ADAMS METHODS: IMPLEMENTATION AS PREDICTOR-CORRECTOR METHODS

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Abstract

In this paper, Adams explicit and implicit formulas are obtained in a simple way and a relationship between them is established, allowing for their joint implementation as predictor-corrector methods. It is shown the purposefulness, from a didactic point of view, of Excel spreadsheets for calculations and for the orderly presentation of results in the application of Adams methods to solving initial value problems in ordinary differential equations.

1. Introduction

Adams formulas are most popular methods in the whole family of linear multistep formulas for the numerical solution of nonstiff problems of ordinary differential equations. Formulas of Adams-Bashforth (explicit) have a simple implementation, while Adams-Moulton formulas (implicit) require
an iterative process prior to implementation in order to obtain an explicit expression for the term \( z_{n+1} \). In return, implicit formulas provide a better approximation to the value sought. This is why Adams formulas are often used in a combined way by means of the so-called prediction-correction procedures, in such a way to take advantage of implicit formulas and thus avoid its drawbacks: a value of \( z_{n+1} \) is predicted with an explicit Adams formula and then corrected with the corresponding implicit formula. In Sections 2 and 3 of this paper, Adams explicit and implicit formulas are obtained in a simple way and a relationship between them is established, allowing for their joint implementation. Finally in Section 4, the above formulas are applied to solving two initial value problems and analyzing results achieved. Basic tool used both for calculations and for the orderly presentation of results is an Excel spreadsheet, which greatly facilitates operations and is very useful from a didactic point of view.

2. Adams-Bashforth Formulas of 2, 3 and 4 Steps

Adams formulas are used for the numerical solution of initial value problems of ordinary differential equations, i.e., to obtain approximate values for the solution of problem (P)

\[
\begin{align*}
\dot{y} &= f(x, y) \\
y(x_0) &= y_0
\end{align*}
\]

in which the function \( f(x, y) \) fulfils the regularity conditions that allow us to assume the problem has a unique solution (Picard-Lindelöf theorem).

The discrete set of points that we consider is \( x_n = x_0 + nh \), being \( n = 0, 1, 2, \ldots \). Let us call \( y_n = y(x_n) \) the exact value of the solution of problem (P) at the point \( x_n \) and \( z_n \) the value that approximates the solution at the point \( x_n \), i.e., \( z_n \approx y_n \). The parameter \( h \) represents the step length.

The solution of (P) can be expressed as:

\[
y(x) = y_0 + \int_{x_0}^{x} f(t, y(t)) dt = y_n + \int_{x_n}^{x} f(t, y(t)) dt.
\]
Assuming values $y_0, y_1, ..., y_n$, are known, the value of $y_{n+1}$ can be obtained from the expression

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y(x)) \, dx.$$

Main difficulty to apply this formula lies in the fact that it is not possible to integrate $f(x, y(x))$ without knowing the solution $y(x)$. However, if we know the $k$ points $(x_n, z_n), ..., (x_{n-(k-1)}, z_{n-(k-1)})$, we may replace the function $f(x, y(x))$ by the interpolating polynomial, the single polynomial $P_k(x)$ of a degree less than or equal to $k - 1$ that fulfils $P_k(x_i) = f(x_i, z_i)$ with $i = n - (k - 1), ..., n$, and then obtain an approximate value of $y_{n+1}$ by integrating the polynomial instead of the function:

$$z_{n+1} = z_n + \int_{x_n}^{x_{n+1}} P_k(x) \, dx. \quad (1)$$

Henceforth we will use the notation $f_i = f(x_i, z_i)$.

All Adams methods are built based on the scheme presented in the previous paragraph. In this section, we will develop the 2, 3 and 4 step-formulas of Adams-Bashforth that will be implemented later in Section 4.

For obtaining the Adams-Bashforth method of $k = 2$ steps, we first build the interpolating polynomial $P_2(x)$ that passes through the points $(x_n, f_n)$ and $(x_{n-1}, f_{n-1})$,

$$P_2(x) = f_n + \frac{f_n - f_{n-1}}{h}(x - x_n)$$

and then we substitute into the formula (1) and integrate:

$$z_{n+1} = z_n + \int_{x_n}^{x_{n+1}} \left( f_n + \frac{f_n - f_{n-1}}{h}(x - x_n) \right) \, dx$$

$$= z_n + f_n h + \frac{f_n - f_{n-1}}{h} \frac{h^2}{2}.$$

Finally, we have $z_{n+1} = z_n + \frac{h}{2}(3f_n - f_{n-1})$ with $n = 1, 2, ...$ or its equivalent

$$z_{n+2} = z_{n+1} + \frac{h}{2}(3f_{n+1} - f_n) \quad \text{with } n = 0, 1, ....$$
The above expression is known as *Adams-Bashforth formula of two steps*.

Adams formulas can also be expressed by means of the so-called backward differences, which in many cases facilitate their implementation.

The value \( f_n - f_{n-1} = \nabla f_n \) is called *first order backward difference* for \( f_n \).

With this notation, the interpolator polynomial can be expressed as

\[
P_2(x) = f_n + \frac{\nabla f_n}{h} (x - x_n),
\]

and the method of Adams-Bashforth 2 takes the form:

\[
z_{n+1} = z_n + h \left( f_n + \frac{1}{2} \nabla f_n \right) \text{ with } n = 1, 2, \ldots
\]

The Adams-Bashforth method of \( k = 3 \) steps can be obtained in a similar way with the interpolating polynomial \( P_3(x) \) that passes through points \((x_n, f_n), (x_{n-1}, f_{n-1})\) and \((x_{n-2}, f_{n-2})\):

\[
P_3(x) = P_2(x) + \frac{f_n - 2f_{n-1} + f_{n-2}}{2h^2} (x - x_n)(x - x_{n-1}).
\]

For obtaining \( P_3(x) \), we use all calculations made in the case \( k = 2 \) and we only need to get the value of the integral \( \int_{x_n}^{x_{n+1}} (x - x_n)(x - x_{n-1})\) \(dx\),

which is equal to \( \frac{5h^3}{6} \).

Therefore,

\[
z_{n+1} = z_n + \frac{h}{2} (3f_n - f_{n-1}) + \frac{f_n - 2f_{n-1} + f_{n-2}}{2h^2} \frac{5h^3}{6}
\]

with \( n = 2, 3, \ldots \); and carrying out calculations, we arrive to:

\[
z_{n+1} = z_n + \frac{h}{12} (23f_n - 16f_{n-1} + 5f_{n-2}) \text{ with } n = 2, 3, \ldots,
\]

which is known as the *Adams-Bashforth formula of three steps*. 
Using second-order backward differences

\[ \nabla^2 f_n = \nabla f_n - \nabla f_{n-1} = f_n - 2f_{n-1} + f_{n-2}, \]

we obtain \( P_2(x) = P_2(x) + \frac{\nabla^2 f_n}{2h^2} (x - x_n)(x - x_{n-1}) \), and the method can also be written in the form:

\[ z_{n+1} = z_n + h \left( f_n + \frac{1}{2} \nabla f_n + \frac{5}{12} \nabla^2 f_n \right) \] with \( n = 2, 3, \ldots \)

Similarly, it follows the 4-step formula of Adams-Bashforth

\[ z_{n+4} = z_{n+3} + \frac{h}{24} (55f_{n+3} - 59f_{n+2} + 37f_{n+1} - 9f_n) \] with \( n = 0, 1, \ldots \)

or by using backward differences,

\[ z_{n+1} = z_n + h \left( f_n + \frac{1}{2} \nabla f_n + \frac{5}{12} \nabla^2 f_n + \frac{3}{8} \nabla^3 f_n \right) \] with \( n = 3, 4, \ldots \),

being \( \nabla^3 f_n = \nabla^2 f_n - \nabla^2 f_{n-1} \) the regressive difference of order 3.

The general expression of the Adams-Bashforth method of \( k \) steps is:

\[ z_{n+1} = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \gamma_2 \nabla^2 f_n + \cdots + \gamma_k \nabla^{k-1} f_n) \]

with \( n = k - 1, k, \ldots \),

where

\[ \gamma_0 = 1 \text{ and } \gamma_i = \frac{1}{i!} h^{i+1} \int_{x_n}^{x_{n+1}} \prod_{j=n-i+1}^{n} (x - x_j) dx \] for \( i = 1, \ldots, k - 1, \)

\[ \nabla^0 f_n = f_n, \quad \nabla^i f_n = \nabla^{i-1} f_n - \nabla^{i-1} f_{n-1} \] for \( i = 1, \ldots, k - 1. \)

We have already calculated the first coefficients: \( \gamma_0 = 1, \ \gamma_1 = 1/2, \gamma_2 = 5/12 \text{ and } \gamma_3 = 3/8. \)

One can also check that coefficients of Adams-Bashforth formulas verify the relationship \( \gamma_i + \frac{\gamma_{i-1}}{2} + \frac{\gamma_{i-2}}{3} + \cdots + \frac{\gamma_1}{i} + \frac{\gamma_0}{i+1} = 1 \) for \( i = 0, \ldots, k - 1. \)
The previous expression allows us to successively obtain the coefficients \( \gamma_i \) from the preceding ones. Thus, for example,

\[
\gamma_4 = 1 - \left( \frac{\gamma_3}{2} + \frac{\gamma_2}{3} + \frac{\gamma_1}{4} + \frac{\gamma_0}{5} \right) = \frac{251}{720}.
\]

The Adams-Bashforth method of steps \((k \geq 1)\) is convergent of order \(k\), and the truncation error of the method can be expressed as

\[
T_{n+k} = \gamma_k y_n h^{k+1} + O(h^{k+2}).
\]

### 3. Adams-Moulton Formulas

In this section, we will see how to deduce the implicit Adams formulas, known as *Adams-Moulton formulas*.

The structure of Adams-Moulton formulas of \(k\) steps is similar to that of the Adams-Bashforth formulas, but in this case, function \(f(x, y(x))\) is replaced by the interpolating polynomial passing through the points \((x_n, f_n), (x_{n-1}, f_{n-1}), \ldots, (x_{n-(k-2)}, f_{n-(k-2)}), (x_{n+1}, f_{n+1})\). It is noteworthy that \(f_{n+1} = f(x_{n+1}, z_{n+1})\) involves the actual value \(z_{n+1}\) we want to calculate and, therefore, the formula we get is implicit.

For example, to build the Adams-Moulton formula of \(k = 3\) steps, we consider the polynomial \(Q_4(x)\) of a degree less than or equal to 3 that passes through \((x_n, f_n), (x_{n-1}, f_{n-1}), (x_{n-2}, f_{n-2}), (x_{n+1}, f_{n+1})\):

\[
Q_4(x) = P_3(x) + \frac{\nabla^3 f_{n+1}}{3! h^3} (x - x_n)(x - x_{n-1})(x - x_{n-2})
\]

\[
= f_n + \frac{\nabla f_n}{h} (x - x_n) + \frac{\nabla^2 f_n}{2 h^2} (x - x_n)(x - x_{n-1})
\]

\[
+ \frac{\nabla^3 f_{n+1}}{6h^3} (x - x_n)(x - x_{n-1})(x - x_{n-2}).
\]
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One then performs the calculation of $z_{n+1}$:

$$z_{n+1} = z_n + \int_{x_n}^{x_{n+1}} Q_4(x) \, dx$$

$$= z_n + h \left( f_n + \frac{1}{2} \nabla f_n + \frac{5}{12} \nabla^2 f_n \right) + h \frac{3}{8} \nabla^3 f_{n+1}, \quad n = 2, 3, \ldots$$

and obtains the Adams-Moulton formula of $k = 3$ steps. The first terms of this formula are those of the Adams-Bashforth method of $k = 3$ steps and the last sum term is a corrector term of the value that provides the explicit formula of the same number of steps.

Regressive differences can be expressed in terms of values $f_{n+j}$ and we get another expression of the same method:

$$z_{n+3} = z_{n+2} + \frac{h}{24} (9 f_{n+3} + 19 f_{n+2} - 5 f_{n+1} + f_n), \quad n = 0, 1, \ldots$$

The general expression of the $k$-step Adams-Moulton method is:

$$z_{n+1} = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_{k-1} \nabla^{k-1} f_n)$$

$$+ h \gamma_k \nabla^k f_{n+1}, \quad n = k - 1, k, \ldots$$

where the coefficients $\gamma_i$ are those defined in Section 2.

This method is convergent of order $k + 1$. It is then concluded that implicit Adams formulas have faster convergence than the corresponding explicit ones. We further noted that if we call $z^0_{n+1}$ the approximate value obtained from the $k$-step Adams-Bashforth formula, and $z^1_{n+1}$ that obtained by the implicit Adams formula with the same number of steps, it holds that:

$$z^1_{n+1} = z^0_{n+1} + h \gamma_k \nabla^k f_{n+1}.$$

This tells us that if we know the value $z^0_{n+1}$ from an explicit formula, we can calculate the value provided by the corresponding implicit formula,
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$z_{n+1}^1$, without further to do a little extra effort calculation, thus achieving a greater degree of approximation.

The prediction-correction procedure with Adams formulas can also be applied to two formulas with the same order of convergence: if the explicit formula has $k$ steps, then the implicit one must have $k - 1$ steps. In this case, both formulas can also be combined. In fact, it is

$$z_{n+1}^0 = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_{k-1} \nabla^{k-1} f_n),$$

$$z_{n+1}^1 = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_{k-2} \nabla^{k-2} f_n + \gamma_{k-1} \nabla^{k-1} f_n) + h\gamma_{k-1} \nabla^{k-1} f_{n+1}.$$

We add and subtract the same amount to the second expression:

$$z_{n+1}^1 = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_{k-2} \nabla^{k-2} f_n + \gamma_{k-1} \nabla^{k-1} f_n + h\gamma_{k-1} \nabla^{k-1} f_{n+1} - h\gamma_{k-1} \nabla^{k-1} f_n)$$

and we obtain

$$z_{n+1}^1 = z_n + h(\gamma_0 \nabla^0 f_n + \gamma_1 \nabla f_n + \cdots + \gamma_{k-2} \nabla^{k-2} f_n + \gamma_{k-1} \nabla^{k-1} f_n) + h\gamma_{k-1} \nabla^{k} f_{n+1}$$

$$= z_{n+1}^0 + h\gamma_{k-1} \nabla^{k} f_{n+1}.$$

It is then obtained in this case the expression:

$$z_{n+1}^1 = z_{n+1}^0 + h\gamma_{k-1} \nabla^{k} f_{n+1}.$$

4. Application to the Resolution of Two Initial Value Problems

We present thereafter the results obtained by applying the Adams formulas to solve two initial value problems. The exact solution in the first one is known and we can then compare this value with those obtained by the different methods applied. On the contrary, in the second one the solution cannot be obtained explicitly and only approximate values can be obtained.

In both cases, we follow the same procedure to obtain the approximate value of the solution at $x = 1$: we first apply different Adams-Bashforth
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formulas with different initial additional values and analyze the results achieved. Then we apply the prediction correction formula obtained by combining the 4-step Adams-Bashforth formula with the 3-step Adams-Moulton formula, both with convergence order 4, and we compare the values achieved with those obtained above.

**Problem 1.** Given the differential equation \( y' = 2xy \) with the initial condition \( y(0) = 1 \), obtain the approximate value of the solution at \( x = 1 \).

The solution of the IVP is \( y(x) = \exp(x^2) \), and therefore \( y(1) = e = 2.71828183 \ldots \).

We will first use the methods of Adams-Bashforth of 2, 3 and 4 steps, with \( h = 0.2, \ 0.1 \) and \( 0.05 \), to obtain approximate values of the solution at \( x = 1 \).

We can apply these methods on the IVP using an Excel sheet and compare the different results obtained with the exact value.

The approximate values of \( y(1) \) obtained by using the methods of Adams-Bashforth of 2, 3 and 4 steps (AB2, AB3 and AB4), taking \( h = 0.2, \ 0.1 \) and \( 0.05 \), are represented in bold in Table 4.1. The initial additional values are obtained by different one-step methods: Euler, Runge-Kutta 4 (RK4) and exact values. Errors that have occurred in each case are also represented.

**Table 4.1.** Approximate values of \( y(1), y(x) \) solution of Problem 1

<table>
<thead>
<tr>
<th>( h )</th>
<th>AB2+Euler</th>
<th>AB2+exact</th>
<th>AB3+Euler</th>
<th>AB3+exact</th>
<th>AB4+Euler</th>
<th>AB4+RK4</th>
<th>AB4+exact</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>2.42040064</td>
<td>2.51917906</td>
<td>2.40939989</td>
<td>2.62549227</td>
<td>2.34056178</td>
<td>2.68586806</td>
<td>2.68588428</td>
</tr>
<tr>
<td>Error</td>
<td>0.29788119</td>
<td>0.19910276</td>
<td>0.30888194</td>
<td>0.09278956</td>
<td>0.37772005</td>
<td>0.03241377</td>
<td>0.03239755</td>
</tr>
<tr>
<td>0.1</td>
<td>2.62338018</td>
<td>2.64974558</td>
<td>2.64379751</td>
<td>2.69823208</td>
<td>2.63035899</td>
<td>2.71334472</td>
<td>2.71334476</td>
</tr>
<tr>
<td>Error</td>
<td>0.09490165</td>
<td>0.06853624</td>
<td>0.07448432</td>
<td>0.02004975</td>
<td>0.08792284</td>
<td>0.00493711</td>
<td>0.00493707</td>
</tr>
<tr>
<td>0.05</td>
<td>2.6916606</td>
<td>2.69839817</td>
<td>2.7014941</td>
<td>2.71510034</td>
<td>2.69735449</td>
<td>2.71783957</td>
<td>2.71783957</td>
</tr>
<tr>
<td>Error</td>
<td>0.02662123</td>
<td>0.01988366</td>
<td>0.01678772</td>
<td>0.00318149</td>
<td>0.02092734</td>
<td>0.00044226</td>
<td>0.00044226</td>
</tr>
</tbody>
</table>
Table 4.1 shows the behaviour of the Adams-Bashforth formulas: we can see that the results obtained for the value of $y(1)$ generally improve the error incurred if the formula has a higher number of steps, provided that the initial values have been properly chosen. This can be seen by comparing columns 3, 5, 7 and 8.

However, if the initial additional values are taken from a formula with lower convergence order, it may happen that a formula with a greater number of steps cannot compensate errors incurred in obtaining the initial additional values. This is what happens when we get the approximate value of $y(1)$, with $h = 0.2$, (row 2 of Table 4.1) by AB2, AB3 and AB4 methods, when they are taken as initial additional values those obtained by Euler’s formula: the approximate value obtained with AB2 is better than with AB3, and this in turn is better than with AB4.

We then apply the combined method of Adams-Bashforth-Moulton 4 (ABM4) to improve the results. Then we use the 4-step Adams-Bashforth and 3-step Adams-Moulton combined formulas. Both have convergence order 4:

$$z_{n+1}^0 = z_n + h \left( f_n + \frac{1}{2} \nabla f_n + \frac{5}{12} \nabla^2 f_n + \frac{3}{8} \nabla^3 f_n \right),$$

$$z_{n+1}^1 = z_n + h \left( f_n + \frac{1}{2} \nabla f_n + \frac{5}{12} \nabla^2 f_n \right) + h^3 \frac{3}{8} \nabla^3 f_{n+1}.$$

Both formulas can be related by the expression

$$z_{n+1}^1 = z_{n+1}^0 + h^3 \frac{3}{8} \nabla^4 f_{n+1}.$$

We again use an Excel sheet and obtain the corresponding results shown in the third column of Table 4.2.
The results obtained by applying ABM4 clearly improve those obtained with the Adams-Bashforth method 4 (column 2).

**Problem 2.** Given the differential equation \( y' = x^2 + y^2 \) with the initial condition \( y(0) = 0 \), obtain the approximate value of the solution at \( x = 1 \).

In this case, we do not know the solution and therefore, we apply different Adams-Bashforth methods for obtaining an approximate result of \( y(1) \), by dividing the step size a larger number of times.

We will use as before Adams-Bashforth methods of 2, 3 and 4 steps, but now we take \( h = 0.2, 0.1, 0.05, 0.025 \) and \( 0.0125 \).

We perform the calculations easily by using an Excel sheet and will compare the results. Table 4.3 summarizes the results obtained in the application of each method.

**Table 4.3.** Approximate values of \( y(1), y(x) \) solution of Problem 2

<table>
<thead>
<tr>
<th>( h )</th>
<th>AB2+Euler</th>
<th>AB3+Euler</th>
<th>AB4+Euler</th>
<th>AB4+RK4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.31131468</td>
<td>0.330064477</td>
<td>0.310185206</td>
<td>0.347292904</td>
</tr>
<tr>
<td>0.1</td>
<td>0.338924768</td>
<td>0.347222491</td>
<td>0.345093961</td>
<td>0.349819849</td>
</tr>
<tr>
<td>0.05</td>
<td>0.347184899</td>
<td>0.349812959</td>
<td>0.349601634</td>
<td>0.350194441</td>
</tr>
<tr>
<td>0.025</td>
<td>0.349441778</td>
<td>0.350176269</td>
<td>0.350154879</td>
<td>0.350229015</td>
</tr>
<tr>
<td>0.0125</td>
<td>0.350030776</td>
<td>0.350239349</td>
<td>0.350250957</td>
<td>0.350231649</td>
</tr>
</tbody>
</table>
Table 4.3 shows again the behaviour of Adams-Bashforth formulas: To calculate the values shown in column 5, we have used at any time fast-convergence formulas (fourth order), and therefore the approximations obtained must be “good”. We can say at least that the first four decimal figures must match the exact solution and that the error we made must be less than $10^{-5}$. If we now look at the values obtained in column 4, we see that the values of $y(1)$ with the four-step Adams-Bashforth method are worse than those obtained with Adams-Bashforth 3 (column 3). This is because initial additional values were calculated by using the slow convergence Euler’s formula. This highlights the importance of taking initial additional values with a minimal error.

We then apply the combined method of Adams-Bashforth-Moulton 4 as in Problem 1 applied to improve the results. Again, we use an Excel sheet and obtain the corresponding results shown in the third column of Table 4.4.

<table>
<thead>
<tr>
<th>$h$</th>
<th>AB4+RK4</th>
<th>ABM4+RK4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.347292904</td>
<td>0.350537266</td>
</tr>
<tr>
<td>0.1</td>
<td>0.349819849</td>
<td>0.350268805</td>
</tr>
<tr>
<td>0.05</td>
<td>0.350194441</td>
<td>0.350234934</td>
</tr>
<tr>
<td>0.025</td>
<td>0.350229015</td>
<td></td>
</tr>
<tr>
<td>0.0125</td>
<td>0.350231649</td>
<td></td>
</tr>
</tbody>
</table>

We can see that it suffices to apply the ABM4 prediction-correction method with initial additional values obtained from RK4 and $h = 0.05$ to obtain an approximate value similar to that obtained with AB4 and $h = 0.0125$ (column 2), which also in this case represents a clear improvement over previously obtained results.

References

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