The numerical solution of second-order differential equations not containing the first derivative explicitly

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Several methods are obtained for the numerical solution of the differential equation $y'' = f(x, y)$ starting from initial values of y and y' at some point x_0. These methods may be considered as generalizations of the Runge–Kutta method and De Vogelaere's method.

Some previously known methods

Collatz (1960) has shown that for the equation $y'' = f(x, y)$ the standard fourth-order Runge–Kutta process can be put into the simplified form

$$\left.\begin{aligned} k_0 &= h^2 f(x_0, y_0) \\ k_1 &= h^2 f\left(x_0 + \tfrac{1}{2}h, y_0 + \tfrac{1}{2}hy_0' + \tfrac{1}{8}k_0\right) \\ k_2 &= h^2 f\left(x_0 + h, y_0 + hy_0' + \tfrac{1}{2}k_1\right) \\ y_1 &= y_0 + hy_0' + \tfrac{1}{6}(k_0 + 2k_1) + O(h^5) \\ hy_1' &= hy_0' + \tfrac{1}{6}(k_0 + 4k_1 + k_2) + O(h^6). \end{aligned}\right\} \quad (A)$$

This process requires three evaluations of the function $f(x, y)$ for each step; unless $f(x, y)$ is a very simple function, these evaluations comprise the bulk of the computational work.

De Vogelaere has shown (1955) that the same degree of accuracy can be obtained with only two function evaluations per step. His process may be put in the form

$$\left.\begin{aligned} y_{\frac{1}{2}} &= y_0 + \tfrac{1}{2}hy_0' + \tfrac{1}{6}\left(F_0 - \tfrac{1}{4}F_{-\frac{1}{2}}\right) + O(h^4) \\ y_1 &= y_0 + hy_0' + \tfrac{1}{6}(F_0 + 2F_{\frac{1}{2}}) + O(h^5) \\ hy_1' &= hy_0' + \tfrac{1}{6}(F_0 + 4F_{\frac{1}{2}} + F_1) + O(h^6) \end{aligned}\right\} \quad (B)$$

where $F_p = h^2 f(x_p, y_p)$. This process requires the value of $F_{-\frac{1}{2}}$ from the previous step and is therefore not self-starting. For the initial step $F_{-\frac{1}{2}}$ may be obtained from

$$y_{-\frac{1}{2}} = y_0 - \tfrac{1}{2}hy_0' + \tfrac{1}{8}F_0 + O(h^3). \quad (B')$$

A similar procedure must be used at each change of interval.

It will be noted that in both the above processes, the error in hy' is of a higher order than that in y. This is essential if the order of accuracy is to be preserved throughout the tabulation, for each subsequent value of y contains, in effect, the sum of all previous values of hy'.

Runge–Kutta type processes

A general process of the Runge–Kutta type is of the form

$$\begin{aligned} k_0 &= h^2 f(x_0, y_0) \\ k_r &= h^2 f\left(x_0 + a_r h, y_0 + a_r hy_0' + \sum_{s=0}^{r-1} b_{rs}k_s\right) \\ &\qquad r = 1, 2, \ldots, n. \\ y_1 &= y_0 + hy_0' + W_0k_0 + \sum_{r=1}^{n} W_r(1 - a_r)k_r \\ hy_1' &= hy_0' + \sum_{r=0}^{n} W_r k_r. \end{aligned}$$

It is possible to write down a set of equations for the unknowns a_r, W_r, b_{rs}, depending on the order of accuracy required. The solution of these equations involves some cumbersome algebra which need not be discussed here; the general method is described in detail by Collatz (1960).

Below are given fifth- and sixth-order processes requiring four and five function evaluations per step, respectively. Neither of these processes is unique; it is possible to derive a variety of similar processes.

Fifth-order process

$$\left.\begin{aligned} k_0 &= h^2 f(x_0, y_0) \\ k_1 &= h^2 f\left(x_0 + \tfrac{1}{4}h, y_0 + \tfrac{1}{4}hy_0' + \tfrac{1}{32}k_0\right) \\ k_2 &= h^2 f\left(x_0 + \tfrac{7}{10}h, y_0 + \tfrac{7}{10}hy_0' - \tfrac{7}{1000}k_0 + \tfrac{63}{250}k_1\right) \\ k_3 &= h^2 f\left(x_0 + h, y_0 + hy_0' + \tfrac{2}{7}k_0 + \tfrac{3}{14}k_2\right) \\ y_1 &= y_0 + hy_0' + \tfrac{1}{14}k_0 + \tfrac{8}{27}k_1 + \tfrac{25}{189}k_2 + O(h^6) \\ hy_1' &= hy_0' + \tfrac{1}{14}k_0 + \tfrac{32}{81}k_1 + \tfrac{250}{567}k_2 + \tfrac{5}{54}k_3 + O(h^7) \end{aligned}\right\} \quad (C)$$

Sixth-order process

$$\left.\begin{aligned}
k_0 &= h^2f(x_0, y_0)\\
k_1 &= h^2f\Big(x_0+\tfrac{1}{4}h,\ y_0+\tfrac{1}{4}hy_0'+\tfrac{1}{32}k_0\Big)\\
k_2 &= h^2f\Big(x_0+\tfrac{1}{2}h,\ y_0+\tfrac{1}{2}hy_0'-\tfrac{1}{24}k_0+\tfrac{1}{6}k_1\Big)\\
k_3 &= h^2f\Big(x_0+\tfrac{3}{4}h,\ y_0+\tfrac{3}{4}hy_0'\\
&\qquad +\tfrac{3}{32}k_0+\tfrac{1}{8}k_1+\tfrac{1}{16}k_2\Big)\\
k_4 &= h^2f\Big(x_0+h,\ y_0+hy_0'+\tfrac{3}{7}k_1\\
&\qquad -\tfrac{1}{14}k_2+\tfrac{1}{7}k_3\Big)\\
y_1 &= y_0+hy_0'+\tfrac{1}{90}(7k_0+24k_1+6k_2+8k_3)\\
&\qquad + O(h^7)\\
hy_1' &= hy_0'+\tfrac{1}{90}(7k_0+32k_1+12k_2\\
&\qquad +32k_3+7k_4) \quad + O(h^8).
\end{aligned}\right\}\quad \text{(D)}$$

It is tempting to assume from processes (A), (C) and (D) that it is always possible to derive an nth-order process requiring $(n-1)$ function evaluations per step; this is not, however, correct. It may be possible to obtain a seventh-order process requiring only six function evaluations, though no such process has been obtained; it can be shown that an eighth-order process would require at least eight, and a ninth-order at least ten. Processes of this complexity would be of little practical use.

Methods based on Radau Quadrature

It was shown by Radau (1880) that for any value of n a closed quadrature formula may be obtained in the form

$$\int_{x_0}^{x_1} g(x)dx = h\left[W_0g(x_0)+\sum_{r=1}^{n-1} W_rg(x_0+a_rh)+W_ng(x_1)\right] + O(h^{2n+1}).$$

It can be deduced that

$$\begin{aligned}
y_1 &= y_0+hy_0'+W_0F_0+\sum_{r=1}^{n-1} W_r(1-a_r)F_{a_r} + O(h^{2n+1})\\
hy_1' &= hy_0'+W_0F_0+\sum_{r=1}^{n-1} W_rF_{a_r}+W_nF_1 + O(h^{2n+2})
\end{aligned}$$

where $F_p = h^2y_p'' = h^2f(x_p, y_p)$. A process based on these formulae would be of the $2n$th order and yet require only n function evaluations per step, thus improving on the Runge–Kutta processes. It is necessary, however, to obtain the intermediate values of F correct to order h^{2n+1} and this entails the evaluation of the corresponding y to order h^{2n-1}. These latter values must be obtained by extrapolation using the data of previous steps; the processes are not therefore self-starting, but require special starting procedures.

The simplest Radau formula ($n = 1$) is the trapezium rule, which gives rise to the trivial process:

$$\left.\begin{aligned}
y_1 &= y_0+hy_0'+\tfrac{1}{2}F_0 && + O(h^3)\\
hy_1' &= hy_0'+\tfrac{1}{2}(F_0+F_1) && + O(h^4).
\end{aligned}\right\}\quad \text{(E)}$$

This requires no starting procedure.

With $n = 2$, the appropriate Radau formula is Simpson's rule, and the corresponding process is De Vogelaere's process (B). Higher-order processes of this type may thus be regarded as generalizations of De Vogelaere's process.

Radau's four-point formula ($n = 3$) is

$$\int_{x_0}^{x_1} g(x)dx = \frac{h}{12}(g_0+5g_a+5g_{1-a}+g_1) \quad + O(h^7)$$

where $a = \dfrac{5-\sqrt{5}}{10} = 0\cdot2763{,}9320$. The corresponding process is given below:

$$\left.\begin{aligned}
y_a &= y_0 + 0\cdot2763{,}9320\,hy_0'\\
&\quad + 0\cdot0645{,}7768\,F_0 - 0\cdot0387{,}4353\,F_{-a}\\
&\quad + 0\cdot0187{,}1643\,F_{a-1} - 0\cdot0063{,}5398\,F_{-1}\\
&\qquad + O(h^6)\\
y_{1-a} &= y_0 + 0\cdot7236{,}0680\,hy_0'\\
&\quad + 0\cdot2971{,}1983\,F_a - 0\cdot1294{,}4272\,F_0\\
&\quad + 0\cdot1098{,}7164\,F_{-a} - 0\cdot0157{,}4536\,F_{a-1}\\
&\qquad + O(h^6)\\
y_1 &= y_0 + hy_0' + \tfrac{1}{12}F_0 + 0\cdot3015{,}0283\,F_a\\
&\quad + 0\cdot1151{,}6383\,F_{1-a} \qquad + O(h^7)\\
hy_1' &= hy_0' + \tfrac{1}{12}(F_0+5F_a+5F_{1-a}+F_1)\\
&\qquad + O(h^8).
\end{aligned}\right\}\quad \text{(F)}$$

For the initial step, the values of F_{-a}, F_{a-1}, F_{-1}, can be obtained to an adequate degree of accuracy from the following values of y:

$$\left.\begin{aligned}
y_{-\frac{1}{2}} &= y_0 - \tfrac{1}{2}hy_0' + \tfrac{1}{8}F_0 && + O(h^3)\\
y_{-1} &= y_0 - hy_0' + \tfrac{1}{6}(F_0+2F_{-\frac{1}{2}}) && + O(h^5)\\
y_{-a} &= y_0 - 0\cdot2763{,}9320\,hy_0' + 0\cdot0286{,}1197F_0\\
&\quad + 0\cdot0121{,}3107\,F_{-\frac{1}{2}} - 0\cdot0025{,}4644\,F_{-1}\\
&\qquad + O(h^5)\\
y_{a-1} &= y_0 - 0\cdot7236{,}0680\,hy_0' + 0\cdot1180{,}5469F_0\\
&\quad + 0\cdot1612{,}0227\,F_{-\frac{1}{2}} - 0\cdot0174{,}5356\,F_{-1}\\
&\qquad + O(h^5).
\end{aligned}\right\}\quad \text{(F}'\text{)}$$

Table 1

Solutions, obtained by various methods, to the differential equation $y'' = -xy$, where $y = 1$ and $y' = 0$ when $x = 0$

x	CORRECT SOLUTION	METHOD (A) RUNGE-KUTTA	METHOD (B) DE VOGELAERE	METHOD (C) 5TH-ORDER	METHOD (D) 6TH-ORDER	METHOD (F) RADAU
0·0	1·000000	1·000000	1·000000	1·000000	1·000000	1·000000
0·5	0·979253	0·979167 (−86)	0·979219 (−34)	0·979258 (+5)	0·979253 (−)	0·979254 (+1)
1·0	0·838812	0·838609 (−203)	0·838704 (−108)	0·838824 (+12)	0·838812 (−)	0·838814 (+2)
1·5	0·497890	0·497757 (−133)	0·497830 (−60)	0·497915 (+25)	0·497890 (−)	0·497894 (+4)
2·0	−0·014979	−0·014487 (+492)	−0·014571 (+408)	−0·014947 (+32)	−0·014976 (+3)	−0·014976 (+3)
2·5	−0·509797	−0·508159 (+1638)	−0·508499 (+1298)	−0·509806 (−9)	−0·509791 (+6)	−0·509807 (−10)
3·0	−0·694729	−0·692671 (+2058)	−0·693099 (+1630)	−0·694857 (−128)	−0·694723 (+6)	−0·694757 (−28)

The figures in brackets show the errors in units of the sixth decimal place.

This process is of the same order of accuracy as process (D), though it requires two fewer function evaluations per step.

For $n > 3$, the extrapolation must make use of the values of both y and F obtained during the previous step; alternatively, the values of F from the previous two steps may be used. In either case, there is a considerable increase in the complexity of the starting procedure, and this to a large extent limits the usefulness of such processes.

Numerical example

It is not practicable to make a theoretical comparison of the truncation errors of the various methods, owing to the complexity of the error terms in the Runge–Kutta type processes. Nor is it intended to discuss here the question of stability.

In order to illustrate the accuracy which can be obtained, a numerical example is shown in Table 1. This shows the solution of the differential equation $y'' = -xy$, where $y = 1$ and $y' = 0$ when $x = 0$, obtained by the various methods, with an interval $h = 0 \cdot 5$. Alongside is shown the correct solution, which is easily obtained in terms of Bessel functions. It will be seen that methods (D) and (F) yield results of considerable accuracy in spite of the large interval used.

References

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