

A Matrix System for Computing the Coefficients of the Adams Bashforth-Moulton Predictor-Corrector formulae

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Abstract

This paper seeks to show that the k^{th} order Adams Bashforth and Adams Moultons methods are derivable from simple systems of linear equations. The paper uses the often used method of Taylor series expansion to derive matrix systems that can be solved to give the coefficients of the Adams Bashforth and Adams Moultons predictor-corrector formulae used in the solution of first order ordinary differential equations. The contribution in this paper is meant to reduce the work needed during the derivation of the predictor-corrector formulae. A MATLAB m-file is also include for MATLAB implementation of the method. An illustrative example is given to prove the simplicity of the contribution.

Keywords: Ordinary Differential Equations, Numerical Solution, Multistep methods, Predictor-Corrector methods.

Introduction

The solution of first order ordinary differential equations of the form $y' = \frac{dy}{dx} = f(x, y)$ is of so much importance in numerical methods due to the fact that even higher order partial differential equations can be transformed into first order ordinary differential equations and solved. Thus, methods of solution of equations of the form $y' = \frac{dy}{dx} = f(x, y)$ have attracted attention of researchers for a very long time. Several schemes for solutions of ODEs exist. Some include the single step methods (Runge-Kutta, Euler, Heuns, etc) and multi-step methods. Examples of the multistep methods are the predictor-corrector methods of Adams Bashforth and Moulton. These schemes involve the use of explicit formulae to make a prediction of the current value of the dependent variable y and then use implicit (corrector) formulae to make a final

approximation to the current value of y . These predictor-corrector methods can be obtained using a number of methodologies; among which is the use Taylor series expansion of y_n about h [4]. The process of generating these formulae is straight forward but gets very tedious as the order of the method gets higher. The purpose of this paper is to present an easier and simpler way of generating these formulae even for higher order.

Derivation of Adams Bashforth Predictor System

We seek to find a simpler way out in deriving the Adams Bashforth formulae in this brief. There are several methods used in deriving these formulae. These methods however require Taylor series expansions and other simplifications. We seek to find a way of deriving the formulae without having to follow these tedious Taylor series expansions and simplifications. It can be shown that the Adams Bashforth formulae can be generated by solving a system of linear equations. We seek to develop a recipe for these systems here. The general Adams Bashforth formulae is of the form

$$y_{n+1} = y_n + h \sum_{i=1}^k b_i y'_{n-i+1} \quad (1.1)$$

Where k is the order of the Adams method.

Thus, the k^{th} order predictor formula is given by:

$$y_{n+1} = y_n + h \left(b_1 y'_n + b_2 y'_{n-1} + b_3 y'_{n-2} + \dots + b_{k-1} y'_{n-k+2} + b_k y'_{n-k+1} \right) \quad (1.2)$$

The terms $y'_n, y'_{n-1}, y'_{n-2}, \dots, y'_{n-k+2}$, and y'_{n-k+1} are then expanded using Taylor series, truncated after the k^{th} terms and substituted into the above equation.

Thus, expanding the terms $y'_n, y'_{n-1}, y'_{n-2}, \dots, y'_{n-k+2}$, and y'_{n-k+1} and substituting them into equation (1.2) we have

$$\begin{aligned} y_{n+1} = & y_n + h \left\{ b_1 y'_n + b_2 \left(y'_n - h y''_n + \frac{1}{2!} h^2 y'''_n - \frac{1}{3!} h^3 y''''_n + \dots \pm \frac{1}{(k-1)!} h^{(k-1)} y_n^{(k)} \right) \right. \\ & + b_3 \left(y'_n - 2h y''_n + \frac{1}{2!} (2h)^2 y'''_n - \frac{1}{3!} (2h)^3 y''''_n + \dots \pm \frac{1}{(k-1)!} (2h)^{(k-1)} y_n^{(k)} \right) + \dots \\ & + b_{k-1} \left(y'_n - (k-2)h y''_n + \frac{1}{2!} ((k-2)h)^2 y'''_n - \frac{1}{3!} ((k-2)h)^3 y''''_n + \dots \pm \frac{1}{(k-1)!} ((k-2)h)^{(k-1)} y_n^{(k)} \right) \\ & \left. + b_k \left(y'_n - (k-1)h y''_n + \frac{1}{2!} ((k-1)h)^2 y'''_n - \frac{1}{3!} ((k-1)h)^3 y''''_n + \dots \pm \frac{1}{(k-1)!} ((k-1)h)^{(k-1)} y_n^{(k)} \right) \right\} \end{aligned}$$

Expanding and grouping like terms gives

$$\begin{aligned} y_{n+1} = & y_n + (b_1 + b_2 + b_3 + \dots + b_{k-1} + b_k) h y'_n - [b_2 + 2b_3 + \dots + (k-2)b_{k-1} + (k-1)b_k] h^2 y''_n + \\ & \frac{1}{2!} [b_2 + 2^2 b_3 + \dots + (k-2)^2 b_{k-1} + (k-1)^2 b_k] h^3 y'''_n - \frac{1}{3!} [b_2 + 2^3 b_3 + \dots + (k-2)^3 b_{k-1} + (k-1)^3 b_k] h^4 y''''_n + \dots \end{aligned}$$

$$\pm \frac{1}{(k-1)!} [b_2 + 2^{(k-1)}b_3 + \dots + (k-2)^{(k-1)}b_{k-1} + (k-1)^k b_k] h^{(k-1)} y_n^{(k)}$$

Comparing this equation with the Taylor series expansion of y_{n+1} :

$$y_{n+1} = y_n + h y'_n + \frac{1}{2} h^2 y''_n + \frac{1}{3!} h^3 y'''_n + \dots + \frac{1}{(k-1)!} h^{(k-1)} y_n^{(k-1)} + \frac{1}{k!} h^k y_n^{(k)} + \dots$$

we have the following system of equations:

$$\begin{aligned} b_1 + b_2 + b_3 + \dots + b_{k-1} + b_k &= 1 \\ b_2 + 2b_3 + \dots + (k-2)b_{k-1} + (k-1)b_k &= -\frac{1}{2} \\ b_2 + 2^2b_3 + \dots + (k-2)^2b_{k-1} + (k-1)^2b_k &= \frac{1}{3} \\ b_2 + 2^3b_3 + \dots + (k-2)^3b_{k-1} + (k-1)^3b_k &= -\frac{1}{4} \\ &\vdots \\ &\vdots \\ b_2 + 2^{(k-1)}b_3 + \dots + (k-2)^{(k-1)}b_{k-1} + (k-1)^{(k-1)}b_k &= (-1)^{(k-1)} \frac{1}{k} \end{aligned} \tag{1.3}$$

Writing this system as a matrix equation gives

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 & 1 \\ 0 & 1 & 2 & \dots & k & (k-1) \\ 0 & 1 & 2^2 & \dots & k^2 & (k-1)^2 \\ 0 & 1 & 2^3 & \dots & k^3 & (k-1)^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2^{(k-1)} & \dots & k^{(k-1)} & (k-1)^{(k-1)} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ \vdots \\ b_k \end{bmatrix} = \begin{bmatrix} 1 \\ -\frac{1}{2} \\ \frac{1}{3} \\ -\frac{1}{4} \\ \vdots \\ (-1)^{(k-1)} \frac{1}{k} \end{bmatrix} \tag{1.4}$$

Thus, the coefficients of the explicit Adams Bashforth predictor formula can be found by solving the matrix system $[a_{ij}][b_i] = [c_i]$,

Where $a_{ij} = (j-1)^{i-1}$, and $c_i = (-1)^{(i-1)} \frac{1}{i}$, $i = 1, 2, \dots, k$

Adams Moulton Corrector Coefficients

The k^{th} order Adams Moulton corrector formula is given by [4]

$$y_{n+1} = y_n + h \sum_{i=1}^k b_i y'_{n-i+2}$$

Hence

$$y_{n+1} = y_n + h (b_1 y'_{n+1} + b_2 y'_n + b_3 y'_{n-1} + \dots + b_{k-1} y'_{n-k+3} + b_k y'_{n-k+2}) \tag{1.5}$$

Expanding the terms $y'_{n+1}, y'_n, y'_{n-1}, y'_{n-2}, \dots, y'_{n-k+3}$, and y'_{n-k+2} using Taylor series, truncating them after the k th terms and substituting them into the above equation gives:

$$y_{n+1} = y_n + h \left\{ b_1 \left(y'_n + h y''_n + \frac{1}{2!} h^2 y'''_n + \frac{1}{3!} h^3 y''''_n + \dots + \frac{1}{(k-1)!} h^{(k-1)} y_n^{(k)} \right) + \right.$$

$$\begin{aligned}
 & b_2 y'_n + b_3 \left(y'_n - h y''_n + \frac{1}{2!} h^2 y'''_n - \frac{1}{3!} h^3 y''''_n + \dots \pm \frac{1}{(k-1)!} h^{(k-1)} y_n^{(k)} \right) + \dots + \\
 & b_{k-1} \left(y'_n - (k-3) h y''_n + \frac{1}{2!} ((k-3)h)^2 y'''_n - \frac{1}{3!} ((k-3)h)^3 y''''_n + \dots \pm \frac{1}{(k-1)!} ((k-3)h)^{(k-1)} y_n^{(k)} \right) + \\
 & b_k \left(y'_n - (k-2) h y''_n + \frac{1}{2!} ((k-2)h)^2 y'''_n - \frac{1}{3!} ((k-2)h)^3 y''''_n + \dots \pm \frac{1}{(k-1)!} ((k-2)h)^{(k-1)} y_n^{(k)} \right) \}
 \end{aligned}$$

Expanding and grouping like terms, we have

$$\begin{aligned}
 y_{n+1} = & y_n + (b_1 + b_2 + b_3 + \dots + b_{k-1} + b_k) h y'_n + [b_1 - b_3 - \dots - (k-3)b_{k-1} - (k-2)b_k] h^2 y''_n + \\
 & \frac{1}{2!} [b_1 + b_3 + \dots + (k-3)^2 b_{k-1} + (k-2)^2] h^3 y'''_n + \frac{1}{3!} [b_1 - b_3 - \dots - (k-3)^3 b_{k-1} - (k-2)^3] h^4 y''''_n + \\
 & \dots \frac{1}{(k-2)!} [b_1 \pm b_3 \pm \dots \pm (k-3)^{(k-2)} b_{k-1} \pm (k-2)^{(k-2)}] h^{(k-1)} y_n^{(k-1)} + \\
 & \frac{1}{(k-1)!} [b_1 \pm b_3 \pm \dots \pm (k-3)^{(k-1)} b_{k-1} \pm (k-2)^{(k-1)}] h^k y_n^{(k)}
 \end{aligned}$$

Comparing this formula with the Taylor series expansion gives the following set of linear equations

$$\begin{aligned}
 & b_1 + b_2 + b_3 + \dots + b_{k-1} + b_k = 1 \\
 & b_1 - b_3 - \dots - (k-3)b_{k-1} - (k-2)b_k = \frac{1}{2} \\
 & b_1 + b_3 + \dots + (k-3)^2 b_{k-1} + (k-2)^2 = \frac{1}{3} \\
 & b_1 - b_3 - \dots - (k-3)^3 b_{k-1} - (k-2)^3 = \frac{1}{4} \\
 & \vdots \\
 & \vdots \\
 & \vdots \\
 & b_1 \pm b_3 \pm \dots \pm (k-3)^{(k-2)} b_{k-1} \pm (k-2)^{(k-2)} = \frac{1}{(k-1)} \\
 & b_1 \pm b_3 \pm \dots \pm (k-3)^{(k-1)} b_{k-1} \pm (k-2)^{(k-1)} = \frac{1}{k}
 \end{aligned}$$

Or in matrix form, we have

$$\begin{bmatrix}
 1 & 1 & 1 & 1 & \dots & 1 & 1 \\
 -1 & 0 & 1 & 2 & \dots & (k-3) & (k-2) \\
 1 & 0 & 1 & 2^2 & \dots & (k-3)^2 & (k-2)^2 \\
 \vdots & \vdots & \dots & \dots & \vdots & \dots & \vdots \\
 \pm 1 & 0 & 1 & (2)^{(k-2)} & \dots & (k-3)^{(k-2)} & (k-2)^{(k-2)} \\
 \pm 1 & 0 & 1 & 2^{(k-1)} & \dots & (k-3)^{(k-1)} & (k-2)^{(k-1)}
 \end{bmatrix}
 \begin{bmatrix}
 b_1 \\
 b_2 \\
 b_3 \\
 \vdots \\
 b_{k-1} \\
 b_k
 \end{bmatrix}
 =
 \begin{bmatrix}
 1 \\
 -\frac{1}{2} \\
 \frac{1}{3} \\
 \vdots \\
 \pm \frac{1}{k-1} \\
 \pm \frac{1}{k}
 \end{bmatrix}
 \tag{1.6}$$

Thus, the coefficients for the Adams Moulton corrector formula can be obtained by solving the system $[a_{ij}][b_i] = [c_i]$ where $a_{ij} = (j-2)^{i-1}$, $c_i = (-1)^{i-1} \frac{1}{i}$

MATLAB implementation

```

% This function finds the coefficients of the Adams
Bashforth predictor formulae of order 'order'
function [Adamsbashcoefficients]=Abashcoefficients(order)
format rat
    
```

```

A=zeros(order);
c=ones(order,1);
for i=1:order
    for j=1:order
        A(i,j)=(j-1)^(i-1);
    end
    c(i,1)=(-1)^(i-1)/i;
end
Adamsbashcoefficients=inv(A)*c;
% This function finds the coefficients of the Adams
Moulton corrector formulae of order 'order'
function
AdamsMoultonmoultonCoefficients=Amoultoncoefficients(orde
r)
format rat
A=zeros(order);
c=ones(order,1);
for i=1:order
    for j=1:order
        A(i,j)=(j-2)^(i-1);
    end
    c(i)=(-1)^(i-1)/i;
end
solution=(inv(A)*c)';
[N,D]=rat(solution);
temp1=abs(max(D));temp2=temp1./D;temp3=N.*temp2;
AdamsMoultonmoultonCoefficients=['1/'      num2str(temp1)
mat2str(temp3') ]';

```

Illustration

In this section, we illustrate the veracity of our proposed method. We shall use the proposed method to derive the coefficients of the 3rd order Adams Bashforth predictor formula which is given by $y_{n+1} = y_n + \frac{1}{12}h(23f_n - 16f_{n-1} + 5f_{n-2})$ and the Adams Moulton corrector formula which is given by $y_{n+1} = y_n + \frac{1}{12}h(5f_{n+1} + 8f_n - 1f_{n-1})$, where $f = y'$

For Adams Bashforth predictor coefficients, using the proposed system form

We have:

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \\ 0 & 1 & 4 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -\frac{1}{2} \\ \frac{1}{3} \end{bmatrix}$$

Solving this system gives $b_1 = \frac{23}{12}$, $b_2 = -\frac{16}{12}$, and $b_3 = \frac{5}{12}$

For Adams Moulton corrector coefficients, using the proposed system we have:

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -1/2 \\ 1/3 \end{bmatrix}$$

Solving this system gives

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} \frac{5}{12} \\ 8/12 \\ -1/12 \end{bmatrix} \quad (1.7)$$

References

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