - 3x_{meas}^i)) + \\ &+ f_1 y_{meas}^i + \frac{3}{2} f_2 (y_{meas}^i)^2 + \frac{3}{2} f_3 (5(y_{meas}^i)^3 - 3y_{meas}^i) + \\ &+ x_{meas}^i \cdot (c_1 y_{meas}^i + \frac{3}{2} c_2 (y_{meas}^i)^2 + \frac{3}{2} c_3 (5(y_{meas}^i)^3 - 3y_{meas}^i)) \end{aligned} \right)^2 \right) \quad (8.58)
 \end{aligned}$$

The minimum value of F arrives when the gradient is zero [45, 46], i.e.:

$$\frac{\partial F}{\partial \beta_i} = 0 \quad (8.59)$$

Where F is the objective function, β_i represents the parameters of coefficients to be determined. There are 18 parameters in this part of work, hence there are 18 partial derivatives:

$$\frac{\partial F}{\partial a_1} = \sum_{i=1}^n 2 \left(\begin{aligned} & x_{nom}^i - x_{meas}^i + a_1 x_{meas}^i + \frac{3}{2} a_2 (x_{meas}^i)^2 + \frac{3}{2} a_3 (5(x_{meas}^i)^3 - 3x_{meas}^i) + \\ & + b_1 y_{meas}^i + \frac{3}{2} b_2 (y_{meas}^i)^2 + \frac{3}{2} b_3 (5(y_{meas}^i)^3 - 3y_{meas}^i) - \\ & - y_{meas}^i \cdot (c_1 y_{meas}^i + \frac{3}{2} c_2 (y_{meas}^i)^2 + \frac{3}{2} c_3 (5(y_{meas}^i)^3 - 3y_{meas}^i)) \end{aligned} \right) \cdot x_{meas}^i = 0 \quad (8.60)$$

$$\frac{\partial F}{\partial a_2} = \sum_{i=1}^n 2 \left(\begin{aligned} & x_{nom}^i - x_{meas}^i + a_1 x_{meas}^i + \frac{3}{2} a_2 (x_{meas}^i)^2 + \frac{3}{2} a_3 (5(x_{meas}^i)^3 - 3x_{meas}^i) + \\ & + b_1 y_{meas}^i + \frac{3}{2} b_2 (y_{meas}^i)^2 + \frac{3}{2} b_3 (5(y_{meas}^i)^3 - 3y_{meas}^i) - \\ & - y_{meas}^i \cdot (c_1 y_{meas}^i + \frac{3}{2} c_2 (y_{meas}^i)^2 + \frac{3}{2} c_3 (5(y_{meas}^i)^3 - 3y_{meas}^i)) \end{aligned} \right) \cdot \frac{3}{2} (x_{meas}^i)^2 = 0 \quad (8.61)$$

$$\vdots$$

$$\vdots$$

$$\frac{\partial F}{\partial f_3} = \sum_{i=1}^n 2 \left(\begin{aligned} & y_{nom}^i - y_{meas}^i + d_1 x_{meas}^i + \frac{3}{2} d_2 (x_{meas}^i)^2 + \frac{3}{2} d_3 (5(x_{meas}^i)^3 - 3x_{meas}^i) + \\ & + x_{meas}^i \cdot (e_1 x_{meas}^i + \frac{3}{2} e_2 (x_{meas}^i)^2 + \frac{3}{2} e_3 (5(x_{meas}^i)^3 - 3x_{meas}^i)) + \\ & + f_1 y_{meas}^i + \frac{3}{2} f_2 (y_{meas}^i)^2 + \frac{3}{2} f_3 (5(y_{meas}^i)^3 - 3y_{meas}^i) + \\ & + x_{meas}^i \cdot (c_1 y_{meas}^i + \frac{3}{2} c_2 (y_{meas}^i)^2 + \frac{3}{2} c_3 (5(y_{meas}^i)^3 - 3y_{meas}^i)) \end{aligned} \right) \cdot \frac{3}{2} (5(y_{meas}^i)^3 - 3y_{meas}^i) = 0 \quad (8.62)$$

Those equations can be first solved by equation solving for the initial solutions. The initial solutions might be far from the correct solutions as there are too many more constraints than unknown coefficients. Those initial solutions can be used as the started point for finding the nonlinear least square solutions iteratively. Extensive work has been done on the nonlinear least squares algorithms [47, 48]. Let the model for data fitting to be [48]:

$$\begin{aligned} E(y) &= f(x_1, x_2, \dots, x_m; b_1, b_2, \dots, b_k) \\ &= f(\mathbf{x}, \mathbf{b}) \end{aligned} \quad (8.63)$$

Where $x_1, x_2, \dots, x_m$ are independent variables, $b_1, b_2, \dots, b_k$ are k parameters of coefficients to be determined, $E(y)$ is the expected value of the dependent variable y . Denote the data points as:

$$(Y_i, X_{1i}, X_{2i}, \dots, X_{mi})$$

Where, $i = 1, 2, \dots, n$. The objective is to calculate the k parameters of coefficients which will minimize the squares of the residuals:

$$\min \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 = \min \|\mathbf{Y} - \hat{\mathbf{Y}}\|^2 \quad (8.64)$$

This problem can be written as an objective function which aims at optimizing coefficients of each function $Y_i - \hat{Y}_i$, denote the vector of the parameters to be optimized as $\mathbf{t}$, where $\mathbf{t} = [a_1, a_2, \dots, g_3]$ in this work. The objective function is:

$$\min F(\mathbf{t}) = \sum_{i=1}^k f_i^2(\mathbf{t}) \quad (8.65)$$

Where, $f_i(\mathbf{t})$ are functions of those to be optimized vector $\mathbf{t}$. When $f_i(\mathbf{t})$ are nonlinear functions with respect to $\mathbf{t}$, this problem is about nonlinear optimization. The solution is to use Taylor expansion to convert $f_i(\mathbf{t})$ into linear functions. As only the first order of Taylor series is linear, here approximate it by the first order:

$$\begin{aligned} \varphi_i(\mathbf{t}) &= f_i(\mathbf{t}^{(k)}) + \nabla f_i(\mathbf{t}^{(k)})^T (\mathbf{t} - \mathbf{t}^{(k)}) \\ &= \nabla f_i(\mathbf{t}^{(k)})^T \mathbf{t} - \nabla f_i(\mathbf{t}^{(k)})^T \mathbf{t}^{(k)} + f_i(\mathbf{t}^{(k)}) \end{aligned} \quad (8.66)$$

Where $\nabla f_i(\mathbf{t}^{(k)})$ is the value of the first derivative of $f_i(\mathbf{t}^{(k)})$ on vector $\mathbf{t}$ evaluated at the point $\mathbf{t}^{(k)}$.

Substituting $f_i(\mathbf{t})$ in Equation 8.66 by its Taylor Expansion approximation indicated by Equation 8.67, the approximation of $F(\mathbf{t})$ is:

$$\begin{aligned} \min \phi(\mathbf{t}) &= \sum_{i=1}^k \phi_i^2(\mathbf{t}) \\ &= \sum_{i=1}^k \left(\nabla f_i(\mathbf{t}^{(k)})^T \mathbf{t} - \nabla f_i(\mathbf{t}^{(k)})^T \mathbf{t}^{(k)} + f_i(\mathbf{t}^{(k)}) \right)^2 \end{aligned} \quad (8.67)$$

To simplify the above equation, use $\mathbf{A}_k$ to represent $\nabla f_i(\mathbf{t}^{(k)})^T$, and $\mathbf{b}$ to represent $\nabla f_i(\mathbf{t}^{(k)})^T \mathbf{t}^{(k)} - f_i(\mathbf{t}^{(k)})$. Equation 8.68 is simplified into:

$$\min \phi(\mathbf{t}) = \sum_{i=1}^k (\mathbf{A}_k - \mathbf{b})^2 \quad (8.68)$$

Where,

$$\mathbf{A}_k = \begin{bmatrix} \nabla f_1(\mathbf{t}^{(k)})^T \\ \vdots \\ \nabla f_m(\mathbf{t}^{(k)})^T \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(\mathbf{t}^{(k)})}{\partial t_1} & \frac{\partial f_1(\mathbf{t}^{(k)})}{\partial t_2} & \dots & \frac{\partial f_1(\mathbf{t}^{(k)})}{\partial t_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_m(\mathbf{t}^{(k)})}{\partial t_1} & \frac{\partial f_m(\mathbf{t}^{(k)})}{\partial t_2} & \dots & \frac{\partial f_m(\mathbf{t}^{(k)})}{\partial t_n} \end{bmatrix} \quad (8.69)$$

$$\mathbf{b} = \begin{bmatrix} \nabla f_1(\mathbf{t}^{(k)})^T \mathbf{t}^{(k)} - f_1(\mathbf{t}^{(k)}) \\ \vdots \\ \nabla f_m(\mathbf{t}^{(k)})^T \mathbf{t}^{(k)} - f_m(\mathbf{t}^{(k)}) \end{bmatrix} = \mathbf{A}_k \mathbf{t}^{(k)} - \mathbf{f}^{(k)} \quad (8.70)$$

$$\mathbf{f}^{(k)} = \begin{bmatrix} f_1(\mathbf{t}^{(k)}) \\ f_2(\mathbf{t}^{(k)}) \\ \vdots \\ f_m(\mathbf{t}^{(k)}) \end{bmatrix} \quad (8.71)$$

Therefore, it can be obtained

$$\phi(\mathbf{t}) = (\mathbf{A}_k \mathbf{t} - \mathbf{b})^T (\mathbf{A}_k \mathbf{t} - \mathbf{b}) \quad (8.72)$$

The solution of this equation is:

$$\mathbf{t}^{(k+1)} = \mathbf{t}^{(k)} - (\mathbf{A}_k^T \mathbf{A}_k)^{-1} \mathbf{A}_k^T \mathbf{f}^{(k)} \quad (8.73)$$

This solution can be simplified as:

$$\mathbf{t}^{(k+1)} = \mathbf{t}^{(k)} - \mathbf{H}_k^{-1} \nabla F(\mathbf{t}^{(k)}) \quad (8.74)$$

Where, $\mathbf{H}_k$ is the Hessian matrix.

$$\mathbf{H}_k = 2\mathbf{A}_k^T \mathbf{A}_k \quad (8.75)$$

$$\nabla F(\mathbf{t}^{(k)}) = 2\mathbf{A}_k^T \mathbf{f}^{(k)} \quad (8.76)$$

The Equation 8.75 can be solved iteratively by starting with an initial solution.

8.5 Uncertainty evaluation of the geometric error correction coefficients

A statement of measurement is complete only if it provides an estimate of the quantity concerned as well as a quantitative evaluation of the estimate's reliability, i.e., the associated uncertainty [49]. Accompany measurement results by quantitative statements about their accuracy is very important particularly when the result is part of a measurement chain tracking back to national standards or when decisions about product specifications are taken [50].

The document issued by BIPM, *Guide to the Expression of Uncertainty in Measurement* (GUM) provides a method and procedure for the evaluation and expression of measurement uncertainties [51]. This method is termed as GUM uncertainty framework in supplement 1 and supplement 2 (GUM-S1 and GUM-S2) [62, 63] and other bibliographies [49, 50]. The GUM uncertainty framework has two main limitations [51, 54]. The first limitation is lacking generality of the procedure to obtain an interval to contain the values of the measurand with a stipulated coverage probability [54]. In the GUM uncertainty framework, the way a coverage interval is constructed to contain values of the measurand with a stipulated coverage

probability is approximate [51]. The second limitation is that insufficient guidance is given for the multivariate case in which there is more than one measurand, namely, more than one output quantity [51, 54]. In order to address these limitations, Working Group 1 of the Joint Committee for Guides in Metrology (JCGM) has produced two specific guidance documents, namely GUM-S1 and GUM-S2 [62, 63], on Monte Carlo method respectively for uncertainty evaluation and extensions to any number of measurand (output quantity) [51].

In part 4.6 of Chapter 4, a general and basic introduction of GUM uncertainty framework and Monte Carlo method have been made. Further explanations of Monte Carlo method and its application on evaluation of uncertainties of the geometric error coefficients are introduced here.

MCM provides a general approach to obtain a numerical representation $\mathbf{G}$ of the distribution function $G_Y(\boldsymbol{\eta})$ for $\mathbf{Y}$. The heart of the approach is making repeated draws from the PDFs for the input variables X_i (or joint PDF for $\mathbf{X}$) and the evaluation of the output quantity. Assignment of the PDFs for the input variables will be dependent on each experiment and be explained in the part of experimental studies. The same case applies to the evaluation of the output quantity. Here explains the mathematical models and algorithms for the implementation of MCM for uncertainty evaluation. These models and algorithms are generic for all cases.

The distribution function $G_Y(\boldsymbol{\eta})$ encodes all information known about the output quantity $\mathbf{Y}$. Properties of $\mathbf{Y}$ can be approximated using $G_Y(\boldsymbol{\eta})$. The numerical representation $\mathbf{G}$, which provides a discrete representation of the distribution function $G_Y(\boldsymbol{\eta})$, constitutes the matrix of dimension $m \times M$:

$$\mathbf{G} = (\mathbf{y}_1, \dots, \mathbf{y}_M) \quad (8.77)$$

The quality of $\mathbf{G}$ depends on the number of draws made. The symbol $\mathbf{y}$ represent the output measurement results. It is determined by the input measurement results $\mathbf{x}_i$:

$$\mathbf{y} = f(\mathbf{x}_1, \dots, \mathbf{x}_N) \quad (8.78)$$

Where, f is the multivariate function, $\mathbf{x}_i$ is determined by a series of input quantities $\mathbf{X}_1, \dots, \mathbf{X}_N$:

$$\mathbf{x}_i = \int \mathbf{g}_{\mathbf{X}_1, \dots, \mathbf{X}_N}(\xi_1, \dots, \xi_N) \xi_i d_{\xi_1, \dots, \xi_N} \quad (8.79)$$

Where $\mathbf{g}_\mathbf{x}(\xi)$ is the probability density function, ξ denotes possible values that can be attributed to $\mathbf{X}$. Given the PDF $\mathbf{g}_\mathbf{y}(\boldsymbol{\eta})$, the output measurement results $\mathbf{y}$ is:

$$\mathbf{y} = \int \mathbf{g}_\mathbf{y}(\boldsymbol{\eta}) \boldsymbol{\eta} d\boldsymbol{\eta} \quad (8.80)$$

The relationship between the PDF of output measurement results and input measurement results is:

$$\mathbf{g}_\mathbf{y}(\boldsymbol{\eta}) = \int \mathbf{g}_{\mathbf{X}_1, \dots, \mathbf{X}_N}(\xi_1, \dots, \xi_N) \times \delta[\boldsymbol{\eta} - f(\xi_1, \dots, \xi_N)] d\xi_1 \dots d\xi_N \quad (8.81)$$

Where $\boldsymbol{\eta}$ denotes possible values that can be distributed to $\mathbf{Y}$, $\delta[\dots]$ denotes the Dirac delta function. The relationship between the CDF $G_\mathbf{y}(\boldsymbol{\eta})$ and PDF $\mathbf{g}_\mathbf{y}(\boldsymbol{\eta})$ is:

$$G_\mathbf{y}(\boldsymbol{\eta}) = \int_{-\infty}^{\boldsymbol{\eta}} \mathbf{g}_\mathbf{y}(\boldsymbol{\eta}') d\boldsymbol{\eta}' \quad (8.82)$$

Where, $G_\mathbf{y}(\boldsymbol{\eta})$ expresses the probability that the value of $\mathbf{Y}$ is less than or equal to $\boldsymbol{\eta}$, $\mathbf{g}_\mathbf{y}(\boldsymbol{\eta})$ is the derivative of $G_\mathbf{y}(\boldsymbol{\eta})$ with respect to $\boldsymbol{\eta}$.

Fig. 8.22 Illustration of the propagation of distributions for input quantities and the obtained output quantities [50].

The expectation of the output quantities can be obtained by its PDF $\mathbf{g}_Y(\boldsymbol{\eta})$ as:

$$E(Y_i) = \int_{-\infty}^{\infty} \eta_i g_{Y_i}(\eta_i) d\eta_i \quad (8.83)$$

The variance of the output quantities can be obtained by its PDF $\mathbf{g}_Y(\boldsymbol{\eta})$ as:

$$V(Y_i) = \int_{-\infty}^{\infty} [\eta_i - E(Y_i)]^2 g_{Y_i}(\eta_i) d\eta_i \quad (8.84)$$

The covariance of the output quantities can be obtained by its PDF $\mathbf{g}_Y(\boldsymbol{\eta})$ as:

$$\text{Cov}(Y_i, Y_j) = \text{Cov}(Y_j, Y_i) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\eta_i - E(Y_i)][\eta_j - E(Y_j)] g_{Y_i, Y_j}(\eta_i, \eta_j) d\eta_i d\eta_j \quad (8.85)$$

Where $g_{Y_i, Y_j}(\eta_i, \eta_j)$ is the joint PDF for the two random variables Y_i, Y_j .

The correlation of the output quantities can be obtained by its PDF $\mathbf{g}_Y(\boldsymbol{\eta})$ as:

$$\text{Corr}(Y_i, Y_j) = \text{Corr}(Y_j, Y_i) = \frac{\text{Cov}(Y_i, Y_j)}{\sqrt{V(Y_i)V(Y_j)}} \quad (8.86)$$

8.6 Validation of the algorithm

8.6.1 Validation of the algorithm for determination of dots' centres and distance

To validate the algorithm for dots' centres determination, a synthetic data with known cylinder centres and point cloud distributions is generated in this work. This generated data contains 35 cylinders of point cloud, distributed as 5×7 along X-axis and Y-axis, as shown in Fig. 8.22.

Fig. 8.23 Plot of the created data for algorithm validation: (a) The 3D view of the point cloud; (b) View of the vertical projection.

For each point cloud, the radius of the cylinder is $31.25 \mu\text{m}$, with a uniform distribution of $r \sim U(-0.1, 0.1) \mu\text{m}$. The values of Z-coordinate of each point follows a standard normal distribution $z \sim N(0, 1) \mu\text{m}$. The centres of each cylinder, as indicated by red asterisks in Fig. 8.22 (b), have an interval of $125 \mu\text{m}$ between each other. Their X-coordinates are $[0, 125, 250, 375, 500] \mu\text{m}$ and Y-coordinates are $[0, 125, 250, 375, 500, 625, 750] \mu\text{m}$. The generated data contains X-, Y-, and Z-coordinates' values. Those data is saved in a Matlab® file with suffix name '.dat' for processing by the algorithm to be validated.

The generated data is processed by our developed algorithm for the determinations of dots' centres. The first step is to separate the data into individual point cloud. The result of the point cloud separation is shown in Fig. 8.23, with each individuals indicated by numbers and

different colours. In this step, the algorithm not only separate the point cloud into individuals, but also give an indication of those initial centroids of each cloud.

Fig. 8.24 The separation of cylinders into individual point clouds.

After the separation, each individual point cloud is processed by our developed algorithm for fitting the circle centres. The calculated centres are exactly the same with the generated ones. Fig. 8.24 makes a plot of the calculated centres of the synthetic data generated for algorithm validation.

Fig. 8.25 Plots of the calculated centres of the generated data.

The results indicate that the algorithm developed in this work for the determination of the centres of cylinder point cloud is valid.

8.6.2 Validation of the algorithm for determination of coefficients

Here use two methods for the validation of the algorithm for coefficients' determination.

a. Method one for algorithm validation

The first method is to create a dataset containing points with intervals of 125 μm as certified positions, while make a little displacement with each point. Calculate the correction coefficients and correct the points with displacement using the algorithm defined in part 7.7.3. The points with displacement with respect to certified points represent the measured points in the experiments. Therefore, two residuals can be obtained, i.e. the residual between the certified points and the points with displacement and the residual between the certified points and the corrected points. Compare those two residuals to check whether they have become smaller.

The values of the X- and Y- coordinates of created certified points and created points with displacement from certified points are shown in Tab.8.4 and Tab.8.5.

Tab.8.4 Values of the X- and Y- coordinates of the created certified points.

y_5	(0,500)	(125,500)	(250,500)	(375,500)	(500,500)	(625,500)	(750,500)
y_4	(0,375)	(125,375)	(250,375)	(375,375)	(500,375)	(625,375)	(750,375)
y_3	(0,250)	(125,250)	(250,250)	(375,250)	(500,250)	(625,250)	(750,250)
y_2	(0,125)	(125,125)	(250,125)	(375,125)	(500,125)	(625,125)	(750,125)
y_1	(0,0)	(125,0)	(250,0)	(375,0)	(500,0)	(625,0)	(750,0)
$P_{cert}(x_i, y_i)$	x_1	x_2	x_3	x_4	x_5	x_6	x_7

Tab.8.5 Values of the X- and Y- coordinates of the created points with displacement from certified points.

y_5	(8.25,511.14)	(129.15,512.47)	(256.68,505.56)	(385.44,491.01)	(511.13,509.87)	(628.01,508.14)	(753.12,502.21)
y_4	(6.98,386.12)	(124.32,365.98)	(245.04,388.01)	(382.99,380.28)	(492.25,382.98)	(629.24,380.87)	(756.96,379.01)
y_3	(4.98,259.11)	(128.68,251.14)	(255.99,255.65)	(382.14,248.21)	(503.01,257.03)	(636.14,255.98)	(761.28,256.65)
y_2	(2.22,129.66)	(129.38,128.88)	(259.66,129.51)	(384.96,130.30)	(509.62,119.04)	(627.58,131.91)	(760.88,130.05)

y_1	(0,0)	(128.17,2.98)	(258.16,4.25)	(385.55,6.66)	(510.56,8.01)	(635.88,7.35)	(755.01,8.24)
$P_{meas}(x_i, y_i)$	x_1	x_2	x_3	x_4	x_5	x_6	x_7

The algorithm first creates the two data described above. Then make a rotation of the points with displacement to the certified points, aiming at makes the axis parallel. This comes from the methodology of this work, which requires locating the standard artefact parallel with the axis. As it is impossible to realize it manually, the coordinate axes are adjusted mathematically. After that, the 18 error coefficients are calculated by the algorithm. With those coefficients, the values of the X- and Y- coordinates of the corrected points can be obtained, which is shown in Tab.8.6. Fig. 8.22 indicates the comparison of the positions of certified, measured and corrected points. Contour of the errors between certified and measured points is manifested in Fig. 8.23, while contour of the errors between certified and measured points is shown in Fig. 8.24. It is obvious that almost all the errors are smaller after correction.

Tab.8.6 Values of the X- and Y- coordinates of the corrected points.

y_5	(-7.08,499.50)	(113.18,502.12)	(242.79,497.16)	(375.80,484.95)	(506.37,504.96)	(629.44,504.06)	(761.87,497.94)
y_4	(-1.88,376.36)	(115.28,358.29)	(235.68,381.86)	(376.30,376.75)	(488.41,381.06)	(629.90,380.24)	(762.20,378.16)
y_3	(1.51,252.97)	(123.88,246.39)	(250.79,252.43)	(377.79,246.72)	(499.93,256.72)	(634.89,256.14)	(761.71,255.87)
y_2	(2.08,127.36)	(127.12,126.41)	(256.12,127.27)	(380.72,128.31)	(504.54,116.50)	(622.18,128.88)	(754.07,124.39)
y_1	(0,0)	(125.56,0.52)	(253.28,-0.25)	(378.54,0.26)	(501.14,-0.67)	(623.29,-4.66)	(738.60,-8.09)
$P_{corr}(x_i, y_i)$	x_1	x_2	x_3	x_4	x_5	x_6	x_7

Fig. 8.26 Comparison of the positions of certified, measured and corrected points

Fig. 8.27 Contour of the errors between certified and measured points

Fig. 8.28 Contour of the errors between certified and corrected points

The error is calculated by the Euclidean distance between the certified point and its corresponding point with displacement. The same goes with the error between the certified point and the corrected point. Tab.8.7 makes a comparison of the error before correction and after correction. The difference is calculated as:

$$Diff(i) = Err_c(i) - Err_m(i) \quad (8.87)$$

Where, $Diff(i)$ is the difference between the error after correction and before correction.

When $Diff(i)$ is negative, it means the error is smaller after correction. In Tab.8.7, the negative value is highlighted by green colour, while the positive value is highlighted by red colour. $Err_c(i)$ is the Euclidean distance between the certified point and corrected point.

$Err_m(i)$ is the Euclidean distance between the certified point and the measured point. The mean residual after correction is $5.6 \mu\text{m}$ while the mean error between measured and certified point is $9.65 \mu\text{m}$. The square residual of all the 35 corrected points is $1587.99 \mu\text{m}^2$ while it is $3684.85 \mu\text{m}^2$ before correction. The errors are plotted and shown in Fig. 8.27.

Tab.8.7 The values of error of each individual points.

Point No. i	$Err_c(i)$ [μm]	$Err_m(i)$ [μm]	$Diff(i)$ [μm]	Point No. i	$Err_c(i)$ [μm]	$Err_m(i)$ [μm]	$Diff(i)$ [μm]
1	0	0	0	19	4.66	7.65	-2.99
2	2.92	4.35	-1.43	20	4.72	12.64	-7.93
3	4.87	9.20	-4.31	21	4.16	13.09	-8.94
4	6.36	12.48	-6.12	22	8.26	13.13	-4.87
5	5.55	13.25	-7.70	23	12.87	9.05	3.82
6	5.27	13.13	-7.86	24	13.52	13.92	-0.41
7	2.63	9.64	-7.01	25	3.56	9.58	-6.01
8	3.08	5.16	-2.08	26	14.17	11.12	3.04
9	2.86	5.85	-2.99	27	3.39	7.24	-3.86
10	5.36	10.66	-5.31	28	1.61	8.03	-6.43
11	4.63	11.28	-6.65	29	7.47	13.86	-6.39
12	11.90	11.32	0.59	30	3.73	13.14	-9.41
13	4.17	7.38	-3.20	31	2.88	8.69	-5.81
14	3.82	11.99	-8.17	32	15.93	13.78	2.15
15	7.19	10.38	-3.20	33	6.59	14.88	-8.28
16	0.62	3.85	-3.23	34	4.15	8.68	-4.53
17	3.99	8.23	-4.25	35	4.49	3.82	0.67
18	4.72	7.36	-2.64	-			
mean error [μm]	5.60	9.65					
Sum of Squared error [μm^2]	1587.99	3684.85

Fig. 8.29 Comparison of the error vectors between the measured and corrected points

Based on this data, another 10 data are created by varying the displacement from the certified positions. In these 10 simulations, the certified positions are all the same with those certified positions introduced above. The measured points' positions are assigned with displacements, which values are shown in Tab.8.8.

Tab.8.8 Further displacements of the measured points of the 10 simulations.

Simulation	N° 1	N° 2	N° 3	N° 4	N° 5	N° 6	N° 7	N° 8	N° 9	N° 10
X [μm]	-20	-16	-12	-8	-4	0	4	8	12	16
Y [μm]	-15	-12	-9	-6	-3	0	3	6	9	12

The 10 data are processed by this algorithm. The results of each simulation are compared and analysed. Fig. 8.25 indicates the positions of certified, measured, and corrected points of those 10 simulations. It is obvious that almost all the corrected points are closer than the measured points to the certified points.

Fig. 8.30 Comparison of the certified, measured, and corrected positions of the 10 simulations.

Tab.8.9 lists two mean residual and two squared residuals. One of the mean residual comes from the displacements of the measured points from the certified points, while the other mean residual comes from the corrected points from the certified points. The mean residual is calculated by Equation 8.79 and Equation 8.80:

$$\text{Re}s_{\text{meas}}^M = \frac{1}{n} \sum_{i=1}^n \|P_{\text{cert}}(i) - P_{\text{meas}}(i)\|_2 \quad (8.88)$$

$$\text{Re}s_{\text{corr}}^M = \frac{1}{n} \sum_{i=1}^n \|P_{\text{cert}}(i) - P_{\text{corr}}(i)\|_2 \quad (8.89)$$

Where, $\text{Re}s_{\text{meas}}^M$ and $\text{Re}s_{\text{corr}}^M$ represent the mean residual of the measured points and the mean residual of the corrected points individually, $P_{\text{cert}}(i)$ represent the position of the i_{th} point of certified positions, $P_{\text{corr}}(i)$ represent the position of the i_{th} point of corrected positions.

The two squared residuals include the squared residual of the measured points to the certified points and the squared residual of the corrected points to the certified points. The squared residual is calculated by:

$$\text{Re } s_{\text{meas}}^S = \sum_{i=1}^n (\|P_{\text{cert}}(i) - P_{\text{meas}}(i)\|_2)^2 \quad (8.90)$$

$$\text{Re } s_{\text{corr}}^S = \sum_{i=1}^n (\|P_{\text{cert}}(i) - P_{\text{corr}}(i)\|_2)^2 \quad (8.91)$$

Tab.8.9 Mean residuals and squared residuals of the measured and corrected points to the certified points.

N° Simulation	mean residuals [μm]		squared residuals [μm^2]	
	measured	corrected	measured	corrected
1	17.94	9.33	12155.65	3858.43
2	13.13	9.13	6961.49	3501.34
3	8.56	7.93	3517.33	2674.56
4	5.81	5.45	1823.17	1201.65
5	6.42	6.08	1879.01	1290.61
6	9.65	7.18	3684.85	2629.28
7	13.93	5.86	7240.69	1720.72
8	18.53	8.24	12546.53	3429.29
9	23.31	8.39	19602.37	3093.64
10	28.18	10.67	28408.21	5490.36

Fig. 8.31 Comparison of the mean residuals before correction and after correction.

Fig. 8.32 Comparison of the squared residuals before correction and after correction.

Fig. 8.26 and Fig. 8.27 plot the mean residuals and squared residuals of the 10 simulations. It can be observed that both the mean residual curve and the squared residual curve of measured points are concave in the middle and convex in the two sides. The two residuals of the corrected points are much smoother. The larger the original residuals, the more the correction can be realized.

The results of the Simulation N° 10 are shown. Fig. 8.29 compare the positions of the certified, measured, and corrected points of Simulation N° 10. Fig. 8.33 and Fig. 8.31 presents contours of the mean residual and the squared residual between certified and measured points of Simulation N° 10. Fig. 8.34 manifests the error vectors between the measured and corrected points of Simulation N° 10.

Fig. 8.35 Comparison of the positions of the certified, measured, and corrected points of Simulation N° 10.

Fig. 8.36 Contour of the mean residual between certified and measured points of Simulation N° 10.

Fig. 8.37 Contour of the mean residual between certified and corrected points of Simulation N° 10.

Fig. 8.38 Comparison of the error vectors between the measured and corrected points of Simulation N° 10.

8.7 Experimental study of the lateral calibration

The work of experimental study includes two measurements and analysis of measurement results. The experiment is the measurement of the standard artefact of dot grid targets. This experiment aims at obtaining the parameters of the coefficients of the kinematic rigid body errors.

8.7.1 Experiment 1: Determination of error coefficients using a dot pattern standard

The standard artefact of dot grid targets is introduced in the part 8.7. This artefact is measured in an environment under controlled temperature of 20 ± 1 °C, using the Leica DCM-3D Confocal Microscopy. A magnification objective of 50X was used, with a numerical aperture of 0.90. The acquisition parameter of measurement area was defined as the topography stitching measurement, with a 4×4 extended topographies, covering an area of 0.828×0.621 mm². The parameter of overlapping area is 25% and the correlation takes XYZ option. The level of resolution is 1, and the measured extended topographies contain 2496×1872 pixels.

After the measurement, the confocal system generated a file with suffix name '.dat', containing three vectors, which are values of X-, Y-, and Z-coordinates. Data of this file is imported and analysed by our developed algorithms. The raw measurement data is shown in Fig. 8.38, which forms an inclined surface as well as some outliers. This surface is rotated to be parallel with the X- and Y- coordinate plane using our developed surface rotation methods introduced in part 7.8. The rotated surface is shown in Fig. 8.39. The distribution of the values of the X-, Y-, and Z-coordinates of the surface after rotation is indicated by Fig. 8.40.

(a)

(b)

Fig. 8.39 Surface reconstruction by the raw measurement data: (a) 2D plot; (b) 3D plot.

(a)

(b)

Fig. 8.40 Surface reconstruction after rotation of the raw measured surface: (a) 2D plot; (b)) 3D plot.

Fig. 8.41 Histograms of the X-, Y-, and Z-coordinates of the rotated surface.

After rotation, the data is separated as surface plane and cylinders. The surface reconstruction of the data of cylinders is shown in Fig. 8.41. It is obvious that this data has many outliers. Those outliers are detected and deleted by the method introduced in Chapter 6. The distribution of the measurement values of the X- and Y- coordinates as well as the threshold for outlier detections are shown in Fig. 8.42 and Fig. 8.43 individually. The surface reconstruction by the data of cylinders with outliers removed is shown in Fig. 8.44.

Fig. 8.42 Surface reconstruction of the data of cylinders.

Fig. 8.43 Distribution of the X-coordinates values and the thresholds for outlier detection.

Fig. 8.44 Distribution of the Y-coordinates values and the thresholds for outlier detection.

Fig. 8.45 Surface reconstruction of the data of cylinders with outliers removed.

The separated cylinders are shown in Fig. 8.44. They are denoted by different colours and numbers.

Fig. 8.46 Separation of the cylinders.

Those individual cylinders are fitted by our introduced algorithms. Their centres are fitted and shown in Fig. 8.46, in comparison with their corresponding certified positions.

Fig. 8.47 Plot of the cylinders' centres and their corresponding certified positions.

The measured points shown in Fig. 8.46 are calibrated to the certified points using our developed mathematical models and algorithms. The results of the coefficients are indicated in Tab.8.10.

Tab.8.10 Parameters of the coefficients of the mathematical models for lateral geometric error correction.

Parameter	Value	Parameter	Value	Parameter	Value
a_1	7.38×10^{-3}	c_1	4.36×10^{-6}	e_1	6.00×10^{-6}
a_2	-1.46×10^{-6}	c_2	1.05×10^{-8}	e_2	-6.24×10^{-9}
a_3	3.19×10^{-11}	c_3	-1.20×10^{-12}	e_3	9.69×10^{-14}
b_1	1.05×10^{-3}	d_1	-7.22×10^{-3}	f_1	-2.01×10^{-2}
b_2	-1.11×10^{-5}	d_2	4.00×10^{-6}	f_2	1.25×10^{-5}
b_3	-3.15×10^{-11}	d_3	-1.01×10^{-10}	f_3	-3.10×10^{-9}

With those obtained parameters of the coefficients, the corrected points are calculated. Fig. 8.46 shows the corresponding positions of certified, measured, and corrected points. The results of the mean errors, maximum errors, sum of squared errors, and standard deviations of the errors are indicated in Tab.8.11.

Fig. 8.48 Comparison of the positions of certified, measured and corrected points.**Tab.8.11** Errors with respect to the certified positions before correction and after correction.

Data types	Mean Error [μm]	Maximum error [μm]	Sum of squared errors [μm^2]	Standard deviations of the errors [μm]
Measured points	18.295	33.058	1.337×10^4	6.971
Corrected points	3.794	8.932	628.063	1.911

The Euclidean residuals of each point are plotted by contours, as shown in Fig. 8.48, which is the Contour of the Euclidean residuals between each certified and measured points.

Fig. 8.49 Contour of the Euclidean residuals between each certified and measured points.

Fig. 8.50 Contour of the Euclidean residuals between each certified and corrected points.

Uncertainty evaluation of the geometric error coefficients based on the algorithms introduced in the part 7.9. As mentioned in 7.9, the heart of the approach is making repeated draws from the PDFs for the input variables X_i (or joint PDF for $\mathbf{X}$) and the evaluation of the output quantity. Here defines the determinations of the number of repeated draws, namely, the

number of simulation trials, the PDFs for the input variables, and the evaluation of the output quantity.

According to GUM-S2 [63] the main stages of uncertainty evaluation constitute formulation, propagation, and summarizing.

i) The first stage of formulation includes:

- a) Define the output quantity, namely, the geometric error correction coefficients $\mathbf{Cc} = (a_1, \dots, g_3)$;
- b) Determine the input quantity upon which $\mathbf{Cc}$ depends, namely, the measurement results $(\mathbf{x}, \mathbf{y})$ and their corresponded certified values $(\mathbf{P}_x, \mathbf{P}_y)$;
- c) Develop a measurement function f or measurement model relating the input and output quantities, namely, Equations 8.44 and 8.45;
- d) On the basis of available knowledge assign PDFs to the components of the input quantities. As indicated by Tab.8.3, the certified values $(\mathbf{P}_x, \mathbf{P}_y)$ follow a rectangular distribution $U(-1,1) \mu\text{m}$. As there are no more information about the sources of uncertainties for $(\mathbf{P}_x, \mathbf{P}_y)$ neither information for the measured coordinates $(\mathbf{x}, \mathbf{y})$, here does not assign more uncertainties to the input quantities, for not introducing unnecessary uncertainties.

ii) The second stage is propagation:

Propagate the PDFs for the components of input quantities through the model to obtain the (joint) PDF for the output quantity.

iii) The final step is summarizing:

Use the PDF for the output quantity to obtain the expectation of the output quantity, the uncertainty matrix, also named covariance matrix, associated with the expectation of the output quantity, and a coverage region containing the output quantity with a specified probability p (the coverage probability).

Tab.8.12 Parameters of the coefficients of the mathematical models for lateral geometric error correction.

Parameter	Mean Value	Expanded Uncertainty	95% coverage Interval	
			Lower Boundary	Upper Boundary
a_1	7.50×10^{-3}	4.74×10^{-3}	5.07×10^{-3}	1.61×10^{-2}
a_2	-2.13×10^{-6}	5.41×10^{-6}	-1.28×10^{-5}	-6.12×10^{-8}
a_3	2.00×10^{-10}	7.14×10^{-10}	-1.35×10^{-10}	1.21×10^{-9}
b_1	-5.91×10^{-6}	8.85×10^{-3}	-1.62×10^{-2}	2.99×10^{-3}
b_2	-9.91×10^{-6}	9.19×10^{-6}	-1.50×10^{-5}	2.08×10^{-6}
b_3	-6.86×10^{-12}	2.36×10^{-9}	-8.94×10^{-10}	2.67×10^{-9}
c_1	3.41×10^{-6}	7.89×10^{-6}	-6.22×10^{-6}	7.41×10^{-6}
c_2	1.26×10^{-8}	1.86×10^{-8}	2.21×10^{-10}	3.86×10^{-8}
c_3	-8.16×10^{-13}	3.44×10^{-12}	-5.74×10^{-12}	1.56×10^{-13}
d_1	-6.57×10^{-3}	4.97×10^{-3}	-8.53×10^{-3}	3.52×10^{-3}
d_2	3.93×10^{-6}	1.94×10^{-6}	1.39×10^{-6}	5.37×10^{-6}
d_3	-5.88×10^{-11}	3.78×10^{-10}	-4.59×10^{-10}	1.53×10^{-10}
e_1	5.89×10^{-6}	2.95×10^{-6}	2.00×10^{-6}	8.04×10^{-6}
e_2	-6.57×10^{-9}	6.71×10^{-9}	-1.44×10^{-8}	-4.88×10^{-11}
e_3	-2.34×10^{-15}	3.80×10^{-13}	-2.36×10^{-13}	3.30×10^{-13}
f_1	-2.21×10^{-2}	1.42×10^{-2}	-5.15×10^{-2}	-1.43×10^{-2}
f_2	1.40×10^{-5}	1.73×10^{-5}	6.71×10^{-6}	4.98×10^{-5}
f_3	-2.94×10^{-9}	2.92×10^{-9}	-5.37×10^{-9}	-1.14×10^{-11}

Fig. 8.51 Distributions of the uncertainties of some geometric error correction coefficients.

8.7.2 Experiment 2: measurement correction of the dot grid targets standard

This experiment measures the dot grid targets standard used in Part 7.11.1 Experiment 1. This standard artefact was introduced in part 7.7. It has 40401 dots as manifested in Tab.8.3. The Experiment 1 only measured 35 dots for the determination of kinematic geometric error coefficients. Here measures another area of this standard, using the same Image Confocal Microscopy, with all the environmental and operational parameters the same with that in Experiment 1. Processing the measurement data with the same procedures used in Experiment 1 until the fitted cylinder circle centres are approximated parallel with the X-axis. The fitted centres are corrected by the error coefficients determined in Experiment 1. By comparing the mean residuals, sum of squared residuals, and standard deviation of residuals of measured

points and corrected points with respect to certified positions, the effectiveness of the calculated error coefficients can be observed.

The raw measurement data with form removed is shown in Fig. 8.56. The cylinders are separated from the base with our developed algorithms. The results are demonstrated in Fig. 8.57. Fig. 8.57 (a) shows the initial separated cylinders. Fig. 8.57 (b) manifests the cylinders with outliers removed and with clusters classified. Fig. 8.58 indicates the histograms of the three coordinates of the cylinders.

Fig. 8.52 The measured surface with form removed: (a) 3D reconstruction; (b) 2D reconstruction.

Fig. 8.53 Separation of the cylinders: (a) The separated cylinders from the base; (b) Separate cylinders into individual clusters.

Fig. 8.54 Histogram of the three coordinates of the separated cylinders

The separated clusters are fitted for their centres using our developed algorithms. The results of the fitted cylinder centres are shown in Tab.8.15. Fig. 8.59 manifests the fitted cylinder centres as well as the centroids of each cluster data.

Tab. 8.13 The raw coordinate values of fitted cylinder centres.

Cluster N°	X-Coordinate $[\mu\text{m}]$	Y-Coordinate $[\mu\text{m}]$	Cluster N°	X-Coordinate $[\mu\text{m}]$	Y-Coordinate $[\mu\text{m}]$
1	47.3	42.6	19	541.8	298.1
2	172.3	42.9	20	667.7	301.3
3	294.8	44.0	21	796.8	298.4
4	425.1	49.5	22	40.2	420.6
5	544.9	48.1	23	163.3	417.8
6	669.2	46.6	24	291.1	421.0
7	796.4	48.3	25	415.9	424.6
8	42.4	166.5	26	538.9	423.9
9	167.7	171.9	27	666.1	430.0
10	292.6	172.3	28	794.6	430.3
11	419.3	172.6	29	41.2	530.7
12	544.1	175.2	30	163.3	548.3
13	666.6	174.6	31	289.5	546.6
14	797.0	176.0	32	415.0	548.2
15	40.1	295.9	33	539.9	551.7
16	163.4	294.6	34	662.6	550.7
17	293.0	294.5	35	796.9	550.8
18	417.9	295.3

Fig. 8.55 Comparison of the fitted circle centre and the centroid of the data.

As it can be observed in Fig. 8.59, the cluster numbered 29 has too many outliers. Therefore, here only choose the first 28 clusters for kinematic geometric error correction. The correction employs the mathematical model 7.45 and 7.46 as well as our calculated error coefficients determined in Experiment 1 in Part 7.11.1. Before correction, the data are rotated to be parallel with the X-coordinate as much as possible. After that, the data are corrected by the error coefficients determined in Experiment 1. Tab.8.16 manifests both the rotated measurement data and the corrected data.

Tab. 8.14 The aligned and corrected measurement data.

Cluster N°	Rotated measurement data		Corrected data by error coefficients	
	X-coordinate [μm]	Y-coordinate [μm]	X-coordinate [μm]	Y-coordinate [μm]
1	47.2	42.8	47.5	41.6
2	172.2	43.4	173.4	41.7
3	294.7	44.8	296.7	42.7
4	425.1	50.6	427.7	48.2
5	544.8	49.5	548.2	46.8
6	669.0	48.3	673.1	45.2
7	796.2	50.3	800.9	46.4
8	42.0	166.6	42.1	163.2
9	167.2	172.3	168.2	168.3
10	292.1	173.1	293.9	168.9

Cluster N°	Rotated measurement data		Corrected data by error coefficients	
	X-coordinate [μm]	Y-coordinate [μm]	X-coordinate [μm]	Y-coordinate [μm]
11	418.9	173.6	421.3	169.3
12	543.7	176.6	546.8	172.1
13	666.2	176.3	669.9	171.5
14	796.6	178.1	801.0	172.6
15	39.3	296.0	39.1	290.6
16	162.6	295.0	163.2	289.3
17	292.3	296.4	293.7	289.6
18	417.2	299.4	419.3	290.7
19	541.0	303.0	543.8	293.7
20	666.9	300.4	670.4	297.2
21	796.1	420.7	800.2	294.2
22	39.1	418.2	38.6	413.4
23	162.2	418.2	162.5	410.9
24	290.0	421.7	291.1	414.6
25	414.8	425.7	416.7	418.8
26	537.9	425.3	540.4	418.6
27	665.1	431.7	668.3	425.1
28	793.5	432.2	797.4	425.5

Both the rotated measurement data and corrected data are adjusted to a beginning of (0,0), which is realized by making every pair of coordinates minus the first pair of coordinates. The results of the measured positions and corrected positions are compared with the certified positions in Tab.8.17. Fig. 8.60 illustrates the measured, corrected, and the certified positions. The mean error, maximum error, sum of squared errors, and the standard deviations of the errors are indicated in Tab.8.18. The mean error/residual between the measured positions and the certified positions is 8.1 μm, while the mean error/residual between corrected positions and the certified positions is 5.7 μm, improved 29.6%. The maximum error between the measured positions and the certified positions is 15.6 μm, while the maximum error between corrected positions and the certified positions is 11.5 μm, reduced 26.3%. The sum of squared errors reduced from 2173.3 μm² to 1136.2 μm², which is 47.7%. It can be observed that all four types of errors are much smaller after correction with the error coefficients.

Tab. 8.15 Comparison of the certified, measured, and corrected positions.

Cluster N°	Certified position		Measured position		Corrected position	
	X- coordinate [μm]	Y- coordinate [μm]	X- coordinate [μm]	Y- coordinate [μm]	X- coordinate [μm]	Y- coordinate [μm]
1	0.0	0.0	0.0	0.0	0.0	0.0
2	125.0	0.0	125.1	0.6	125.9	0.1
3	250.0	0.0	247.6	2.0	249.2	1.1
4	375.0	0.0	377.8	7.8	380.2	6.6
5	500.0	0.0	497.7	6.7	500.7	5.2
6	625.0	0.0	621.9	5.5	625.6	3.6
7	750.0	0.0	749.1	7.5	753.4	4.9
8	0.0	125.0	-5.1	123.8	-5.4	121.6
9	125.0	125.0	120.1	129.5	120.7	126.8
10	250.0	125.0	245.0	130.3	246.4	127.3
11	375.0	125.0	371.7	130.9	373.8	127.8
12	500.0	125.0	496.5	133.8	499.3	130.5
13	625.0	125.0	619.0	133.5	622.4	129.9
14	750.0	125.0	749.4	135.2	753.5	131.0
15	0.0	250.0	-7.8	253.2	-8.4	249.0
16	125.0	250.0	115.5	252.2	115.7	247.8
17	250.0	250.0	245.1	252.5	246.2	248.0
18	375.0	250.0	370.1	253.6	371.8	249.1
19	500.0	250.0	493.9	256.6	496.3	252.2
20	625.0	250.0	619.8	260.2	622.9	255.6
21	750.0	250.0	748.9	257.7	752.7	252.6
22	0.0	375.0	-8.0	377.9	-8.9	371.8
23	125.0	375.0	115.1	375.4	115.1	369.3
24	250.0	375.0	242.9	378.9	243.7	373.0
25	375.0	375.0	367.7	382.9	369.2	377.2
26	500.0	375.0	490.7	382.5	492.9	377.0
27	625.0	375.0	617.9	388.9	620.8	383.5
28	750.0	375.0	746.4	389.5	749.9	383.9

Fig. 8.56 Comparison of the certified, measured, and corrected positions.

Tab. 8.16 Errors with respect to the certified positions before correction and after correction.

Data types	Mean Error [μm]	Maximum error [μm]	Sum of squared errors [μm^2]	Standard deviations of the errors [μm]
Measured points	8.1	15.6	2173.3	3.5
Corrected points	5.7	11.5	1136.2	2.8

Fig. 8.61 and Fig. 8.62 manifests the contour of the mean errors of the measured data and the corrected data individually. Fig. 8.63 compares the error vectors from the certified positions to the measured positions and the vectors from the certified positions to the corrected positions.

Fig. 8.57 Contour of the Euclidean residuals between each certified and measured points.

Fig. 8.58 Contour of the Euclidean residuals between each certified and corrected points.

Fig. 8.59 Comparison of the error vectors between the measured and corrected points.

According to the above results, it can be found that the errors/residuals between the corrected positions and the certified positions are much smaller than the errors/residuals between the measured positions and certified positions. This indicates that our developed algorithms and procedures for the X- and Y- coordinate calibration/correction is effective and useful.

8.8 Summary

- i. The method of using kinematic geometric errors for lateral calibrations of X- and Y- coordinates is useful and meaningful, as the experimental results shown, that the measurement quality can be improved after correction by the calculated coefficients. As shown in Experiment 2, the mean residual between certified positions and

measured positions is 8.1 μm . After correction, the mean residual between certified positions and corrected positions is 5.7 μm . All the 4 types of errors, namely the mean errors/residuals, the maximum residuals, the sum of squared residuals, and the standard deviation of the residuals, decrease obviously

- ii. The calculated coefficients seem only effective for the calibrated area of movement. Namely, if only a 4×4 extended topography, i.e. an area of $0.828\times 0.621\text{ mm}^2$, is measured for the determinations of coefficients, the obtained coefficients can only be applied for a 4×4 extended topography or a smaller one. The coordinates' correction with those calculated coefficients might not work well when the measured area is larger. This is consistent with the idea of the kinematic error correction method. The kinematic errors characterize the movement characteristics of the probes and work bases. When their movement scope changes, it is reasonable if their kinematic characteristics change, since longer movement might cause higher scales of uncertainties.
- iii. This phenomenon can also be explained from the mathematical model of the method. As indicated by formula 8.44 and 8.45, those coefficients are determined by two groups of input pairs, i.e. the measured results (x_i, y_i) and their corresponding certified values (Px_i, Py_i) . Moreover, the coefficients are approximated by the nonlinear Least Squares method. Therefore, when the quantities of inputs changes, the approximation for determination of the values of those coefficients could change accordingly.
- iv. According the above analysis, here we have a guess that both the movement scope and measurement resolutions have influences on the effectiveness of the determined coefficients. Those determined coefficients might only work well for the same size of or smaller measurement area but not for a larger measurement area. The coefficients determined by higher resolution might work well for a measurement of lower resolution, but a controversy way might does not work. Our future work will examine those guests and provide a guidance for the applications of the kinematic geometric error method for lateral calibration of the confocal instrumentation.
- v. The influence of measurement intervals on correction efficiency deserves a profound study. As shown in Fig. 8.31, when the errors between measured points and certified

points are large, the correction is obvious. When the errors between measured points and certified points are small, the correction is small. This might be the nature of the mathematical model, also possibly because of the space intervals of points is large, which is 125 μm in this work. The future work can study the influences of space intervals of points for correction on the efficiency of the calibration.

8.9 References of Chapter 8

- [1] G. Zhang, R. Ouyang, B. Lu, R. Hocken, R. Veale, A. Donmez, A Displacement Method for Machine Geometry Calibration, *Annals of the CIRP* 37 (1) (1988) 515–518.
- [2] G. Hermann, Geometric Error Correction in Coordinate Measurement, *Acta Polytechnica Hungarica* 4 (1) (2007) 47–62.
- [3] Z. Hou, Z. Wang, Y. Zhang, Position determination and measurement error analysis for the spherical proof mass with optical shadow sensing, *Acta Astronautica* 126 (2016) 215–228.
- [4] J. C. Waters, Accuracy and precision in quantitative fluorescence microscopy, *The journal of cell biology* 185 (7) (2009) 1135–1148.
- [5] H. Nouira, N. E. Hayek, X. Yuan, and N. Anwer, Characterization of the main error sources of chromatic confocal probes for dimensional measurement, *Measurement Science and Technology* 25 (044011) (2014) 14pp.
- [6] Kevin Harding (Ed.), *Handbook of Optical Dimensional Metrology*, CRC Press, Taylor & Francis Group, 2013.
- [7] T. R. Corle, G. S. Kino, *Confocal Scanning Optical Microscopy and Related Imaging Systems*, Academic Press, 1996.
- [8] H. E. Keller, Objective lenses for confocal microscopy. In: *Handbook of Biological Confocal Microscopy*, New York: Plenum Press, 1995.
- [9] D. G. Bailey, A new approach to lens distortion correction, *Proceedings Image and Vision Computing New Zealand* (2002) 59–64.
- [10] J. Wang, F. Shi, J. Zhang, Y. Liu, A new calibration model of camera lens distortion, *Pattern Recognition* 41 (2007) 607–615.

- [11] T.H. Besseling, J. Jose, and A. Van Blaadenren, Methods to calibrate and scale axial distances in confocal microscopy as a function of refractive index, *Journal of Microscopy* 257 (2) (2015) 142–150.
- [12] R. W. Cole, T. Jinadasa, C. M. Brown, Measuring and interpreting point spread functions to determine confocal microscope resolution and ensure quality control, *Nature Protocols* 6 (12) (2011) 1929–1941.
- [13] C. Wang, Current issues on 3D volumetric positioning accuracy: measurement, Compensation and Definition, *Proceedings of SPIE* (2008) 7128.
- [14] N. A. Barakat, M. A. Elbestawi, A. D. Spence, Kinematic and geometric error compensation of a coordinate measuring machine, *International Journal of Machine Tools & Manufacture* 40 (2000) 833–850.
- [15] G. Zhang, R. Veale, T. Charlton, B. Borchardt, R. Hocken, Error Compensation of Coordinate Measuring Machines, *Annals of the CIRP* 34 (1) (1985) 445–448.
- [16] H. Schwenke, W. Knapp, H. Haitjema, A. Weckenmann, R. Schmitte, F. Delbressine, Geometric error measurement and compensation of machines - An update, *CIRP Annals - Manufacturing Technology* 57 (2008) 660–675.
- [17] K. Umetsu, R. Furutani, S. Osawa, T. Takatsuji, T. Kurosawa, Geometric calibration of a coordinate measuring machine using a laser tracking system, *Measurement Science and Technology* 16 (12) (2005) 2466–2472.
- [18] Lateral scale calibration for focus variation microscopy, A. Alburayt, W. P. Syam, R. Leach, *Measurement Science and Technology*.
- [19] Richard Leach, *Optical measurement of surface topography*, Springer, 2011.
- [20] R. Leach, D. Chetwynd, L. Blunt, J. Haycocks, P. Harris, K. Jackson, S. Oldfield, S. Reilly, Recent advances in traceable nanoscale dimension and force metrology in the UK, *Measurement science and technology* 17 (2006) 467–476.
- [21] M. Ritter, T. Dziomba, A. Kranzmann, L. Koenders, A landmark-based 3D calibration strategy for SPM, *Measurement Science and Technology* 18 (2007) 404–414.

- [22] R. K. Leach, C. L. Giusca, K. Naoi, Development and characterization of a new instrument for the traceable measurement of areal surface texture, *Measurement Science and Technology* 20 (2009) 125102(8pp).
- [23] D. Semwogerere, E. R. Weeks, *Confocal Microscopy*, Taylor & Francis, 2005.
- [24] K.E. Jensen, D.A. Weitz, and F. Spaepen, Note: A three-dimensional calibration device for the confocal microscope, *Review of Scientific Instruments* 84 (2013) 016108.
- [25] R. Artigas, *Optical Measurement of Surface Topography*, Springer, Berlin, Heidelberg, 2011, Ch. Chapter 11 Imaging Confocal Microscopy, pp. 237–287.
- [26] N. S. Claxton, T. J. Fellers, M. W. Davidson, *Laser scanning confocal microscopy*, Tech. rep., Department of Optical Microscopy and Digital Imaging, Florida State University, Tallahassee (2006).
- [27] ISO 25178 - 600. Geometrical product specifications (GPS) -Surface texture: Areal-Part 600:Metrological characteristics for areal-topography measuring methods.
- [28] R. K. Leach, C. L. Giusca, H. Haitjema, C. Evans, X. Jiang, Calibration and verification of areal surface texture measuring instruments, *CIRP Annals - Manufacturing Technology* 64 (2015) 797–813.
- [29] H. Noura, N. El-Hayek, X. Yuan, N. Anwer, J. Salgado, Metrological characterization of optical confocal sensors measurements (20 and 350 travel ranges), *Journal of Physics: Conference Series* 483 (2015) 012015.
- [30] S. Sartori, G. X. Zhang, Geometric Error Measurement and Compensation of Machines, *Annals of the CIRP* 44 (2) (1995) 599–609.
- [31] W. G. Weekers, Compensation for Dynamic Errors of Coordinate Measuring Machines, Ph.D. thesis, Eindhoven University of Technology (1996).
- [32] J. Yang and Y. Ren, C. Wang, G. Liotto, Theoretical derivations of 4 body diagonal displacement errors in 4 machine configurations, *Proceedings of the LAMDAMAP Conference Cransfield, UK, June 27-30*.
- [33] K. Tong, E. A. Lehtihet, S. Joshi, Parametric error modeling and software error compensation for rapid prototyping, *Rapid Prototyping Journal* 9 (5) (2003) 301–313.

- [34] H. Wang, S. Xiang, On the convergence rates of Legendre approximation, *Mathematics of computation* 81 (278) (2012) 861–877.
- [35] E. W. Weisstein, Legendre Polynomial. From MathWorld - A Wolfram Web Resource. <http://mathworld.wolfram.com/LegendrePolynomial.html>.
- [36] J. Caja, *Técnicas Avanzadas de Metrología Dimensional Indirecta Mediante el Empleo de Maquinas de Medicion por Vision en Entornos Industriales. Modelo para la Estimacion de Incertidumbres*, phdthesis, Technical University of Madrid (2014).
- [37] J. A. Hartigan, M. A. Wong, A K-means Clustering Algorithm, *Journal of the Royal Statistial Society. Series C (Applied Statistics)* 28 (1) (1979) 100–108.
- [38] A. K. Jain, Data clustering: 50 years beyond K-means , *Pattern Recognition Letters* 31 (2010) 651–666.
- [39] S. P. Lloyd, Least Squares Quantization in PCM, *IEEE Transactions on Information Theory* IT-28 (2) (1982) 129–137.
- [40] A. Ghodsi, Dimensionality Reduction - A Short Tutorial, techreport, University of Waterloo (2006).
- [41] C. O. S. Sorzano, J. Vargas, A. P. Montano, A survey of dimensionality reduction techniques, Tech. rep., Preprint at <http://arxiv.org/abs/1403.2877> (2014).
- [42] W. Gander, G. H. Golub, R. Strebels, Least squares fitting of circles and ellipses, *Bull. Belgian Math. Soc.* 3 (1996) 63–84.
- [43] I. D. Coope, Circle fitting by linear and nonlinear least squares, *Journal of Optimization Theory and Applications* 76 (1993) 381–388.
- [44] D. Umbach, K. N. Jones, A few methods for fitting circles to data, *IEEE Transactions on Instrumentation and Measurement* 52 (6) (2003) 1881–1885.
- [45] S. J. Miller, The Method of Least Squares, in Brown University,.
- [46] E. W. Weisstein, Least Squares Fitting, From MathWorld—A Wolfram Web Resource. <http://mathworld.wolfram.com/LeastSquaresFitting.html>.
- [47] J. E. Dennis, D. M. Gay, R. E. Welsch, An adaptive nonlinear least-squares algorithm, *ACM Transactions on Mathematical Software* 7 (3) (1981) 348–368.

- [48] D. W. Marquardt, An algorithm for Least-Squares estimation of nonlinear parameters, *Journal of the Society for Industrial and Applied Mathematics* 11 (2) (1963) 431–441.
- [49] M. G. Cox, B. R. L. Siebert, The use of a Monte Carlo method for evaluating uncertainty and expanded uncertainty, *Metrologia* 43 (2006) S178–S188.
- [50] G. Wubbeler, M. Krystek, C. Elster, Evaluation of measurement uncertainty and its numerical calculation by a Monte Carlo method, *Measurement Science and Technology* 19 (4pp) (2008) 084009.
- [51] P. M. Harris, M. G. Cox, On a Monte Carlo method for measurement uncertainty evaluation and its implementation, *Metrologia* 51 (2014) S176–S182.
- [52] JCGM 101: 2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method.
- [53] JCGM 102: 2011 Evaluation of measurement data - Supplement 2 to the "Guide to the expression of uncertainty in measurement" - Extension to any number of output quantities.
- [54] W. Bich, M. G. Cox, R. Dybkaer, C. Elster, W. T. Estler, B. Hibbert, H. Imai, W. Kool, C. Michotte, L. Nielsen, L. Pendrill, S. Sidney, A. M. H. Veen, W. Woger, Revision of the 'Guide to the Expression of Uncertainty in Measurement', *Metrologia* 49 (2012) 702–705.

Chapter 9 Vertical calibration

Abstract: This chapter works on the calibration of the Z-coordinate of the confocal optical measurement system. Some factors that might influence the accuracy of the scale are studied, such as the measurement and determination of the step height, positioning inclination, repeatability, reproducibility, light source, etc.

9.1 Introduction to the vertical axial calibration of the confocal microscopy

This chapter works on the calibration of the optical confocal system on the vertical direction, i.e. the z-axis coordinate. The widely used international standard VIM [17] has given a specification on the definition of calibration: *operation that, under specified conditions, in a first step establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication*. A calibration may be expressed by a statement, calibration function, calibration diagram, calibration curve, or calibration table. In some cases, calibration may consist of an additive correction of the indication with associated uncertainty. Sometimes the first step in the definition is perceived as being calibration. Calibration hierarchy is defined as sequence of calibrations from a stated reference to the final measuring instrument or measuring system, where the outcome of each calibration depends on the outcome of the previous calibration. Also, measurement uncertainty necessarily increases along the sequence of calibrations.

The influence factors on the calibration of z coordinate include correction coefficients for raw measured heights, positioning inclinations, repeatability, reproducibility, light intensity, as

shown in Fig. 9.1. Two standard artefacts were used, i.e. a Type C1 standard and a depth-setting standard. Mathematical models, algorithm development and validation, experimental studies, etc., are all introduced in detail in the latter parts.

Fig. 9.60 Flow chart of the procedure for the calibration on z-coordinate.

9.2 Mathematical models and algorithms for determination of the calibration factors

9.2.1 Mathematical models and algorithms for calculation of the correction coefficient

As there always exist difference between the measured values and real values, correction coefficients aim at revising the raw measurement data to values as closer as possible to the real ones. Several models of fitting, from simple to complicate, are considered and compared. Those models are shown in Equations 9.1 to 9.3:

$$d_m \cdot C_c = d_c \quad (9.92)$$

$$d_m \cdot C_c + C_o = d_c \quad (9.93)$$

$$d_m^2 \cdot C_t + d_m \cdot C_c + C_o = d_c \quad (9.94)$$

Where, d_m is the groove depth calculated from measured z coordinate data, d_c is the certified values of the groove depth, C_c , C_o , C_t are constants, i.e. the correction coefficients that are pended for calculation. Equations for the fitting of several groove depths and repeated measurement results for the groove depth are:

$$\begin{bmatrix} d_{m11} \\ d_{m12} \\ \vdots \\ d_{m1k} \\ d_{m21} \\ d_{m22} \\ \vdots \\ d_{m2s} \\ d_{m31} \\ \vdots \end{bmatrix} \cdot C_c = \begin{bmatrix} d_{c11} \\ d_{c12} \\ \vdots \\ d_{c1k} \\ d_{c21} \\ d_{c22} \\ \vdots \\ d_{c2s} \\ d_{c31} \\ \vdots \end{bmatrix} \quad (9.95)$$

$$\begin{bmatrix} d_{m11} & 1 \\ d_{m12} & 1 \\ \vdots & \vdots \\ d_{m1k} & 1 \\ d_{m21} & 1 \\ d_{m22} & 1 \\ \vdots & \vdots \\ d_{m2s} & 1 \\ d_{m31} & 1 \\ \vdots & \vdots \end{bmatrix} \cdot \begin{bmatrix} C_c \\ C_o \end{bmatrix} = \begin{bmatrix} d_{c11} \\ d_{c12} \\ \vdots \\ d_{c1k} \\ d_{c21} \\ d_{c22} \\ \vdots \\ d_{c2s} \\ d_{c31} \\ \vdots \end{bmatrix} \quad (9.96)$$

$$\begin{bmatrix} (d_{m11})^2 & d_{m11} & 1 \\ (d_{m12})^2 & d_{m12} & 1 \\ \vdots & \vdots & \vdots \\ (d_{m1k})^2 & d_{m1k} & 1 \\ (d_{m21})^2 & d_{m21} & 1 \\ (d_{m22})^2 & d_{m22} & 1 \\ \vdots & \vdots & \vdots \\ (d_{m2s})^2 & d_{m2s} & 1 \\ (d_{m31})^2 & d_{m31} & 1 \\ \vdots & \vdots & \vdots \end{bmatrix} \cdot \begin{bmatrix} C_t \\ C_c \\ C_o \end{bmatrix} = \begin{bmatrix} d_{c11} \\ d_{c12} \\ \vdots \\ d_{c1k} \\ d_{c21} \\ d_{c22} \\ \vdots \\ d_{c2s} \\ d_{c31} \\ \vdots \end{bmatrix} \quad (9.97)$$

Those equations can be concluded as:

$$\mathbf{d}_m \cdot \mathbf{C} = \mathbf{d}_c \quad (9.98)$$

Solutions of the factors are:

$$\mathbf{C} = (\mathbf{d}_m^T \cdot \mathbf{d}_m)^{-1} \cdot \mathbf{d}_m^T \cdot \mathbf{d}_c \quad (9.99)$$

The obtained results of the correction coefficient $\mathbf{C}$ will be implemented for the correction of the measurement data obtained by the same confocal microscope.

9.2.2 Mathematical models and algorithms for determination of depth heights

The calculation of the depth heights of the grooves is referred to ISO 25178-70 [45] for compliance with its specifications. In part 9.5.2 of ISO 25178-70, the measurement of depth d of a PGR (Profile material measures, Groove, Rectangular) is specified. According to ISO 25178-70, the measurand is denoted as d , and it can be expressed using the Equation 9.9:

$$Z = \alpha X + \beta + h\delta \quad (9.100)$$

Where α , β and h are unknown parameters, fitted by the method of least squares to a profile equal in length to three times the width of the groove, as shown in Fig. 9.2. Only portions of

A, B, and C are used for calculation. The variable δ takes the value +1 on regions A and B, and -1 on region C. The depth of the groove d is twice the estimated value of h .

Fig. 9.61 Assessment of values for a standard artefact of type PGR. Source: ISO 25178-70-2014 [45].

This work evaluates the depth not of profiles but areas. As there is no specification of international standards on evaluation of depth measurand for areal material measures, this work develops a method for areal depth evaluations referring to the standard specifications on profile measures. The evaluation area is also three times the width of the groove as shown in Fig. 9.3. The width of the evaluation area in the base is $B/3$, where B is the groove base width described before. The width of each evaluation area in the upper surface is $2B/3$. The length is 80% of the total length of measured area in Y direction, i.e. 10% length is cut off in each bound.

Fig. 9.62 Indication of the evaluation areas for areal standard artefact.

Depth height is determined as the mean value of points to plane in the evaluated area. For example, denote the evaluated left portion as S_L , the evaluated right portion as S_R , the evaluated portion in the groove base as S_B . The depth is calculated as:

$$Depth = \left([S_p] - \text{mean}(S_t) \right) \cdot \vec{S_p} \quad (9.101)$$

Where, $S_p, S_t = C(\{S_L, S_R, S_B\}, 2)$, $[S_p]$ is the matrix of measured x, y, z values of surface

S_L, S_R , or S_B , $\vec{S_p}$ is the normal vector of the fitted plane by LS method, $\cdot$ means inner product in Euclidean geometry. The idea is to calculate the distance from point to plane, and then obtain the projected length of the distance to the normal vector of this plane.

The data file produced by the measurement instrumentation provides a set of values of coordinates x, y, z , which are the coordinates of a surface. Those coordinates can be fitted to a surface expressed as [24]:

$$ax_i + by_i + cz_i + d_i \cong 0 \quad (9.102)$$

This equation can be expressed in a matrix form as:

$$\begin{bmatrix} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots \\ x_n & y_n & z_n \end{bmatrix} \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} + \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} \cong 0 \quad (9.103)$$

To solve this equation, least squares method is used, that is to find a set values of a , b , and c , acquiring the smallest norm value of d_i comparing to other sets of values of a , b , and c .

Singular value decomposition (SVD) is used to calculate the least squares solution. SVD is an eigenvalue decomposition of Matrix which is not square. It provides a convenient way for breaking a matrix, which contains some data that is of interest, into simpler and meaningful pieces.

Consider a system of equations of the form $A \cdot x = b$. Let A be an $m \times n$ matrix, and $\text{rank}(A) = n$. There are three possibilities [4]:

- (i) If $m < n$, there are more unknowns than equations. In this case, there will not be a unique solution, but a vector space of solutions.
- (ii) If $m = n$, there is a unique solution as long as A is invertible.
- (iii) If $m > n$, there are more equations than unknowns. Normally the system will not have a solution unless by chance b lies in the span of the columns of A .

The case in this work is of case (iii). To calculate the least squares solutions is to find the set of x with objective of $\min \|Ax - b\|$, where $\|\cdot\|$ represents the vector norm. Such problems are conveniently solved using the SVD.

Make the singular value decomposition (SVD) of A can obtain:

$$A = UDV^T \quad (9.104)$$

To seek x that minimizes squares of residual is equal to:

$$\min \|Ax - b\| = \min \|UDV^T x - b\| \quad (9.105)$$

Because of the norm-preserving property of orthogonal transforms, there is:

$$\min \|UDV^T x - b\| = \min \|DV^T x - U^T b\| \quad (9.106)$$

Writing $y = V^T x$ and $b' = U^T b$, the problem becomes:

$$\min \|Dy - b'\| \quad (9.107)$$

Where D is an $m \times n$ matrix with vanishing off-diagonal entries, as following:

$$\begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \\ \hline & 0 & & \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b'_1 \\ b'_2 \\ \vdots \\ b'_n \\ b'_{n+1} \\ \vdots \\ b'_m \end{pmatrix} \quad (9.108)$$

The nearest Dy can approach to b' is the vector $(b'_1, b'_2, \dots, b'_n, 0, \dots, 0)^T$, and this is achieved by setting $y_i = b'_i / d_i$ for $i = 1, \dots, n$. As the assumption $r(A) = n$ ensures that $d_i \neq 0$. Finally, one retrieves x from:

$$x = Vy \quad (9.109)$$

The complete algorithm is:

Objective: Find the least-squares solution to the $m \times n$ set of equations $Ax = b$, where $m > n$ and $r(A) = n$.

Algorithm. Find the least-squares solution.

- (i) Find the SVD $A = UDV^T$;
- (ii) Set $b' = U^T b$;
- (iii) Find the vector y defined by $y_i = b'_i / d_i$, where d_i is the i_{th} diagonal entry of D ;
- (iv) The solution is $x = Vy$.

end

The solution of x is the set of coefficients of coordinates x , y , and z , which fit the measurement points to a plane. The normal vector of the plane is obtained using the following equation [24]:

$$\vec{n} = \frac{a\vec{i} + b\vec{j} + c\vec{k}}{\sqrt{a^2 + b^2 + c^2}} \quad (9.110)$$

The finally obtained results of the depth heights indicated in Equation 9.11 is one of the most important parameters for the mathematical model of the calibration of the vertical scales of the confocal microscopy.

9.2.3 Algorithms for evaluation of the uncertainty produced by measurement positioning inclination

Flatness deviation is defined as the deviation of the measured topography from an ideal plane. Flatness deviation can be caused by an imperfect areal reference, by optical setups in the instrument, or by the residual flatness [27].

One important feature of areal measurement instruments is the quality of their reference surface against which the measurand surfaces are measured. The vast majority of areal surface measurement instrumentations use a nominally flat surface as the areal reference and any deviation from it will render an error along the z axis measurement direction. For optical instruments, the residual flatness can be caused by optical aberrations [33].

The residual flatness test is performed on a flat surface. The parameter that describes its effect is the maximum height of the scale limited surface, S_z . The value of S_z is affected by the local height variations, such as scratches, contaminations, etc. The difficulty lies in completely separating the contribution of the instrument system from that of the flat standard and other spurious measurement data. One way to overcome this is to measure this flat at different locations without change the setup of the instrument and to average the height measurement of each point. The contribution of the flat and other spurious data should be diminished and the quality of the areal reference should be reserved. However, this method is not always effective as the measurement results are always affected by spurious data of high z axis amplitude. In order to achieve effective measurement, repeating measures, outlier removal and filtration methods have to be employed.

Fig. 9.63 Error caused by inaccurate positioning [7].

A further error is the measurement positioning deviation as shown in Fig. 9.5, caused by an inaccurate positioning of the measurand onto its measurement positions. In this figure, n_p is positioning error (mm), L_p is inclination deviation (arcsec), L_{pl} is base length of the measurand [7].

9.2.4 Algorithms for evaluation of the uncertainty produced by repeatability

Measurement repeatability is defined as measurement precision under a set of repeatability conditions of measurement [17]. Repeatability condition of measurement is condition of measurement in a set of conditions that includes the same measurement procedure, same operators, same measuring system, same operating conditions and same location, and replicate measurements on the same or similar objects over a short period of time.

9.2.5 Algorithms for evaluation of the uncertainty produced by reproducibility

Measurement reproducibility is defined as measurement precision under reproducibility conditions of measurement [17]. Reproducibility condition of measurement is condition of measurement in a set of conditions that includes different locations, operators, measuring systems, and replicate measurements on the same or similar objects.

9.2.6 Algorithms for evaluation of the uncertainty produced by light source

Since the optical confocal microscopy instrument is a Charge-Couple Device (CCD) based image sensor, information of the measurand depends greatly on the signal received by the CCD elements. The signal comes from the light reflected from the surface of the workpieces as well as light from the environment where the experiments were conducted. Fig. 9.5 illustrates the signal acquisition on the image plane. Light source casts light into the surface patch, with some angle such as θ_s . Surface patch reflects the incident light into the image sensor through a pinhole in the confocal system. In Fig. 9.5, point P represents the camera centre, which is a pinhole in the confocal system. A point in surface patch receiving illumination is defined as (x, y) , corresponding to the illuminated point $I(x, y)$ in the image plane. The definition of illuminated point on a surface patch is modelled as a hemisphere visible from the source. According to the type of light reflection, surface patch can be divided into three groups, they are lambertian, specular, and the combination of them. Fig. 9.6 (a) illustrates the interaction between surface patch and incident light. It indicates that the radiosity is depended on its radiance received from the illumination source. Radiance $L(x, xs \rightarrow x)$ is defined as amount of energy at a point travel per unit time per unit area perpendicular to the direction of the radiance per unit solid angle. The unit of radiance is $[Wm^{-2}sr^{-1}]$. Among which $[sr^{-1}]$ is the unit per steradian of the solid angle, an infinitesimal area of the incoming radiance entering the hemisphere. The intensity of illumination on the image plane is linearly depended on the radiosity and formulated as:

$$B(x, y) = \rho(x, y) \int_{\Omega} L(x, y, xs, ys \rightarrow x, y) \left(\frac{\cos \theta_s \cdot \cos \theta}{d^2} \right) \quad (9.111)$$

Where $L(x, y, xs, ys \rightarrow x, y)$ is its radiance and $\rho(x, y)$ is the albedo which is a ration of outgoing radiance to the input radiance and a dimensionless fraction which has value 0 to 1.

Fig. 9.64 Illustration of the signal acquisition from the surface to the image plane [8].

Fig. 9.65 (a) Interaction between surface and incident light, (b) Lambertian surface, (c) Specular surface [8]

Illumination (axial, ring light, and polarizer) have impact to the measurement result since they affect the incoming radiance received by the CCD sensor of the instrument. Besides, light coming from the ambient environment, for instance, room light, as well as drift of the instrument due to long measurement acquisition may have the impact on the measurement result.

9.3 Validation of the algorithms for depth determination

For the validation of the algorithm for depth calculation, the Internet Based Surface Metrology Algorithm Testing System of NIST is utilized, as shown in Fig. 9.8, and 3D Virtual SRM Database is chosen as the testing parameter standards. This testing system provides a number of data files from different creators with various ranges of parameters, as

shown in Fig. 9.7. As this testing system does not provide data for validation of depth calculation, this work creates a data based on the synthetic data provided by this system.

Fig. 9.66 The website of the Internet based surface Metrology Algorithm Teting System of NIST.

Fig. 9.67 Data files provided by the Internet Based Surface Metrology Algorithm Testing System of NIST.

Data indexed as SG_1-2 (Random + roughness + surface) is selected. The 2D and 3D surface of the original data SG_1-2 are shown in Fig. 9.8 (a) and Fig. 9.8 (b). Tab. 9.1 manifests the detailed information about SG_1-2, such as its part information, process and measurement information, spacing in x- and y- directions, filter and uncertainty information, etc. Tab. 9.2 demonstrates the nominal value, mean value, and standard uncertainty of the seven height parameters of data SG_1-2, i.e. S_a , S_q , S_{sk} , S_{ku} , S_p , S_t , and S_v .

Fig. 9.68 Surface reconstruction of the synthetic data SG_1-2: (a) 2D surface; (b) 3D surface.

Tab. 9.17 Information of the synthetic data SG_1-2.

Part Information	
Part Name:	SG_1-2
Created by:	Dr. M. Uchida-Dept. of Mechanical Engineering, Iwate University, Japan
Description:	Random roughness surface
Process Information	
Process Name:	Numerically Generated Process
Measurement Information	
Instrument type:	N/A

Data file	
File Name:	SG_1-2.sdf
Units:	μm
Number Points:	256
Number of Profiles:	256
Spacing X-direction:	1 μm
Spacing Y-direction:	1 μm
Data type:	3D
Filter Information	
Filter type:	N/A
Method:	N/A
Cutoff:	0 mm
Additional Information:	Raw Data
Uncertainty Information	
Assume that Z co-ordinates have standard uncertainty of 10.0 nm (1% of S_q);	
X co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
Y co-ordinates have standard uncertainty of 20.0 nm (2% of sampling interval);	
measurement errors on Z, X, and Y co-ordinates are Gaussian distribution and independent.	
Level of Confidence = 95 %	

Tab. 9.18 Areal height parameters of data SG_1-2.

Label	Nominal Value	Mean Value	Standard Uncertainty
S_a	0.80376 μm	0.8038 μm	0.077 nm
S_q	1 μm	1.00005 μm	0.077 nm
S_{sk}	0.19232	0.19231	0.00037
S_{ku}	2.91199	2.912	0.00062
S_t	6.60403 μm	6.60477 μm	26.79 nm
S_p	3.58892 μm	3.58905 μm	17.86 nm
S_v	3.0151 μm	3.0145 μm	18.01 nm

Based on the data SG_1-2, a new data file of step height 10 μm is created in the software MATLAB®. Algorithm for the creation of the new data set is:

Objective: Create a data with step height of 10 μm based on the synthetic data SG_1-2.

Algorithm.

- (i) Read the synthetic data SG_1-2, allocating data into coordinates x , y , z ;
- (ii) Generate two data in z coordinate, with difference of 10 from the original data z ,

i.e. $z_1 = z - 10$, $z_2 = z - 10$;

(iii) Combine data z_1 , z , z_2 in one surface;

(iv) Save the new coordinates values in x-, y- and z- axis.

end

The created data is manifested in Fig. 9.11. It is a combination of the data SG_1-2 but with a step of 10 μm in z-axis direction. Fig. 9.12 shows the distributions of the values in x- and y-direction. As it can be seen, the distributions of values in z-axis direction follow two Gaussian distributions. The difference between the mean values of these two distributions is 10 μm .

Fig. 9.69 Reconstruction of the created data with step height of 10 μm .

Fig. 9.70 Distributions of the coordinates values of the created data: (a) x-axis direction; (b) z-axis direction.

For the validation of the algorithm developed in this work for step height evaluation, this data is loaded and processed. Value of the calculated step height is indicated in Tab. 9.3, which is 9.985 μm . Comparing to the nominal value 10 μm , the algebraic difference, i.e. $Step_calculated - Step_nominal$, is -0.015 μm . The difference in percentage, i.e. $(Step_calculated - Step_nominal) / Step_nominal * 100$, is -0.15. Distribution of the calculated heights from points to the corresponding plane is manifested in Fig. 9.13. The difference between the calculated step height and the nominal height is negligible, which demonstrates that the algorithm developed by this work for step height evaluation is favourable.

Tab. 9.19 Results of processing the created data in our developed algorithm for step calculation.

Nominal Step [μm]	Calculated Step [μm]	Difference [μm]	Difference in percentage [%]	Standard deviation
10	9.985	-0.015	-0.15	2.4213

Fig. 9.71 Histogram of the distribution of the calculated step height of the created data.

9.4 Mathematical model for axial scale calibrations of Z coordinate

Accurate measurement in scales is important for 3D confocal microscopy, as which counts for quantitative analysis, volume visualization and image restoration [50]. However, axis distances may be distorted due to both the point spread function (PSF) and the mismatch of the refractive index between the sample and the immersion liquid [10]. In the case of our experimental studies, the immersion liquid is air. Errors might happen due to thermal expansions of some exponents within the frame of the instrumentation. Also, errors could arise from the changes in refractive index of air because of the changes in ambient conditions.

Intensive researches have been carried out on calibrations of areal surface topography measuring instruments. Some of the researches on calibrations of scales studied the metrological characteristics of instruments. These metrological characteristics generally involve measurement noise, flatness deviation, linearity errors, amplification coefficient, perpendicularity of the axes and resolution of the measurements along the axis of operation [46]. ISO 25178-602: 2010 [47] have a detailed specification on the metrological characteristics. Recently, quite a few of work has been done in the scope of determination of metrological characteristics for calibration of measurement instrumentation. As an example, C. L. Giusca, *et al* proposed methods for determining the measurement noise and residual

flatness[13] of areal surface topography measurement instruments, methods for determining the amplification coefficient, linearity and squareness of the axes of areal surface topography measuring instruments [14], and a method for determining the lateral resolution of areal topography measuring instruments. A multitude of researches on studying metrological characteristics for instrumentation calibrations can be found [15, 16]. Besides these, some investigators studied the correction and calibration of the image systems of confocal microscopy [17, 18].

This chapter investigates the Z-axis scale calibration, proposing a mathematical model as indicated by Equation 9.21

$$Z_c = Z_b \cdot C_c + \delta_{lt} + \delta_{inc} + \delta_r + \delta_{rpt} + \delta_{rpd} \quad (9.112)$$

Where, Z_c is the corrected measured height in z coordinate, Z_b is the raw data in z coordinate measured by instrumentations, C_c is the correction coefficient of the z coordinate measurements, δ_{lt} is the uncertainty source of light, δ_{inc} is the uncertainty generated by inclination of the base of the equipment, δ_r is the uncertainty related with the resolution in z coordinate, δ_{rpt} is the uncertainty related with measurement repeatability, δ_{rpd} is the uncertainty generated by measurement reproducibility.

9.5 Experiments and calibrations on z-axis coordinate

9.5.1 Experiments and calculation of step heights

To obtain the correction coefficients of the measurement in z coordinate, one depth-setting standard artefact is used, as shown in Fig. 9.13. The measured point height values are processed in the algorithms for the calculation of correction coefficients. Fig. 9.14 indicates the general information of this standard. This standard consists of 6 grooves, denoted as R1 to R6, with groove depths about 0.24 μm , 0.75 μm , 2.4 μm , 7.5 μm , 24 μm , 75 μm .

Fig. 9.72 Photograph of the depth-setting standard

Fig. 9.73 General information of the depth-setting standard

The depth-setting standard artefact is measured using the Leica DCM-3D Confocal Microscopy at the Metrology Laboratory of the Technical University of Madrid. A magnification objective of L-20X was used, with a numerical aperture of 0.50. The experiments were conducted under a controlled environment, ensuring thermal stability in the range of $20 \pm 1^\circ\text{C}$. This condition is applied to all the experiments carried out by this work. Each groove was measured 5 times under the reproducibility condition. The measurement data file produced by the confocal microscopy for all those measurements are imported into Matlab and processed by our developed and validated algorithms for step height evaluations. The calculated step heights of the grooves of the depth-setting standard are shown in Tab. 9.4. Distribution of the 5 processed heights for grooves 1, 2, and 3 are shown in Fig. 9.14.

Tab. 9.20 Groove depths of the depth-setting standard processed by our developed algorithms.

Groove No.	Processed values of depth [μm]				
	Expt. 1	Expt. 2	Expt. 3	Expt. 4	Expt. 5
1	74.741	74.810	74.914	75.227	75.180
2	24.385	24.454	23.805	24.036	24.306
3	7.555	7.647	7.555	7.446	7.529

Fig. 9.74 Distribution of the processed results of groove depths of the depth-setting standard.

9.5.2 Calculation of correction coefficients

The calibrated groove depths of this standard are demonstrated in Tab. 9.5. Mean step height of Groove 1 is $75.470 \mu\text{m}$, with uncertainty of $0.120 \mu\text{m}$. Groove 2 has a mean height of depth of $24.060 \mu\text{m}$, with uncertainty of $0.040 \mu\text{m}$. The mean step height of Groove 3, 4, 5, 6, are $7.513 \mu\text{m}$, $2.416 \mu\text{m}$, $0.751 \mu\text{m}$, $0.245 \mu\text{m}$, sharing the same uncertainty of $0.032 \mu\text{m}$. These values are also demonstrated in Fig. 9.14.

Tab. 9.21 Certified values of groove depth of the depth-setting standard.

Groove No.	Depth [μm]	Uncertainty [μm] k???
1	75.470	0.120
2	24.060	0.040
3	7.513	0.032

4	2.416	0.032
5	0.751	0.032
6	0.245	0.032

Fig. 9.75 Certified values of the groove depths of the depth-setting standard.

The correction coefficients aim to fit the processed values as closer as possible to the certified values. For equation 9.2, the correction coefficient C_c is 1.0053, as shown in equation 9.22, error between the certified and the fitted values is calculated according to equation 9.23. For the fitting of the equation 9.22, the error is 0.2506. Fig. 9.16 manifests Comparison of the corrected and certified values of step heights of the depth-setting standard.

$$\begin{bmatrix} d_{m1} \\ d_{m2} \\ \vdots \\ d_{mn} \end{bmatrix} \cdot 1.0053 \cong \begin{bmatrix} d_{c1} \\ d_{c2} \\ \vdots \\ d_{cn} \end{bmatrix} \quad (9.113)$$

$$e = \sqrt{\frac{\sum (d_m - d_c)^2}{m - n}} \quad (9.114)$$

Where e represents the error, d_m is the calculated step height based on the measured data files, d_c is the certified step heights, m is the number of processed step heights, n is the number of parameters, such as C_c , C_o , C_t .

Fig. 9.76 Comparison of the corrected and certified values of step heights of the depth-setting standard.

For equation 9.3, the correction coefficient C_c is 1.0089, C_o is -0.2077, as shown in equation 9.24, error between the certified and the fitted values is 0.1893. Fig. 9.17 manifests the comparison of the corrected and certified values of step heights of the depth-setting standard.

$$\begin{bmatrix} d_{m1} \\ d_{m2} \\ \vdots \\ d_{mn} \end{bmatrix} \cdot \begin{bmatrix} 1.0089 \\ -0.2077 \end{bmatrix} \cong \begin{bmatrix} d_{c1} \\ d_{c2} \\ \vdots \\ d_{cn} \end{bmatrix} \quad (9.115)$$

Fig. 9.77 Comparison of the corrected and certified values of step heights of the depth-setting standard.

For equation 9.4, the correction coefficients C_i is 0.0003, C_c is 0.9849, C_o is 0.0658, as shown in equation 9.25, error between the certified and the fitted values is 0.1483. Fig. 9.18 manifests the comparison of the corrected and certified values of step heights of the depth-setting standard.

$$\begin{bmatrix} d_{m1}^2 & d_{m1} & 1 \\ d_{m2}^2 & d_{m2} & 1 \\ \vdots & \vdots & \vdots \\ d_{mn}^2 & d_{mn} & 1 \end{bmatrix} \cdot \begin{bmatrix} 0.0003 \\ 0.9849 \\ 0.0658 \end{bmatrix} \cong \begin{bmatrix} d_{c1} \\ d_{c2} \\ \vdots \\ d_{cn} \end{bmatrix} \quad (9.116)$$

Fig. 9.78 Comparison of the corrected and certified values of step heights of the depth-setting standard.

9.5.3 Experimental study of the uncertainty contributed by positioning inclination

A Type C1 spacing standard with grooves having a sine wave profile, as shown in Fig. 9.19, with a certified value of S_a equal to $1.003 \mu\text{m}$ and expanded uncertainty of $0.03 \mu\text{m}$ ($k = 2$), was measured using the Leica DCM-3D Confocal Microscopy at the Metrology Laboratory of the Technical University of Madrid. A magnification objective of L-20X was used, with a numerical aperture of 0.50. The measurement was performed under a controlled temperature at $20 \pm 1^\circ\text{C}$. The standard was placed on a base as shown in Fig. 9.20, which is used for the adjustment of plane angles. Four measurements were carried out with different surface inclination. Every two planes of those 4 measured surfaces are compared by points. For 4 surfaces, there are 6 combinations of surface pairs, i.e. z_1 and z_2 , z_2 and z_3 , z_1 and z_3 , z_1 and z_4 , z_2 and z_4 , z_3 and z_4 . Those 4 measured surfaces are shown in Fig. 9.21. The mean value of the height difference is 0, and the standard deviation of the difference is 1.2149. The distribution of the difference is manifested in Fig. 9.22.

$$\mathbf{D}_p = \left\{ \begin{array}{cccccccc} z_{i11} & z_{i12} & \cdots & z_{i1n} & z_{j11} & z_{j12} & \cdots & z_{j1n} \\ z_{i21} & z_{i22} & \cdots & z_{i2n} & z_{j21} & z_{j22} & \cdots & z_{j2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ z_{im1} & z_{im2} & \cdots & z_{imn} & z_{jm1} & z_{jm2} & \cdots & z_{jmn} \end{array} \right\} \quad (9.117)$$

$z_i, z_j = z_1, z_2, z_3, z_4$

Fig. 9.79. Photograph of the Type C1 spacing standard.

Fig. 9.80 Photograph of the base for inclination.

Fig. 9.81 Reconstruction of the 4 inclined Surface.

Fig. 9.82 Distribution of the measured height difference due to inclination.

9.5.4 Experimental study of the uncertainty contributed by measurement repeatability

The same standard used in Part 9.3.3 was measured for the study of the repeatability of the confocal system. The experiments were conducted at the same laboratory, used the same measurement instrumentation, under the same conditions of environment. The difference between the experiments in this part and that in the previous part is that the objective of this study is the investigation of the measurement repeatability. Hence, the measurement of the standard artefact was carried out under the repeatability condition. These experiments were performed under the same measurement procedure, by the same operator, using the same measuring system, under the same operating conditions and at the same location. Four replicate measurements on the same location of this artefact over a short period of time. Every two planes of those 4 measured surfaces are compared by points. For 4 surfaces, there are 6 combinations of surface pairs, i.e. z1 and z2, z2 and z3, z1 and z3, z1 and z4, z2 and z4, z3 and z4. Those 4 measured surfaces are shown in Fig. 9.23. The mean value of the height

difference is 0, and the standard deviation of the difference is 0.0354. The distribution of the difference is manifested in Fig. 9.24.

Fig. 9.83 Reconstruction of the 4 surfaces measured under repeatability conditions.

Fig. 9.84 Distribution of the measured height difference due to repeatability.

9.5.5 Experimental study of the uncertainty contributed by measurement reproducibility

The same standard used in Part 9.3.3 was measured for the study of the reproducibility of the confocal system. The experiments were conducted at the same laboratory, used the same measurement instrumentation, under the same conditions of environment. The difference between the experiments in this part and that in the previous part is that the objective of this study is the investigation of the measurement reproducibility. Hence, the measurement of the standard artefact was carried out under the reproducibility condition. The reproducibility condition of this study was long period for replicate measurements on the same standard artefact, other conditions such as locations, operators, measuring systems are all the same. Four replicate measurements on the same location of this artefact over a long period of time. Every two planes of those 4 measured surfaces are compared by points. For 4 surfaces, there are 6 combinations of surface pairs, i.e. z_1 and z_2 , z_2 and z_3 , z_1 and z_3 , z_1 and z_4 , z_2 and z_4 , z_3 and z_4 . Those 4 measured surfaces are shown in Fig. 9.25. The mean value of the height difference is 0, and the standard deviation of the difference is 0.0354. The distribution of the difference is manifested in Fig. 9.24.

Fig. 9.85 Reconstruction of the 4 surfaces measured under reproducibility conditions.

Fig. 9.86 Distribution of the measured height difference due to reproducibility.

9.5.6 Experimental study of the uncertainty contributed by illumination

The same standard used in Part 9.3.3 was measured for the study of the influence of illumination on measurements. The experiments were conducted at the same laboratory, used the same measurement instrumentation, under the same conditions of environment. The difference between the experiments in this part and that in the previous parts is that the objective of this study is the investigation of the influence of the intensity of light. Therefore, the measurement of the standard artefact was carried out using different intensities of light. Four replicate measurements on the same standard with different light intensities were performed during a short period of time. Among the four experiments, all the other measurement conditions were the same only except using four different light intensities. The light intensities were 138, 148, 158, 168, which can be controlled on the interface of the software of the confocal system. Every two planes of those 4 measured surfaces are compared by points. For 4 surfaces, there are 6 combinations of surface pairs, i.e. z_1 and z_2 , z_2 and z_3 ,

z_1 and z_3 , z_1 and z_4 , z_2 and z_4 , z_3 and z_4 . Those 4 measured surfaces are shown in Fig. 9.27. The mean value of the height difference is 0, and the standard deviation of the difference is 0.2700. The distribution of the difference is manifested in Fig. 9.28.

Fig. 9.87 Reconstruction of the 4 surfaces measured under different illumination conditions.

Fig. 9.88 Distribution of the measured height difference due to reproducibility.

9.6 Conclusions

This chapter studied the calibration of the vertical scales of the confocal microscopy. Some factors that will influence on the calibration have been studied, i.e. step height measurement, positioning inclination, repeatability, reproducibility, light, etc. Mathematical models and algorithms for each factor have been developed and validated. Experimental studies of those influence factors have been carried out.

9.7 References of Chapter 9

- [1] International Vocabulary of Metrology - Basic and General Concepts and Associated Terms (VIM).
- [2] ISO 25178 - 70: 2014 (en). Geometrical product specification (GPS) - Surface texture: Areal - Part 70: Material measures.
- [3] R. D' Amato, J. Caja, P. Maresca, E. G 贸 mez, Use of coordinate measuring machine to measure angles by geometric characterization of perpendicular planes. Estimating uncertainty, *Measurement* 47 (2014) 598 – 606.
- [4] R. Hartley, A. Zisserman, *Multiple view Geometry in computer vision* Second Edition, Cambridge University Press, New York, 2003.
- [5] ISO 25178 - 600. Geometrical product specifications (GPS) -Surface texture: Areal-Part 600:Metrological characteristics for areal-topography measuring methods.
- [6] Richard Leach, *Optical measurement of surface topography*, Springer, 2011.
- [7] A. Gusel, B. Acko, V. Mudronja, Measurement uncertainty in calibration of measurement surface plates flatness, *Journal of mechanical engineering* 55 (5).
- [8] Wahyudin Permana Syam, *Uncertainty evaluation and performance verification of a 3D Geometric Focus-variation measurement*, Ph.D. thesis, Polytechnic University of Milan (2014).
- [9] T.H. Besseling, J. Jose, and A. Van Blaadenren, Methods to calibrate and scale axial distances in confocal microscopy as a function of refractive index, *Journal of Microscopy* 257 (2) (2015) 142–150.
- [10] J. Haycocks, K. Jackson, Traceable calibration of transfer standards for scanning probe microscopy, *Precision Engineering* 29 (2) (2005) 168 – 175.
- [11] C. L Giusca, and R. K Leach, *Measurement Good Practice Guide No.128: Calibration of the Metrological Characteristics of Imaging Confocal Microscopes (ICMs)*, 2012.
- [12] ISO 25178 - 602: 2010 (en). Geometrical product specifications (GPS) -Surface texture: Areal-Part 602: Nominal characteristics of non-contact (confocal chromatic probe) instruments.

- [13] C. L. Giusca, R. Leach, F. Helary, T. Gutauskas, L. Nimishakavi, Calibration of the scales of areal surface topography-measuring instruments: part 1. Measurement noise and residual flatness, *Measurement Science and Technology* 23 (3) (2012) 035008.
- [14] C. L. Giusca, R. Leach, F. Helary, Calibration of the scales of areal surface topography measuring instruments: part 2. Amplification, linearity and squareness, *Measurement Science and Technology* 23 (6) (2012) 065005.
- [15] T. Yoshizawa (Ed.), *Handbook of Optical Metrology: Principles and Applications*, 2nd Edition, CRC Press, 2015.
- [16] R. K. Leach, C. L. Giusca, Determination of the metrological characteristics of optical surface topography measuring instruments, *Proceedings SPIE 8430, Optical Micro- and Nanometrology IV* 84300Q.
- [17] J. M. Zwier, L. Oomen, L. Brocks, K. Jalink, G. J. Brakenhoff, Quantitative image correction and calibration for confocal fluorescence microscopy using thin reference layers and SIPchart-based calibration procedures, *Journal of Microscopy* 231 (1) (2007) 59–69.
- [18] I. Kweon, J. Kim, P. Gurdjos, Euclidean Structure from Confocal Conics: Theory and Application to Camera Calibration, in: *IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR'06)*, New York, NY, 2006, pp. 1214–1221.

Chapter 10 Conclusions

Abstract: This chapter makes a conclusion of the work by this thesis.

The researches carried out in this thesis include the study of the roughness parameterizations and filtrations of areal surfaces, study and comparison of the statistical methods for outlier identification of measured surfaces, proposal of a new method for outlier identification, calibrations of the X- and Y- scales of confocal microscopy system, and calibrations of the the Z-scale of confocal microscopy system.

The first research, study of the roughness parameterizations and filtrations, mainly includes three parts: development of the original algorithms for 3D roughness parameterization, development of the Gaussian filter algorithms for surface filtration, and the validation of those two parts of algorithms with the data provided by the Testing System of NIST.

The second research, study and comparison of the statistical methods for outlier identification of measured surfaces, studied the statistical methods for outlier identification and applied those methods for surface measurement data. Ten statistical methods for outlier identification which could be implemented in the area of surface metrology were analysed and compared. Twenty-four Mat files were created based on two standard data sets provided by the National Institute of Standards and Technology for experimental study of those statistical methods. Based on processing the same series of contaminated data sets, the number of missed outliers, the difference of the height parameters, and the elapsed time by each method are compared. Algorithm efficiency, robustness, breakdown point, limitations, advantages, etc. are compared and analysed. Two of those ten methods were combined to know their potential. A type C1 spacing standard artefact was measured by 3D image confocal microscopy, and the data was processed by those algorithms.

The third research, proposal of a new method for outlier identification, proposed a new statistical method for outlier identification for surface measurement data obtained by confocal microscopy. The implemented statistical method was Confidence Distance Matrix (CDM). This work introduced and simplified the mathematical model of CDM method. Algorithms for identifying random outliers using Monte Carlo method for uncertainty evaluation and for

identifying outliers in a unique measured surface were developed and validated. Two experiments are carried out, respectively on a Type C1 spacing standard and on a steel surface.

The forth research, calibrations of the X- and Y- scales of confocal microscopy system, presented a method for characterizing and correcting the geometric errors of the movement of the lateral stage of Imaging Confocal Microscope in extended topography measurement. For extended topography measurements, inaccuracies due to linear displacement, vertical and horizontal straightness errors, angular errors, and squareness errors based on the assumption of the rigid body kinematics were described. A mathematical model for the scale calibration of the X- and Y- coordinates was derived according to the system kinematics, the axis chain vector of confocal microscope, and the geometric error functions and their approximations by Legendre polynomials. The correction coefficients of the kinematic modelling were determined by the measured and certified data of a dot grid target standard artefact. Algorithms for data partitions, fittings of cylinder centres, and determinations of coefficients were developed and validated. Form removal, K-means clustering, linear and non-linear Least Squares were implemented.

The fifth research, calibrations of the the Z-scale of confocal microscopy system, proposed methods for the calibration of the Z-coordinate of the confocal system. Factors that might have influences on the accuracy of Z- scales were studied, such as the measurement and determination of the step height, positioning inclinations, repeatability, reproducibility, light. Mathematical models and algorithms of each factor were developed and validated.

References

Standards

- [1] Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement (GUM).
- [2] International Vocabulary of Metrology - Basic and General Concepts and Associated Terms (VIM).
- [3] *Internet Based Surface Metrology Algorithm Testing System.*
<https://physics.nist.gov/3DVSC/jsp/Database3D.jsp?state=0>. 7th Feb 2018.
- [4] ISO 11562: 1996 Geometrical product specifications (GPS) - Surface texture: Profile method - Metrological characteristics of phase correct filters.
- [5] ISO 13565-1:1996. Geometrical Product Specifications (GPS) – Surface texture: Profile method; Surfaces having stratified functional properties – Part 1: Filtering and general measurement conditions.
- [6] ISO 14406:2010 Geometrical product specifications (GPS) - Extraction.
- [7] ISO 16269-4: Statistical interpretation of data - Part 4: Detection and treatment of outliers.
- [8] ISO 16610-1:2015. Geometrical product specifications (GPS) – Filtration – Part 1: Overview and basic concepts.
- [9] ISO 16610-21: 2012 Geometrical product specifications (GPS) - Filtration - Part 21: Linear profile filters: Gaussian filters.
- [10] ISO 16610-22:2015. Geometrical product specifications (GPS) – Filtration – Part 22: Linear profile filters: Spline filters.
- [11] ISO 16610-28: 2015 Geometrical product specifications (GPS) - Filtration - Part 28: Profile filters: End effects.
- [12] ISO 16610-29:2015 Geometrical product specifications (GPS) - Filtration - Part 29: Linear profile filters: Spline wavelets.
- [13] ISO 16610-30: 2015(en). Geometrical product specifications (GPS)-Filtration-Part 30: Robust profile filters: Basic concepts.

- [14] ISO 16610-31:2015 Geometrical product specifications (GPS) - Filtration - Part 31: Robust profile filters: Gaussian regression filters.
- [15] ISO 16610-32: 2015 Geometrical product specifications (GPS) - Filtration - Part 32: Robust profile filters: Spline filters.
- [16] ISO 16610-41: 2015 Geometrical product specifications (GPS) - Filtration - Part 41: Morphological profile filters: Disk and horizontal line - segment filters.
- [17] ISO 16610-49: 2015 Geometrical product specifications (GPS) - Filtration - Part 49: Morphological profile filters: Scale space techniques.
- [18] ISO 16610-60: 2015. Geometrical Product Specimen (GPS) - Filtration - Part 60: Linear areal filters: Basic concepts.
- [19] ISO 16610-61: 2015 Geometrical product specifications (GPS) - Filtration - Part 61: Linear areal filters: Gaussian filters.
- [20] ISO 16610-71: 2015 Geometrical product specifications (GPS) - Filtration - Part 71: Robust areal filters: Gaussian regression filters.
- [21] ISO 16610-85: 2015 Geometrical product specifications (GPS) - Filtration - Part 85: Morphological areal filters: Segmentation.
- [22] ISO 25178 - 1: 2016 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 1: Indication of surface texture.
- [23] ISO 25178 - 600: Geometrical product specifications (GPS) -Surface texture: Areal-Part 600:Metrological characteristics for areal-topography measuring methods.
- [24] ISO 25178 - 602: 2010 (en). Geometrical product specifications (GPS) -Surface texture: Areal-Part 602: Nominal characteristics of non-contact (confocal chromatic probe) instruments.
- [25] ISO 25178 - 70: 2014 (en). Geometrical product specification (GPS) - Surface texture: Areal - Part 70: Material measures.
- [26] ISO 25178-2: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 2: Terms, definitions and surface texture parameters.
- [27] ISO 25178-3: 2012 (en). Geometrical product specifications (GPS) - Surface texture: Areal - Part 3: Specification operators.
- [28] ISO 4287: 1998 Geometrical product specification (GPS) - Surface texture: Profile method - Terms, definitions and surface texture parameter.
- [29] ISO 468:1982 Surface roughness – Parameters, their values and general rules for specifying requirements.

- [30] ISO/TR 13587:2012 (en) Three statistical approaches for the assessment and interpretation of measurement uncertainty.
- [31] JCGM 101: 2008 Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method.
- [32] JCGM 102: 2011 Evaluation of measurement data - Supplement 2 to the "Guide to the expression of uncertainty in measurement" - Extension to any number of output quantities.
- [33] JCGM 104: 2009 Evaluation of measurement data - An introduction to the "Guide to the expression of uncertainty in measurement" and related documents.

Journals, conferences, books

- [34] R. K. Leach, C. L. Giusca, *Determination of the metrological characteristics of optical surface topography measuring instruments, Proceedings SPIE 8430, Optical Micro- and Nanometrology IV 84300Q*, 2012.
- [35] J. M. Zwier, L. Oomen, L. Brocks, K. Jalink, G. J. Brakenhoff. Quantitative image correction and calibration for confocal fluorescence microscopy using thin reference layers and SIPchart-based calibration procedures. *Journal of Microscopy*, 231(1):59–69, 2007.
- [36] A. Basu, H. Shioya, C. Park. *Statistical Inference: The Minimum Distance Approach*. New York: Chapman and Hall/CRC., 2011.
- [37] A. Bhattacharyya. On a measure of divergence between two statistical populations defined by their probability distributions. *Bulletin of the Calcutta Mathematical Society*, 35:99–109, 1943.
- [38] A. Ghodsi. Dimensionality Reduction - A Short Tutorial. techreport, University of Waterloo , 2006.
- [39] A. Godi, A. Kuhle, and L. D. Chiffre. A new procedure for characterizing textured surfaces with a deterministic pattern of valley features. *Measurement Science and Technology*, 24(8):085009, 2013.
- [40] A. Gusel, B. Acko, V. Mudronja. Measurement uncertainty in calibration of measurement surface plates flatness. *Journal of mechanical engineering*, 55(5), 2009.
- [41] A. K. Jain. Data clustering: 50 years beyond K-means . *Pattern Recognition Letters*, 31:651–666, 2010.
- [42] A. Murugarajan, G.L. Samuel. Measurement, modeling and evaluation of surface parameter using capacitive-sensor-based measurement system. *Metrology and measurement systems*, 3:403–418, 2011.
- [43] A. Nurunnabi, G. West, D. Belton. Outlier detection and robust normal-curvature estimation in mobile laser scanning 3D point cloud data. *Pattern Recognition*, 48(4):1404 – 1419, 2015.

- [44] A. S. Soy, C. Ohrstrom. Investigation and Evaluation of Methods for Measuring Surface Texture on Worktops and Kitchen Fronts. mathesis, Lund University, 2013.
- [45] A. Srivania, M. A. Xaviorb. Investigation of Surface Texture Using Image Processing Techniques. *12th Global Congress on Manufacturing and Management, GCMM*, 2014.
- [46] Robert Andersen. *Modern Methods for Robust Regression*. SAGE Publications, 2008.
- [47] Asad Ali, Muhammad F. Qadir. A Modified M-Estimator for the Detection of Outliers. *PJSOR*, 1:49–64, 2005.
- [48] B. Bhushan. *Modern Tribology Handbook*, chapter Chapter 2 Surface Roughness Analysis and Measurement Techniques. CRC Press LLC, 2001.
- [49] B. Muralikrishnan. J. Raja. *Computational Surface and Roundness Metrology*. Springer, 2009.
- [50] B. X. Jiang, and D. J. Whitehouse. Precision metrology. *Philosophical transactions of the royal society A*, 370:4154–4160, 2012.
- [51] B. Y. Lee, H. Juan, S. F. Yu. A study of computer vision for measuring surface roughness in the turning process. *The international journal of advanced manufacturing technology*, 19:295–301, 2002.
- [52] Gleb Beliakov. Fast computation of trimmed means. *Journal of statistical software*, 39(2):1–6, 2011.
- [53] Zhang Bi-Ming, Jiang Qi-Yun, Mo Dan, and Xiao Long-Ying. A novel method for handling gross errors in electromagnetic prospecting data. *CHINESE JOURNAL OF GEOPHYSICS-CHINESE EDITION*, 58(6):2087–2102, JUN 2015.
- [54] Bureau International des Poids et Mesures (BIPM). *The International System of Units (SI)*. Organisation Intergouvernementale de la Convention du Metre, 2006.
- [55] C. F. Cheung, M. Liu, R. Leach, X. Feng, C. Zhao. Hierarchical information based characterization of multiscale structured surfaces. *CIRP Annals*, 67(1):539 – 542, 2018.
- [56] C. L. Giusca, and R. K Leach. *Measurement Good Practice Guide No.128: Calibration of the Metrological Characteristics of Imaging Confocal Microscopes (ICMs)*. 2012.
- [57] C. L. Giusca, R. Leach. *Good Practice Guide No.128: Calibration of the metrological characteristics of Imaging Confocal Microscopy (ICMs)*. 2012.
- [58] C. L. Giusca, R. Leach, F. Helary. Calibration of the scales of areal surface topography measuring instruments: part 2. Amplification, linearity and squareness. *Measurement Science and Technology*, 23(6):065005, may 2012.

- [59] C. L. Giusca, R. Leach, F. Helary, T. Gutauskas, L. Nimishakavi. Calibration of the scales of areal surface topography-measuring instruments: part 1. Measurement noise and residual flatness. *Measurement Science and Technology*, 23(3):035008, feb 2012.
- [60] C. O. S. Sorzano, J. Vargas, A. P. Montano. A survey of dimensionality reduction techniques. Technical report, Preprint at <http://arxiv.org/abs/1403.2877>, 2014.
- [61] C. Teutsch, E. Trostmann, D. Berndt. A parallel point cloud clustering algorithm for subset segmentation and outlier detection. *Proceedings SPIE Optical Metrology*, 8085, 2011.
- [62] C. Wang. Current issues on 3D volumetric positioning accuracy: measurement, Compensation and Definition. *Proceedings of SPIE*, (2008) 7128, 2008.
- [63] C. Wang, J. Caja, E. Gomez. Comparison of methods for outlier identification in surface characterization. *Measurement*, 117:312 – 325, 2018.
- [64] Leica cooperation. *3D Optical Surface Metrology System Leica DCM 3D*. 2015.
- [65] Leica cooperation. *Dual Core 3D Profiler combines Confocal Imaging and Interferometry*. 2015.
- [66] D. B. Sharp. *Measurement Standards*. CRC Press LLC, 1999.
- [67] D. G. Abdelsalam, B. Yao. *Interferometry and its Applications in Surface Metrology, Chapter 5 in Optical interferometry*. InTech, 2017.
- [68] D. G. Bailey. A new approach to lens distortion correction. *Proceedings Image and Vision Computing New Zealand*, pages 59–64, 2002.
- [69] D. Huang, S. Du, G. Li, C. Zhao, Y. Deng. Detection and monitoring of defects on three-dimensional curved surfaces based on high-density point cloud data. *Precision Engineering*, 53:79–95, 2018.
- [70] D. Imkamp. Looking at the future of manufacturing metrology: The VDI/VDE roadmap manufacturing metrology 2020. In *Proceedings of the 5th Manufacturing Engineering Society International Conference - Zaragoza - June 2013*, 2013.
- [71] D Imkamp, J. Berthold, M. Heizmann, K. Kniel, E. Manske, M. Peterrek, R. Schmitt, J. Seidler, and K. D. Sommer. Challenges and trends in manufacturing measurement technology - the "Industrie 4.0" concept. *Journal of sensors and sensor systems*, 5:325–335, 2016.
- [72] D. J. Whitehouse. Surface metrology. *Measurement science and technology*, 8:955–972, 1997.
- [73] D. K. Cohen. Introduction to ASME B46.1-2009: surface texture (surface roughness, waviness, and lay). Technical report, Michigan Metrology, LLC, 2011.
- [74] D. Semwogerere, E. R. Weeks. *Confocal Microscopy*. Taylor & Francis, 2005.

- [75] D. Umbach, K. N. Jones. A few methods for fitting circles to data. *IEEE Transactions on Instrumentation and Measurement*, 52(6):1881–1885, 2003.
- [76] D. W. Marquardt. An algorithm for Least-Squares estimation of nonlinear parameters. *Journal of the Society for Industrial and Applied Mathematics*, 11(2):431–441, 1963.
- [77] David J. Whitehouse. *Hand book of surface and nanotechnology. 2nd Edition*. CRC Press, 2011.
- [78] E. Alegre, J. Barreiro, M. Castejon, and S. Suarez. Computer Vision and Classification Techniques on the Surface Finish Control in Machining Processes. *Image Analysis and Recognition, 5th International Conference, ICIAR 2008*, 2008.
- [79] E. W. Weisstein. Least Squares Fitting. *From MathWorld—A Wolfram Web Resource*. <http://mathworld.wolfram.com/LeastSquaresFitting.html>.
- [80] E. W. Weisstein. Legendre Polynomial. *From MathWorld - A Wolfram Web Resource*. <http://mathworld.wolfram.com/LegendrePolynomial.html>.
- [81] Hanan Elsaied and Roland Fried. Tukey’s M-estimator of the Poisson parameter with a special focus on small means. *STATISTICAL METHODS AND APPLICATIONS*, 25(2):191–209, JUN 2016.
- [82] E.S. Gadelmawla, M.M. Koura, T.M.A. Maksoud, I.M. Elewa, H.H. Soliman. Roughness parameters. *Journal of Materials Processing Technology*, 123:133–145, 2002.
- [83] F. R. Boddeke, L. J. Van Vliet, and I. T. Young. Calibration of the automated z-axis of a microscope using focus functions. *Journal of Microscopy*, 186(3):270–274, 1997.
- [84] F. Wessel, R. Schluter, K. Macherey, H. Ney. Confidence measures for large vocabulary continuous speech recognition. *IEEE Transactions on Speech and Audio Processing*, 9(3):288–298, 2001.
- [85] G. A. Al-Kindi, R. M. Baul, K. F. Gill. An application of machine vision in the automated inspection of engineering surfaces. *International Journal of Production Research*, 30(2):241–253, 1992.
- [86] G. Hermann. Geometric Error Correction in Coordinate Measurement. *Acta Polytechnica Hungarica*, 4(1):47–62, 2007.
- [87] G. L. Goic, C. A. Brown, H. Favreliere, S. Samper, F. Formosa. Outlier filtering: a new method for improving the quality of surface measurements. *Measurement science and technology*, 24:015001(13pp), 2013.
- [88] G. M. Krolczyk, J. B. Krolczyk, R. W. Maruda, S. Legutko, M. Tomaszewski. Metrological changes in surface morphology of high-strength steels in manufacturing processes. *Measurement*, 88:176–185, 2016.

-
- [89] G. M. Krolczyk, R. W. Maruda, P. Nieslony, M. Wieczorowski. Surface morphology analysis of Duplex Stainless Steel (DSS) in Clean Production using the Power Spectral Density. *Measurement*, (94):464–470, 2016.
- [90] G. T. Smith. *Industrial Metrology: Surfaces and Roundness*. Springer, 2002.
- [91] G. Wubbeler, M. Krystek, C. Elster. Evaluation of measurement uncertainty and its numerical calculation by a Monte Carlo method. *Measurement Science and Technology*, 19(4pp):084009, 2008.
- [92] G. Zhang, R. Ouyang, B. Lu, R. Hocken, R. Veale, A. Donmez. A Displacement Method for Machine Geometry Calibration. *Annals of the CIRP*, 37(1):515–518, 1988.
- [93] G. Zhang, R. Veale, T. Charlton, B. Borchardt, R. Hocken. Error Compensation of Coordinate Measuring Machines. *Annals of the CIRP*, 34(1):445–448, 1985.
- [94] Gavin MacAulay. *Characterization of structured surfaces and assessment of associated measurement uncertainty*. NPL, 2015.
- [95] J Gawlowski, J Bartulewicz, T Gierczak, and J Niedzielski. Tests for outliers. A Monte Carlo evaluation of the error of first type. *CHEMIA ANALITYCZNA*, 43(4):743–753, 1998.
- [96] Gilberto A. Ortiz Ka Veng Yuen. Outlier detection and robust regression for correlated data. *Computer methods in applied mechanics and engineering*, 2017.
- [97] H. Bornfleth, K. Saetzler, R. Eils, and C. Cremer. Distance measurements and volume-conserving segmentation of objects near and below the resolution limit in three-dimensional confocal fluorescence microscopy. *Journal of Microscopy*, 189:118–136, 1998.
- [98] H. E. Keller. *Objective lenses for confocal microscopy*. In: *Handbook of Biological Confocal Microscopy*. New York: Plenum Press, 1995.
- [99] H. Huang, D. Li, H. Zhang, U. Ascher, D. Cohen-Or. Consolidation of Unorganized Point Clouds for Surface Reconstruction. *ACM Transactions on Graphics*, 28(5):176:1–176:7, December 2009.
- [100] H. Jia, Y. L. Murphey, J. Shi, T. S. Chang. An Intelligent Real-time Vision System for Surface Defect Detection. In *Proceedings of the Pattern Recognition, 17th International Conference on (ICPR'04) Volume 3*, ICPR '04, pages 239 – 242, Washington, DC, USA, 2004. IEEE Computer Society.
- [101] H. Noura, J. A. Salgado, N. E. Hayek, S. Ducourtieux, A. Delvallee, and N. Anwer. Setup of a high-precision profilometer and comparison of tactile and optical measurements of standards. *Measurement Science and Technology*, 25(044016):12pp, 2014.
- [102] H. Noura, N. E. Hayek, X. Yuan, and N. Anwer. Characterization of the main error sources of chromatic confocal probes for dimensional measurement. *Measurement Science and Technology*, 25(044011):14pp, 2014.
-

- [103] H. Noura, N. El-Hayek, X. Yuan, N. Anwer, J. Salgado. Metrological characterization of optical confocal sensors measurements (20 and 350 travel ranges). *Journal of Physics: Conference Series*, 483:012015, 2015.
- [104] H. Schwenke, W. Knapp, H. Haitjema, A. Weckenmann, R. Schmitte, F. Delbressine. Geometric error measurement and compensation of machines - An update. *CIRP Annals - Manufacturing Technology*, 57:660–675, 2008.
- [105] H. Wang, S. Xiang. On the convergence rates of Legendre approximation. *Mathematics of computation*, 81(278):861–877, 2012.
- [106] Tianming Hu and Sam Yuan Sung. A trimmed mean approach to finding spatial outliers. *Intelligent Data Analysis*, 8(1):79–95, January 2004.
- [107] I. D. Coope. Circle fitting by linear and nonlinear least squares. *Journal of Optimization Theory and Applications*, 76:381–388, 1993.
- [108] I. Kweon, J. Kim, P. Gurdjos. Euclidean Structure from Confocal Conics: Theory and Application to Camera Calibration. In *IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR '06)*, New York, NY, pages 1214–1221, 2006.
- [109] I. Raid, T. Kusnezowa, J. Seewig. Application of ordinary kriging for interpolation of micro-structured technical surfaces. *Measurement Science and Technology*, 24(9):095201, 2013.
- [110] Interagency working group on manufacturing research and development. Instrumentation, metrology, and standards for nanomanufacturing. Technical report, National Institute of Standards and Technology, U.S. Department of Commerce, National Science Foundation, Office of Naval Research, 2008.
- [111] Internet Based Surface Metrology Algorithm Testing System.
<https://physics.nist.gov/3DVSC/jsp/SurfaceParameter3D.jsp?ran=1679>.
- [112] J. A. Hartigan, M. A. Wong. A K-means Clustering Algorithm. *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, 28(1):100–108, 1979.
- [113] J. C. Waters. Accuracy and precision in quantitative fluorescence microscopy. *The journal of cell biology*, 185(7):1135–1148, 2009.
- [114] J. C. Wyant. Guest Editorial Precision Surface Metrology. *Optical Engineering*, 23(4):349, 1984.
- [115] J. Caja. *Técnicas Avanzadas de Metrología Dimensional Indirecta Mediante el Empleo de Maquinas de Medicion por Vision en Entornos Industriales. Modelo para la Estimacion de Incertidumbres*. phdthesis, Technical University of Madrid, 2014.

- [116] J. E. Dennis, D. M. Gay, R. E. Welsch. An adaptive nonlinear least-squares algorithm. *ACM Transactions on Mathematical Software*, 7(3):348–368, 1981.
- [117] J. Haycocks, K. Jackson. Traceable calibration of transfer standards for scanning probe microscopy. *Precision Engineering*, 29(2):168 – 175, 2005.
- [118] J. Vicente, C. Molpeceres, O. Guarneiros, et al. Calibracion de Microscopios Confocales. *XVII Congreso Nacional de IngenierÃ-a MecÃ-jnica*, pages 307–312, 2008.
- [119] J. Wang, F. Shi, J. Zhang, Y. Liu. A new calibration model of camera lens distortion. *Pattern Recognition*, 41:607–615, 2007.
- [120] J. Yang and Y. Ren, C. Wang, G. Liotto. Theoretical derivations of 4 body diagonal displacement errors in 4 machine configurations. *Proceedings of the LAMDAMAP Conference*, Cransfield, UK, June 27-30, 2005.
- [121] J.C. Mullikin, L.J. van Vliet, H. Netten, F.R. Boddeke, G. van der Feltz, and I.T. Young. Methods for CCD camera characterization. *SPIE*, 2173:73–84, 1994.
- [122] K. A. Cychosz, R. G. Nicolas, J. G. MartÃ-nezb, M. Thommes. Recent advances in the textural characterization of hierarchically structured nanoporous materials. *Chemical Society Reviews*, 46:389–414, 2017.
- [123] K. H. Lin, Y. H. Hu. White-light interferometric techniques in microstructure measurement. *Proceedings of the SPIE, Volume 6280, id. 62800X (2006)*, 2006.
- [124] K. Hossain, M. Milton, B. Nimmo. *Metrology for the 2020s*. Fiona Auty, the NPL Graphics Team, 2013.
- [125] K. J. Stout, editor. *Development of methods for the Characterisation of Roughness in Three Dimensions*. Penton Press, 1993.
- [126] K. J. Stout, L. Blunt. *Three-dimensional Surface Topography, 2nd Edition*. Penton Press, 2000.
- [127] K. Miyoshi. Surface characterization techniques: An overview. *NASA/TM*, 2002.
- [128] K. Tong, E. A. Lehtihet, S. Joshi. Parametric error modeling and software error compensation for rapid prototyping. *Rapid Prototyping Journal*, 9(5):301–313, 2003.
- [129] K. Umetsu, R. Furutnani, S. Osawa, T. Takatsuji, T. Kurosawa. Geometric calibration of a coordinate measuring machine using a laser tracking system. *Measurement Science and Technology*, 16(12):2466–2472, 2005.
- [130] K.E. Jensen, D.A. Weitz, and F. Spaepen. Note: A three-dimensional calibration device for the confocal microscope. *Review of Scientific Instruments*, 84:016108, 2013.

- [131] Kevin Harding, editor. *Handbook of Optical Dimensional Metrology*. CRC Press, Taylor & Francis Group, 2013.
- [132] L. Nielsen. Least-squares estimation using Lagrange multipliers. *Metrologia*, 35(2):115–118, 1998.
- [133] L. Nielsen. Evaluation of measurements by the method of least squares. *J. Levesley, I. J. Anderson, J. C. Mason (Eds.), Algorithms for Approximation IV, University of Huddersfield*, pages 170–186, 2002.
- [134] L. Richard, and A. Hart. A comparison of stylus and optical methods for measuring 2D surface texture. *NPL Report CNTLM 15*, pages 1–46, 2002.
- [135] Lateral scale calibration for focus variation microscopy. A. Alburayt, W. P. Syam, R. Leach. *Measurement Science and Technology*, 2018.
- [136] Richard Leach. *Fundamental principles of engineering nanometrology 2nd Edition*. William Andrew, 2014.
- [137] M. F. Ismail, K. Yanagi, A. Fujii. An outlier correction procedure and its application to areal surface data measured by optical instruments. *Measurement science and technology*, 21(10):105105(11pp), 2010.
- [138] M. G. Cox, B. R. L. Siebert. The use of a Monte Carlo method for evaluating uncertainty and expanded uncertainty. *Metrologia*, 43: S178–S188, 2006.
- [139] M. Genevieve, B. Labrousse. Surface characterization. *Physical methods, instruments and measurements*, 3, 2010.
- [140] M. Krystek 1, P.J. Scott 2 and V. Srinivasan. Discrete linear filters for metrology. *Proceedings of the 16th IMEKO World Congress, Hofburg, Wien, Austria*, 2000.
- [141] M. Ritter, T. Dziomba, A. Kranzmann, L. Koenders. A landmark-based 3D calibration strategy for SPM. *Measurement Science and Technology*, 18:404–414, 2007.
- [142] M. S. Fernandez. MATLAB implementation for evaluation of measurements by the generalized method of least squares. *Measurement*, 114:218–225, 2018.
- [143] M.C. Jenkins, S.U. Egelhaaf. Confocal microscopy of colloidal particles: Towards reliable, optimum coordinates. *Advances in Colloid and Interface Science*, 136:65–92, 2008.
- [144] Michigan Metrology, LLC. *3D Spatial Parameters*. 2016.
- [145] N. A. Barakat, M. A. Elbestawi, A. D. Spence. Kinematic and geometric error compensation of a coordinate measuring machine. *International Journal of Machine Tools & Manufacture*, 40:833–850, 2000.

- [146] N. Jouini, A. Gautier, P. Revel, P-E. Mazeran, and M. Bigerelle. Multi-scale analysis of high precision surfaces by Stylus Profiler, Scanning White-Light Interferometry and Atomic Force Microscopy. *International Journal of Surface Science and Engineering*, 3(4), 2015.
- [147] N. S. Claxton, T. J. Fellers, M. W. Davidson. Laser scanning confocal microscopy. Technical report, Department of Optical Microscopy and Digital Imaging, Florida State University, Tallahassee, 2006.
- [148] National Physical Laboratory. *Good Practice Guide No. 80: Fundamental Good Practice in Dimensional Metrology*. Queen's Printer and Controller of HMSO, 2005.
- [149] P. Howarth, F. Redgrave. *Metrology - in short 3rd Edition*. EURAMET project 1011, participants: DFM Denmark, NPL United Kingdom, PTB Germany, 2008.
- [150] P. J. Huber. *Robust Statistics*, pages 1248–1251. Springer Berlin Heidelberg, 2011.
- [151] P. J. Rousseeuw, M. Hubert. Robust statistics for outlier detection. *WIREs Data Mining and Knowledge Discovery*, 1:73–79, 2011.
- [152] P. M-Arguello, J. Barreiro, E. Alegre. An evaluation of surface roughness classes by computer vision using wavelet transform in the frequency domain. *The International Journal of Advanced Manufacturing Technology*, 59:213–220, 2012.
- [153] P. M. Harris, M. G. Cox. On a Monte Carlo method for measurement uncertainty evaluation and its implementation. *Metrologia*, 51:S176–S182, 2014.
- [154] Chanseok Park and Mark Leeds. A highly efficient robust design under data contamination. *COMPUTERS & INDUSTRIAL ENGINEERING*, 93:131–142, MAR 2016.
- [155] Annick M. Leroy Peter J. Rousseeuw. *Robust Regression and Outlier Detection*. John Wiley & Sons, New York, 1987.
- [156] PRIME Faraday Partnership. *An Introduction to MEMS*. Prime Faraday Technology Watch , 2002.
- [157] R. Artigas. *Optical Measurement of Surface Topography*, chapter Chapter 11 Imaging Confocal Microscopy, pages 237–287. Springer, Berlin, Heidelberg, 2011.
- [158] R. C. Luo, M. G. Kay. Multisensor integration and fusion in intelligent systems. *IEEE Transactions on Systems, Man, and Cybernetics*, 19(5):901–931, 1989.
- [159] R. C. Luo, M. H. Lin, R. S. Scherp. Dynamic multi-sensor data fusion system for intelligent robots. *IEEE Journal on Robotics and Automation*, 4(4):386–396, 1988.
- [160] R. D' Amato, J. Caja, P. Maresca, E. GÃmez. Use of coordinate measuring machine to measure angles by geometric characterization of perpendicular planes. Estimating uncertainty. *Measurement*, 47:598–606, 2014.
-

- [161] R. Deltombe, K. Kubiak, M. Bigerelle. How to select the most relevant 3D roughness parameters of a surface. *Scanning*, 36(1):150–160, 2014.
- [162] R. Hartley, A. Zisserman. *Multiple view Geometry in computer vision Second Edition*. Cambridge University Press, New York, 2003.
- [163] R. J. Pike, and T. R. Thomas. Quantitative characterization of micro-topography—A bibliography of industrial surface metrology. Technical report, U.S. Department of the interior and U.S. Geological survey, 1988.
- [164] R. K. Leach, C. L. Giusca, H. Haitjema, C. Evans, X. Jiang. Calibration and verification of areal surface texture measuring instruments. *CIRP Annals - Manufacturing Technology*, 64:797–813, 2015.
- [165] R. K. Leach, C. L. Giusca, K. Naoi. Development and characterization of a new instrument for the traceable measurement of areal surface texture. *Measurement Science and Technology*, 20:125102(8pp), 2009.
- [166] R. Leach. *Characterisation of Areal Surface Texture*. Springer, 2013.
- [167] R. W. Cole, T. Jinadasa, C. M. Brown. Measuring and interpreting point spread functions to determine confocal microscope resolution and ensure quality control. *Nature Protocols*, 6(12):1929–1941, 2011.
- [168] Richard Leach. *Optical measurement of surface topography*. Springer, 2011.
- [169] R. Leach, D. Chetwynd, L. Blunt, J. Haycocks, P. Harris, K. Jackson, S. Oldfield, S. Reilly. Recent advances in traceable nanoscale dimension and force metrology in the UK. *Measurement science and technology*, 17:467–476, 2006.
- [170] Peter J. Rousseeuw and Christophe Croux. Alternatives to the median absolute deviation. *Journal of the American Statistical Association*, 88(424):1273–1283, 1993.
- [171] S. Bell. *Good Practice Guide No.11: The beginner's guide to Uncertainty of measurement*. National Physical Laboratory, 1999.
- [172] S. Carmignato, A. Voltan, E. Savio. Metrological performance of optical coordinate measuring machines under industrial conditions. *CIRP Annals - Manufacturing Technology*, 59:497–500, 2010.
- [173] S. Chen, D. Zhang. Robust Image Segmentation Using FCM With Spatial Constraints Based on New Kernel-Induced Distance Measure. *IEEE Transactions on Systems, Man, and Cybernetics - Part B: Cybernetics*, 34(4):1907–1916, 2004.

- [174] S. I. Chang, J. S. Ravathur. Computer Vision Based Non-contact Surface Roughness Assessment Using Wavelet Transform and Response Surface Methodology. *Quality Engineering*, 17:435–451, 2005.
- [175] S. J. Miller. The Method of Least Squares. in *Brown University*, 2006.
- [176] S. P. Lloyd. Least Squares Quantization in PCM. *IEEE Transactions on Information Theory*, IT-28(2):129–137, 1982.
- [177] S. Sartori, G. X. Zhang. Geometric Error Measurement and Compensation of Machines. *Annals of the CIRP*, 44(2):599–609, 1995.
- [178] S. Sophia, A. Vicithra, S. Sangeetha, V. Mahitha, S. Hedayathbasha. Measurement of Surface Roughness Using Image Processing. *IOSR Journal of Electronics and Communication Engineering*, pages 20–24, 2017.
- [179] M. R. Sindhumol, M. R. Srinivasan, and M. Gallo. A robust dispersion control chart based on modified trimmed standard deviation. *ELECTRONIC JOURNAL OF APPLIED STATISTICAL ANALYSIS*, 9(1):111–121, APR 2016.
- [180] J.A. Sladek. *Coordinate Metrology: Chapter 2 Measurement Uncertainty and Requirements of Production System. Selected Issues of Measurement Uncertainty Theory*. Springer-Verlag Berlin Heidelberg, 2016.
- [181] S.S.Qian. *Measurement Uncertainty: Process and Representation of Experimental Data*. 2002.
- [182] Jan-Philipp Stauffert, Florian Niebling, and Marc Erich Latoschik. Towards Comparable Evaluation Methods and Measures for Timing Behavior of Virtual Reality Systems. In Spencer, SN, editor, *22ND ACM CONFERENCE ON VIRTUAL REALITY SOFTWARE AND TECHNOLOGY (VRST 2016)*, pages 47–50, 1515 BROADWAY, NEW YORK, NY 10036-9998 USA, 2016. ACM; ACM SIGCHI; ACM SIGGRAPH, ASSOC COMPUTING MACHINERY. 22nd ACM Conference on Virtual Reality Software and Technology (VRST), Munich, GERMANY, NOV 02-04, 2016.
- [183] Steven Walfish. A review of statistical outlier methods. *Pharmaceutical Technology*, 30:1–5, 2006.
- [184] T. G. Mathia, P. Pawlus, M. Wiczorowski. Recent trends in surface metrology. *Wear*, 271(3-4):494–508, 2011.
- [185] T. Kailath. The Divergence and Bhattacharyya Distance Measures in Signal Selection. *IEEE Transactions on Communication Technology*, 15:52–60, 1967.
- [186] T. R. Corle, G. S. Kino. *Confocal Scanning Optical Microscopy and Related Imaging Systems*. Academic Press, 1996.
- [187] T. V. Vorburger. *Tutorial in optics: Chapter 8 Methods for characterizing surface topography*. Optical society of America, 2010.

- [188] T. V. Vorburger, J.Raja. *Surface Finish Metrology Tutorial*. NISTIR 89-4088, 1990.
- [189] T. Yoshizawa, editor. *Handbook of Optical Metrology: Principles and Applications, 2nd Edition*. CRC Press, 2015.
- [190] T.D. Visser, J.L. Oud, G.J. Brakenhoff. Refractive index and axial distance measurements in 3-D microscopy. *Optik*, 90:17–19, 1992.
- [191] T.H. Besseling, J. Jose, and A. Van Blaadenren. Methods to calibrate and scale axial distances in confocal microscopy as a function of refractive index. *Journal of Microscopy*, 257(2):142–150, 2015.
- [192] Albrecht Ullrich. Detecting measurement outliers - Remeasure efficiently. In Montgomery, MW and Maurer, W, editor, *PHOTOMASK TECHNOLOGY 2010*, volume 7823 of *Proceedings of SPIE*, 1000 20TH ST, PO BOX 10, BELLINGHAM, WA 98227-0010 USA, 2010. BACUS; SPIE, SPIE-INT SOC OPTICAL ENGINEERING. Conference on Photomask Technology 2010, Monterey, CA, SEP 13-16, 2010.
- [193] F Velasco, SP Verma, and M Guevara. Comparison of the performance of fourteen statistical tests for detection of outlying values in geochemical reference material databases. *MATHEMATICAL GEOLOGY*, 32(4):439–464, MAY 2000.
- [194] W. Bich, M. G. Cox, R. Dybkaer, C. Elster, W. T. Estler, B. Hibbert, H. Imai, W. Kool, C. Michotte, L. Nielsen, L. Pendrill, S. Sidney, A. M. H. Veen, W. Woger. Revision of the 'Guide to the Expression of Uncertainty in Measurement'. *Metrologia*, 49:702–705, 2012.
- [195] W. G. Weekers. *Compensation for Dynamic Errors of Coordinate Measuring Machines*. PhD thesis, Eindhoven University of Technology, 1996.
- [196] W. Gander, G. H. Golub, R. Strebler. Least squares fitting of circles and ellipses. *Bull. Belgian Math. Soc.*, 3:63–84, 1996.
- [197] Wahyudin Permana Syam. *Uncertainty evaluation and performance verification of a 3D Geometric Focus-variation measurement*. PhD thesis, Polytechnic University of Milan, 2014.
- [198] X A. Zheng, J. A. Soons, T. V. Vorburger, J. F. Song, T. B. Renegar, R. M. Thompson. Applications of Surface Metrology in Firearm Identification. *Surface Topography: Metrology and Properties*, 2(014012):10pp, 2014.
- [199] X. J. Jiang, D. J. Whitehouse. Technological shifts in surface metrology. *CIRP Annals - Manufacturing Technology*, 61:815–836, 2012.
- [200] X. Jiang, P. J. Scott, D. J. Whitehouse, and L. Blunt. *Paradigm shifts in surface metrology. Part I. Historical philosophy*. Proceedings of the Royal Society, 2007.

- [201] X. Jiang, P. J. Scott, D. J. Whitehouse, and L. Blunt. *Paradigm shifts in surface metrology. Part II. The current shift*. Proceedings of the Royal Society, 2007.
- [202] Y. Jia, and Q. Xu. MEMS Microgripper actuators and sensors: The state-of-the-art survey. *Recent Patents on Mechanical Engineering*, 6:000–000, 2013.
- [203] Y. Wang, H. Y. Feng. Modeling outlier formation in scanning reflective surfaces using a laser stripe scanner. *Measurement*, 57:108–121, 2014.
- [204] Y. Wang, H. Y. Feng. Outlier detection for scanned point clouds using majority voting. *Computer-Aided Design*, 62:31 – 43, 2015.
- [205] Z. Hou, Z. Wang, Y. Zhang. Position determination and measurement error analysis for the spherical proof mass with optical shadow sensing. *Acta Astronautica*, 126:215–228, 2016.
- [206] Z. Xu, M. Xia. Distance and similarity measures for hesitant fuzzy sets. *Information Sciences*, 181(11):2128 – 2138, 2011.