PREDICTION OF DESTRUCTIVE PROPERTIES USING DESCRIPTIVE ANALYSIS OF ND MEASUREMENTS

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ABSTRACT

Three groups of measurements related to peach maturity were acquired through destructive (D) mechanical tests (Magness Taylor Firmness, MTF), mechanical non destructive (ND) tests, and ND optical spectroscopy (Optical indexes). The relationship between these groups of variables was studied in order to estimate D mechanical measurements (MTF, with higher instrumental and sampling variability, time consuming, generally used as a reference for the assessment of peach handling), from ND measurements (quick, applicable on line, dealing better with the high variability found in fruit products). Multivariate exploratory analysis was used to extract the structure of the data. The information about the data structure of ND measurements, the relationship of MTF with the space defined by ND variables, and the expert knowledge regarding to the dataset was then used for modelling MTF (R^2=0.72 and standard error on validation 5.73 N).

INTRODUCTION

The measurement of peach maturity for harvest is a controversial issue. Optimum maturity needs to be balanced between a minimum, acceptable for the consumer, and a maximum, to minimize fruit loses during the postharvest process.

Three groups of measurements, related with peach maturation are considered in this work: Magness Taylor Firmness (MTF) [1], low mass impact measurements (LMI) [2], and optical indexes related with pigments evolution along maturation [3]. As MTF is the most extensive reference for peach maturity and ripeness [1, 2], there is a need to estimate destructive firmness (MTF) of fruits through non destructive means (quick, applicable on line, dealing better with the high variability found in fruit products). Several variables can be computed from the row measurements acquired from each of these non destructive (ND) techniques (visible spectroscopy [3] and low mass impact [4, 5]), according to different corrections or calibrations applied to the row data acquired. These variables are thus, highly correlated, and variable selection is generally applied for data compression [6, 7].

The objective of this work is to model MTF from ND (optical and mechanical) measurements, taking into account the data structure of ND measurements and its relationship with MTF. A multivariate approach is applied to handle ND measurements co-linearity in an attempt to.

MATERIALS AND METHODS

'Richlady' peaches from 2 seasons were measured on the same region. For each season, sampled peaches were picked sequentially along the maturation process (on the tree) in order to provide the widest feasible variability. Fruit samples were picked weekly from one week prior to commercial harvest date (CH) on season 1 and from the 3 weeks prior to commercial harvest date (season 2) until the week after CH.

Three groups of measurements were acquired, each with an instrumental technique:

X (Input variables to model MTF)

- ✓ **Mechanical (ND):** Low mass impact measurements (LMI). Imp, Imp2, Imp3 and Imp4. They are different parameters extracted from the deceleration curve produced by a low mass impact on the sample (peach fruit)[5].
- ✓ **Optical spectral indexes** related to chlorophyll and other pigments (ND): (Optical indexes). Ind_1, ind_2, ind_3, rir and I_{AD} are optical indexes for chlorophyll estimation based on different spectral corrections on the chlorophyll absorption band (680nm)[3]. I_{carot} is related with carotenoids content [8].

MTF (Variable to model)

In order to summarize and interpret the information of the ND dataset, the relationship among variables was studied through Principal Component Analysis (PCA). The main principal component (PC) directions were interpreted and used first, for studying the feasibility and limitations of MTF modeling (D) from ND measurements; and finally, for building the model.

1 EXPERIMENTAL RESULTS AND DISCUSSION

1.1 Multivariate exploratory analysis to describe data structure

A. Relationship within groups of ND variables ¿Can we compress the information provided by each instrument?

PCA was performed, and by considering two principal components (80,4% of variance), two main factorial directions, optical (Opt) and mechanical (Mec), were identified.Chlorophyll optical indexes based on spectrophotometer and LMI measurements were mainly explained by factors 1 and 2 (0.86 and 0.94 of the explained variance of factor 1 and 2 respectively was explained by these two groups of measurements). Factors 3 and 4were also studied, observing their lesser importance (14.6% of variance) and interpretability. They were mainly explained by I_{carot} (0.5 and 0.4, respectively of the explained variance of the factor was explained by I_{carot}). In this regard, carotenoids content has been observed to increase throughout fruit maturation and decrease or stabilize at the end of the peach maturation process [9]. Its estimation through spectral measurements is though greatly affected by interactions with other pigments [8]. Thus, I_{carot} and factors 3 and 4 were considered a less reliable indicator of maturation than chlorophyll optical indexes and factors 1 and 2. Factors 1 and 2 were considered for further analysis.

As plotted in Fig. 1, two main groups of variables, aggregated in two pertinent directions (each corresponding to an instrumental technique) were found in factors 1 and 2:

- ✓ An optical axis, related with spectral indexes and chlorophyll content.
- ✓ A mechanical axis related to LMI measurements.

Two new (latent) variables were computed as the projection of ND measurements onto optical and mechanical axes (Fig. 2). Both mechanical and optical axis values reflected maturity variability, being aligned from lower values of optical and mechanical axis (associated to less mature fruits) to higher values on both axis (more mature fruits).

B. Relationship between ND groups of variables ¿Are they complementary?

When considering the plane defined by factors 1 and 2, plotted in Fig. 1, optical and mechanical axis showed 70% of complementation and 30% of dependency (the square cosine of the angle between both directions is 0.3). This result agrees with a previous work [7] which observed LMI measurements and reflectance at selected wavelengths to be complementary and related to the maturity of peach fruit, merging several peach varieties.

C. Relationship between the ND and D ¿Can the D measurements be estimated with the ND?

As observed in Fig.1. the response (MTF) is plotted between Mechanical and Optical axis. Thus, MTF is related both to optical and mechanical axis and both should be preferably considered for the estimation of MTF. Fig. 3. plots a multilinear regression (MLR) of MTF as a function of the score projections onto optical and mechanical axes, including both seasons. The model showed a linear relationship with MTF in the range between 20 N and 75 N of observed MTF. Therefore, optical and mechanical axis could be used for MTF estimation (through a linear model) within this range.

1.2 MTF modeling using data structure

MTF estimation from optical and mechanical variables was applicable only within the range from 20-75 N MTF. This range gathers most commercial firmness variability (Crisosto, 1996), being 65N the maximum firmness at harvest established by EU regulations. As plotted in Fig. 2, Season 2 data presented a wider variability, according to the experimental design and seasonal conditions (earlier pre-commercial harvest dates and high temperatures at the end of the maturation period, producing a quick maturation of post-commercial fruits from season 2). All observations over 75 N MTF corresponded to pre-commercial harvests on season 2, which were excluded from further modeling.

Therefore, a total of 391 observations were considered in the model for MTF estimation, 311 from season 1 and 80 observations from season 2. Given the heterogeneity between season 1 and season 2 datasets, both populations were merged and then split into two sets: calibration, (n=206) and validation (n=167), with similar distribution.

The model was built using the optical and mechanical axes observed in the exploratory analysis as input variables for a multilinear regression to estimate MTF. R^2 was 0.72 and standard error of prediction 5.73, this is, 11% of the considered range.

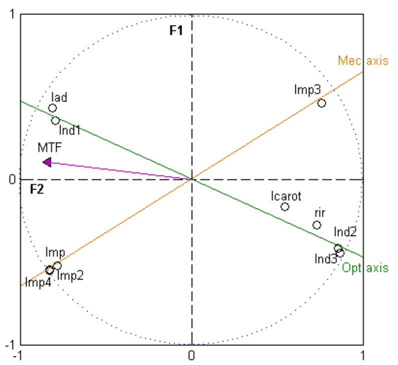

Fig. 1. PCA loadings interpretation of factors 1 and 2. N=311 from season 1. MTF projection onto PCA factors.

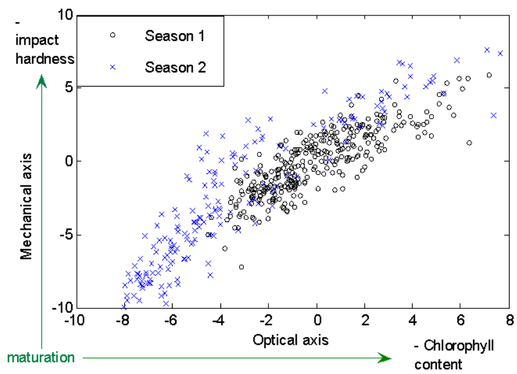

Fig. 2. Scores projection onto mechanical and optical axis. N=311 from season 1 and N= 400 from season 2.

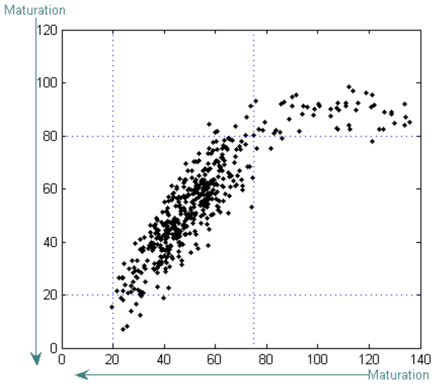

Fig. 3. MLR for the estimation of MTF as a linear function of the projection of PCA scores onto Optical and Mechanical axis (n=311 from season 1 and n=400 samples from season 2). Observed (x axis) against predicted MTF (y axis).

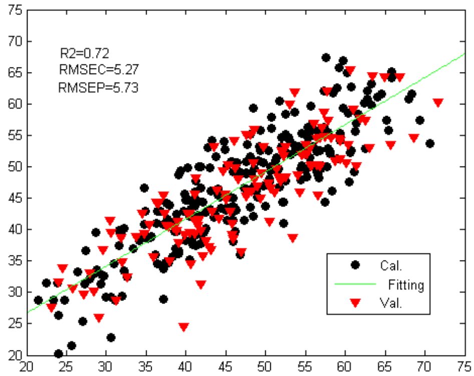

Fig. 4. MLR from mechanical and optical axis. Observed (x axis) against predicted MTF (y axis) and coefficient of determination (R^2), Root Mean Standard Error of Calibration (RMSEC) and Root Mean Standard Error of prediction (RMSEP). Calibration (Cal.) and validation (Val.) populations are represented.

CONCLUSIONS

The structure of a dataset comprised by two groups of non destructive (ND) variables (optical and mechanical) was studied through multivariate analysis. A third variable, Magness-Taylor firmness (MTF), was projected on the space defined by these ND measurements. As a conclusion it was observed that both groups of ND variables were necessary for MTF estimation.

MTF is the widest reference used for assessing postharvest handling in peach fruit, though it has shown to have lower repeatability and accordance to consumer perception of firmness than alternative non destructive measurements [6]. In contrast, ND measurements offer higher reliability, the possibility to extend measurements to a higher portion of the population or even to all fruits and even to allow repeating the analysis on the same samples for monitoring their physiological changes. The transition from MTF, developed in 1925 [10], to ND references is an increasing demand for which it is essential to be able to establish a relationship between both kinds of measurements. In this work, **it was observed the feasibility of using optical and mechanical (low mass impact) ND measurements to estimate MTF** in the usual commercial firmness range through a linear model. Furthermore, **information about data structure was used for modelling MTF.**

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