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MULTISTEP METHODS FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS MADE SELF-STARTING

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INTRODUCTION

Milne's method and other similar multistep ones for the approximate solution of differential equations, are not self-starting. They require the use of known p pivotal points $(x_i, y(x_i))$, $i = 0, 1, \ldots, (p—1)$, where x's are equally spaced and $y = y(x)$ is the solution of the differential equation.

Usually these pivotal points are generated through the use of a set of so-called p-point formulas, preferably p being an odd integer. But these p-point formulas are not self-starting either.

A rational method is established herein which will make these p-point formulas, and consequently also the multistep methods, self-starting.

Subsequently the method is extended to systems of diferantial equations.

We shall be concerned first with the approximate solution of ordinary differential equations,

$$\frac{dy}{dx} = f(x, y) \qquad (1)$$

subject to the initial condition $x = a$, $y = b$, with a multistep method [7a]. Later we shall consider the case of systems of ordinary differential equations.

In these methods a certain number of pivotal points must be determined first, for instance, with a set of p-point formulas [12].

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We have thus the well known three-point formulas:

$$y_n(a+h) = b + \frac{h}{12}\left[5f(a) + 8f_{n-1}(a+h) - f_{n-1}(a+2h)\right] \qquad (2a)$$

$$y_n(a+2h) = b + \frac{h}{3}\left[f(a) + 4f_{n-1}(a+h) + f_{n-1}(a+2h)\right],\ n = 1, 2, \ldots \qquad (2b)$$

where $y(x)$ is the solution of (1) and

$$f(a) = f(a, b)$$

$$f_{n-1}(a+ih) = f(a+ih, y_{n-1}(a+ih)), \quad i = 1, 2.$$

It will be assumed that the step-length « h » is chosen so as to assure the convergence of the process to the limits $\tilde{y}(a+h)$ and $\tilde{y}(a+2h)$ for ($2a$) and ($2b$) respectively [$2a$].

These limiting values, $\tilde{y}(a+h)$ and $\tilde{y}(a+2h)$, are known to be third-order and fourth-order approximations to $y(a+h)$ and $y(a+2h)$, respectively.

As the reader recognizes, [$2b$] is analogous to the well known and highly efficient Newton-Cotes quadrature formula [6, 9] which is often erroneously referred to as Simpson's one third rule or merely Simpson's formula [4, 5, $7c$, $8a$, 10].

Unfortunately, these 3-point formulas, like all other p-point formulas, also are not self-starting and the initial or starting approximations $y_0(a+ih)$, $i = 1, 2$, must be determined either by guess or other systematic ways which may be called « auxiliary starting methods ».

However what is referred to in the literature as « guessed values » is usually obtained through the use of the formulas $y_0(a+ih) = b + ihf(a)$, $i = 1, 2$. These formulas as it is seen require only one substitution or functional evaluation, namely $f(a)$ and provide first-order approximations for the ordinates $y(a+ih)$, $i = 1, 2$, respectively.

A few auxiliary methods are based upon the use of higher-order derivatives of the solution $y(x)$ [$3b$, 11]. This renders the method impractical in most cases except when these derivatives can be expressed in simple analytical form.

In some other auxiliary methods use is made of formulas which require at least three substitutions and yield two second-order approximations $y_0\,(a+ih)$, $i = 1, 2$ for $y\,(a+ih)$, $i = 1, 2$, respectively [3*b*, p. 81]. With one additional substitution, that is, with four substitutions in all, we may obtain the two improved second-order approximations $y_1\,(a+ih)$, $i = 1, 2$; and with a total of five substitutions the value $y_1\,(a+3h)$ is obtained which may also be considered as an improved second-order approximation for $y\,(a+3h)$.

At any rate these approximations are not quite satisfactory and are referred to as « rough values » by Collatz in [3*b*, p. 81].

It is our immediate purpose to establish an auxiliary method, based upon the formulas, (2*a*, *b*), which with four substitutions yield third-order approximations for the ordinates of six appropriate points on the integral curve.

All these results are summarized in the following table of which the last row pertains to the method that will be established in this work.

Number of substitutions	Number of approximated points	Order of approximation
1	2	1st
3	2	2nd
4	2	improved 2nd
5	3	improved 2nd
4	6	3rd

In turn, in various ways these third-order approximations can be improved and their number increased from 6 to a number m. The m known points thus obtained will constitute the pivotal points of the multistep method.

However it is worthwhile mentioning that four pivotal points are sufficient to make self-starting a moderately accurate multistep method (such as the well known Milne's method). For better results one needs more than four pivotal points, since it is a well established fact, at least theoretically, that the bigger the number of pivotal points the better are the obtained approximations.

Another way to generate 6 such third-order approximations or points is to use a Runge-Kutta formula of third-order six consecutive times. But since these formulas require 3 substitutions for each generated point, for the 6 points one would need 18 subtitutions. This far exceeds the number of four substitutions needed in our proposed method.

We shall begin by establishing a theorem which not only will render the 3-point formulas self-starting but which will also provide two third-order approximations of our proposed six. The remaining four points or approximations will be the subject of another theorem.

Theorem I: If one takes

$$y_0(a+h) = b + hf(a,b) \quad \ldots\ldots \text{ in } (2a) \text{ and } (2b) \tag{3a}$$

$$y_0(a+2h) = b + 4hf(a,b) - 2hf(a+h, y_0(a+h)) \quad \ldots \text{ in } (2a) \tag{3b}$$

$$y_0(a+2h) = b - 2hf(a,b) + 4hf(a+h, y_0(a+h)) \quad \ldots \text{ in } (2b) \tag{3c}$$

then $y_1(a+h)$ and $y_1(a+2h)$ become third-order approximations to $y(a+h)$ and $y(a+2h)$, respectively.

Proof: With these starting approximations the formulas (2a, b) become

$$y_1(a+h) = b + \frac{h}{12}\{5f(a,b) + 8f[a+h, b+hf(a,b)] - f[a+2h, b+4hf(a,b)-2hf[a+h, b+hf(a,b)]]\} \tag{4a}$$

$$y_1(a+2h) = b + \frac{h}{3}\{f(a,b) + 4f[a+h, b+hf(a,b)] + f[a+2h, b-2hf(a,b)+4hf[a+h, b+hf(a,b)]]\}. \tag{4b}$$

Expanding the right hand side of (4a) and (4b) in Taylor series about (a, b) and up to and including the term in h^3 we obtain

$$y_1(a+h) = b + hf + \frac{h^2}{2}(f_x + ff_y)$$
$$+ \frac{h^3}{6}[f_{xx} + 2ff_{xy} + f^2 f_{yy} + (f_x + ff_y)f_y] + 0(h^4) \tag{5a}$$

$$y_1(a+2h) = b + 2hf + 2h^2(f_x + ff_y)$$
$$+ \frac{4h^3}{3}[f_{xx} + 2ff_{xy} + f^2 f_{yy} + (f_x + ff_y)f_y] + 0(h^4) \tag{5b}$$

where f stands for $f(a, b)$ and all the partial derivatives are evaluated at (a, b).

On observing that

$$\frac{d^2 y}{dx^2} = f_x + ff_y$$

$$\frac{d^3 y}{dx^3} = f_{xx} + 2ff_{xy} + f^2 f_{yy} + (f_x + ff_y)f_y$$

expansions (5a) and (5b) can be written

$$\begin{aligned} y_1(a+h) &= b + hf + \frac{h^2}{2}y'' + \frac{h^3}{6}h''' + 0(h^4) \\ y_1(a+2h) &= b + 2hf + 2h^2 y'' + \frac{4}{3}h^2 y''' + 0(h^4) \end{aligned} \tag{6a}$$

where the derivatives y'' and y''' are evaluated at $x = a$.

It is readily recognizable that the expansions (6a) and (6b) are none other than Taylor series through the term in h^3 of $y(a+h)$ and $y(a+2h)$ respectively.

Because of this agreement through the term in h^3 of the two pairs of Taylor series in consideration, it follows that $y_1(a+h)$ and $y_1(a+2h)$ constitute third-order approximations to $y(a+h)$ and $y(a+2h)$, respectively. And this completes the proof of the theorem.

It goes without saying that if so desired, the two third-order approximations $y_1(a+h)$, $y_1(a+2h)$ which required 4 substitutions, can be further improved through the use of the iterative 3-point formulas (2a, b).

It should be remarked that the approximation $y_1\,(a+2h)$ furnished by Theorem I, specifically that shown in $(4b)$, is identical with a formula due to Kutta; see (6.16.1) and (6.16.2) of [8b].

We shall now establish another theorem which, with no additional substitutions, that is by making use of the information furnished by Theorem I, will provide us the remaining four third-order approximations of our proposed six.

THOREM II: The following values

$$y_1(a-h) = -\frac{3}{2}b - 3hf + 3y_1(a+h) - \frac{1}{2}y_1(a+2h) \qquad (7a)$$

$$y_1(a-2h) = -12b - 12hf + 16y_1(a+h) - 3y_1(a+2h) \qquad (7b)$$

$$y_1(a+3h) = \frac{11}{2}b + 3hf - 9y_1(a+h) + \frac{9}{2}y_1(a+2h) \qquad (7c)$$

$$y_1(a-3h) = -35b - 30hf + 45y_1(a+h) - 9y_1(a+2h) \qquad (7d)$$

constitute third-order approximations to $y\,(a-h)$, $y\,(a-2h)$, $y\,(a+3h)$ and $y\,(a-3h)$ respectively.

Proof. From $(6a)$ and $(6b)$ it also follows that the quantities $b + (ih)\,f + \frac{(ih)^2}{2}\,y'' + \frac{(ih)^3}{6}\,y'''$, $i = 1, 2$, constitute third-order approximations for $y_1\,(a+ih)$, $i = 1, 2$, respectively.

We thus can set, approximately:

$$y_1(a+h) \approx b + hf + \frac{h^2}{2}y'' + \frac{h^3}{6}y'''$$

$$y_1(a+2h) \approx b + 2hf + 4\left(\frac{h^2}{2}y''\right) + 8\left(\frac{h^3}{6}y'''\right),$$

these approximations being of third order.

Then

$$\left(\frac{h^2}{2}y''\right) + \left(\frac{h^3}{6}y'''\right) \approx y_1(a+h) - b - hf$$

$$4\left(\frac{h^2}{2}y''\right) + 8\left(\frac{h^3}{6}y'''\right) \approx y_1(a+2h) - b - 2hf.$$

Solving this system of simultaneous equations for $\left(\frac{h^2}{2} y''\right)$ and $\left(\frac{h^3}{6} y'''\right)$ we obtain:

$$\frac{h^2}{2} y'' \approx \frac{1}{4}[8y_1(a+h) - y_1(a+2h) - 7b - 6hf] \tag{8}$$

$$\frac{h^3}{6} y''' \approx \frac{1}{4}[y_1(a+2h) - 4y_1(a+h) + 3b + 2hf], \tag{9}$$

these approximations being of third order.

On the other hand we have the following expansions:

$$y(a-h) = b - hf + \frac{h^2}{2} y'' - \frac{h^3}{6} y''' + 0(h^4) \tag{10a}$$

$$y(a-2h) = b - 2hf + 4\frac{h^2}{2} y'' - 8\frac{h^3}{6} y''' + 0(h^4) \tag{10b}$$

$$y(a+3h) = b + 3hf + 9\frac{h^2}{2} y'' + 27\frac{h^3}{6} y''' + 0(h^4) \tag{10c}$$

$$y(a-3h) = b - 3hf + 9\frac{h^2}{2} y'' - 27\frac{h^3}{6} y''' + 0(h^4). \tag{10d}$$

The third degree polynomials in h appearing in the right hand side of (10a), (10b), (10d), and (10c) constitute third-order approximations for $y\,(a—h)$, $y\,(a—2h)$, $y\,(a+3h)$ and $y\,(a—3h)$, respectively. Thus we can set

$$y_1(a-h) = b - hf + \left(\frac{h^2}{2} y''\right) - \left(\frac{h^3}{6} y'''\right) \tag{11a}$$

$$y_1(a-2h) = b - 2hf + 4\left(\frac{h^2}{2} y''\right) - 8\left(\frac{h^3}{6} y'''\right) \tag{11b}$$

$$y_1(a+3h) = b + 3hf + 9\left(\frac{h^2}{2} y''\right) + 27\left(\frac{h^3}{6} y'''\right) \tag{11c}$$

$$y_1(a-3h) = b - 3hf + 9\left(\frac{h^2}{2} y''\right) - 27\left(\frac{h^3}{6} y'''\right) \tag{11d}$$

where $y_1\,(a+ih)$, $i = 1, -2, \pm 3$, represent third-order approximations to $y\,(a+ih)$, $i = -1, -2, \pm 3$ respectively.

Substituting (8) and (9) into formulas (11) and performing obvious simplifications the theorem follows.

A variety of known methods are now at our disposal for the improvement of the third-order approximations $y_1\,(a \pm ih)$, $i = 1, 2, 3$ and the determination of p ($\geqq 4$) pivotal points for the multistep methods. For instance, through the use of the set of 3-point formulas ($2a$, b) and, independently, again the formula ($2b$), converted now to Milne's « 3-point corrector », we can determine three pivotal points. These together with (a, b) constitute a set of four pivotal points. Also we may use 4-point formulas, symmetrical 5-point formulas, a set of 6-point formulas and a « 6-point corrector », symmetrical 7-point formulas and determine 4, 5, 6, 7 pivotal points (including (a, b)), etc.

We observed previously that an increase in the number of pivotal points results, theoretically, in an increase in accuracy of the approximations. However at the same time the step-size «h» of the set of p-point formulas decreases. This implies an increase in the number of substitutions which in turn increases the frequency of rounding error thus distorting the accuracy of the estimates.

We can remedy this, at least partially, by retaining more decimal places than before in our calculations.

It seems to us appropriate at this point to quote a remark of Agnew in [1] which, although made about the Runge-Kutta method, is applicable for p-point formulas also:

« Thus, rounding errors completely destroy the usefulness of the calculations. It is clear that the prohibition against small values of h is more severe when we make 3D (decimal places) or 4D calculations, and would remain if our equipment were used in such a way that it actually or effectively makes 50D cal culations. »

It now becomes evident that one is facing a real paradoxical problem when one wishes to increase the accuracy of approximations by increasing the number p.

This method can readily be extended to systems of differential equations.

It suffices to consider all the equations, formulas and other relations in vectorial form, the vectors being $\vec{y}$ and $\vec{f}$, defined as follows [7b, 2]:

$$\vec{y} = \begin{bmatrix} y^1 \\ y^2 \\ \cdot \\ \cdot \\ y^m \end{bmatrix} \text{ and } \vec{f}(x, \vec{y}) = \begin{bmatrix} f^1(x, y^1, y^2, \ldots, y^m) \\ f^2(x, y^1, y^2, \ldots, y^m) \\ \cdots\cdots\cdots \\ \cdots\cdots\cdots \\ f^m(x, y^1, y^2, \ldots, y^m) \end{bmatrix}.$$

In fact, the vector formulas ($2a$, b) are known to provide vector approximations for $\vec{y}\,(a+h)$ and $\vec{y}\,(y+2h)$, $\vec{y}\,(x)$ being the solution of the vector equation (1) subjected to the initial conditions $x = a, \vec{y} = \vec{b}$.

However the vector p-point formulas, just as their original scalar counterparts, are not self-starting.

Since the Taylor series, in one and several variables, are valid for vectors also, it follows that the Theorem I, where now ($3a$, b, c) are vector formulas, is valid for the vector equation (1) and vector formulas ($2a$, b). Likewise the Theorem II is valid for the vector equation (1) provided that ($7a$, b, c, d) are considered as vector formulas.

Thus not only our vector p-point formulas become self-starting, and consequently their scalar counterparts also, but furthermore we dispose of six third-order approximations to $\vec{y}\,(a \pm ih)$, $i = 1, 2, 3$.

Consider for instance the initial value problem:

$$\begin{cases} \dfrac{dy^j}{dx} = f^j(x, y^1, y^2) \\ y^j(a) = b^j \end{cases} \tag{12}$$

with $j = 1, 2$.

The following 3-point formulas provide third-order approximations to $y^j\,(a+h)$ and $y^j\,(a+2h)$, $j = 1, 2$.

These formulas are:

$$y_n^j(a+h) = b^j + \frac{h}{12}[5f^j(a) + 8f_{n-1}^j(a+h) - f_{n-1}^j(a+2h)] \qquad (13a)$$

$$y_n^j(a+2h) = b^j + \frac{h}{3}[f^j(a) + 4f_{n-1}^j(a+h) + f_{n-1}^j(a+h) + f_{n-1}^j(a+2h)],\ n = 1, 2, \ldots \qquad (13b)$$

where

$$\begin{cases} f^j(a) = f^j(a, b^1, b^2) \\ f_{n-1}^j(a+ih) = f^j(a+ih, y_{n-1}^1(a+ih), y_{n-1}^2(a+ih)) \end{cases} \qquad (14)$$

with $j = 1, 2$.

In order to determine the starting values $y_0^j(a+h)$ and $y_0^j(a+2h)$ and the other third-order approximations we treat (12) and (13a, b) as vector relations.

This can be done without rewriting these relations, but merely regarding y^j, b^j and f^j as equivalent to $\vec{y}$, $\vec{b}$ and $\vec{f}$ respectively.

The starting values for the vector formulas (13a, b) are given by (vector) Theorem I as follows:

$$y_0^j(a+h) = b^j + hf^j(a) \ldots\ldots \text{ for (13}a\text{) and (13}b\text{)} \qquad (15a)$$

$$y_0^j(a+2h) = b^j + 4hf^j(a) - 2hf_0^j(a+h) \ldots \text{ for (13}a\text{)} \qquad (15b)$$

$$y_0^j(a+2h) = b^j - 2hf^j(a) + 4hf_0^j(a+h) \ldots \text{ for (13}b\text{)} \qquad (15c)$$

with the use of notations (14).

We regard (15a, b, c) as scalar formulas again and we have all the necessary starting values for the (scalar) formulas (13a, b) at our disposal.

Then through the use of (13a, b) we determine $y_1^j(a+h)$ and $y_1^j(a+2h)$ respectively.

The formulas (7a, b, c, d) of Theorem II treated as vector formulas (using " j " superscript notation) can be written:

$$y_1^j(a-h) = -\frac{3}{2}b^j - 3hf^j(a) + 3y_1^j(a+h) - \frac{1}{2}y_1^j(a+2h) \qquad (16a)$$

$$y_1^j(a-2h) = -12b^j - 12hf^j(a) + 16y_1^j(a+h) - 3y_1^j(a+2h) \qquad (16b)$$

$$y_1^j(a+3h) = -\frac{11}{2}b^j + 3hf^j(a) - 9y_1^j(a+h) + \frac{9}{2}y_1^j(a+2h) \qquad (16c)$$

$$y_1^j(a-3h) = -35b^j - 30hf^j(a) + 45\,y_1^j(a+h) - 9y_1^j(a+2h)\,. \qquad (16d)$$

We regard now (16*a*, *b*, *c*, *d*) as scalar formulas and determine $y_1^j\,(a+ih)$, $i = -1, -2, \pm 3$, third-order approximations to $y^j\,(a+ih)$, $i = -1, -2, \pm 3$, respectively.

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