NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

TECHNICAL MEMORANDUM 1403

ON THE INSTABILITY OF METHODS FOR THE INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

By Heinz Rutishauser

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ON THE INSTABILITY OF METHODS FOR THE INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS[1]

By Heinz Rutishauser[2]

In spite of the remarkable publication of J. Todd (ref. 1) the essential points of which are related below, the author has since observed several times methods for the nummerical integration of differential equations which, although subject only to a temptingly small truncation error, nevertheless involve the great danger of numerical instability. I want to state beforehand that this danger hardly exists for the well-tested methods of Runge-Kutta and Adams (extrapolation methods) if they are applied correctly.

It is a natural characteristic that a differential equation to be solved numerically is approximated by a difference equation, and that the latter is then solved. In order not to be forced to select an all too small interval, one prefers difference equations which approximate the differential equation as closely as possible but in compensation are of higher order than the original differential equation. Precisely in this, however, there lies a danger because the difference equation thereby has a greater diversity of possible solutions, and it may well happen that the numerical integration yields precisely one of the extraneous solutions which only at the beginning is in any way related to the desired solution of the differential equation. In the paper of J. Todd mentioned before several examples of this type have been enumerated.

Consideration of the pertinent variation equation is particularly informative. It is very well possible that the differential variation equation is stable, that is, that it contains only converging solutions, whereas the difference variation equation is unstable since it possesses, due to the increased diversity of solutions, aside from the converging solutions, also solutions which increase exponentially. A deviation from the correct solution, once it exists, small as it may be - and such

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[1]"Über die Instabilität von Methoden zur Integration gewöhnlicher Differentialgleichungen," ZAMP, Kurze Mitteilungen, vol. III, 1952, pp. 65-74.

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deviations are unavoidable, because of the rounding-off errors - therefore increases rapidly and may finally falsify considerably the solution obtained. Yet - we want to emphasize this once more - this instability is caused only by an inappropriate integration method.

In the following discussion, several customary methods are examined from this viewpoint, and simple criteria for the stability of such methods are indicated. For the rest, this report does not deal with error estimates.

DIFFERENTIAL EQUATIONS OF THE FIRST ORDER

$$y' = f(x,y)$$

Variation equation

$$\eta' = \frac{\partial f}{\partial y} \eta$$

(a) Integration by Means of Simpson's Rule[3]

$$y_{k+1} = y_{k-1} + \frac{h}{3}\left(y'_{k+1} + 4y'_{k} + y'_{k-1}\right) \qquad (1)^{4}$$

This relationship, together with the differential equation, yields two equations for the unknown quantities y_{k+1} and y'_{k+1} which are solved mostly by iteration. If the differential equation is linear or quadratic in y, the iteration can be avoided. We assume, however, that one passes over, in any case, to the next integration interval only when the relationship (1) is satisfied.

The difference variation equation pertaining to (1) is evidently

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[3]The phenomenon was observed on this example, and correctly interpreted, also by Mr. G. Dahlquist, Stockholm (Lecture at the GaMM-convention 1951 at Freiburg im Breisgau). Compare also: Z. angew. Math. Mech., 31, 239, 1951.

[4]Where h signifies the length of the integration interval, and y_k stands as an abbreviation for $y(kh)$.

$$\eta_{k+1}\left(1 - \frac{h}{3} f_{y,k+1}\right) - \frac{4h}{3} f_{y,k}\eta_k - \left(1 + \frac{h}{3} f_{y,k-1}\right)\eta_{k-1} = 0$$

If one assumes f_y to be constant, and chooses the expression $\eta_k = \lambda^k$ for the solution of this equation, one obtains for λ a quadratic equation with the solutions

$$\lambda_1 = 1 + hf_y + \frac{h^2}{2} f_y^2 + \ldots \sim e^{hf_y}$$

$$\lambda_2 = -1 + \frac{h}{3} f_y - \frac{h^2}{18} f_y^2 + \ldots \sim -e^{-hf_y/3}$$

One recognizes easily that, of the two fundamental solutions $\eta_{1,k} = \lambda_1^k$ and $\eta_{2,k} = \lambda_2^k$ of the difference variation equation, the first one approximates the solution of the differential variation equation whereas the second one is brought in by the numerical method.

In particular

$$\lambda_2^k \sim (-1)^k e^{-khf_y/3}$$

represents for $f_y < 0$, thus precisely when the differential equation is stable, an oscillation which is slowly exponentially increasing. This has the effect that a small disturbance of the numerical solution - caused by a rounding-off or a truncation error - is intensified in the further course of the integration and finally gets completely out of hand. In Collatz' (ref. 2) book, the phenomenon is denoted as "roughening phenomenon"; means for elimination of this inconvenience are given. On the other hand, the explanation given there is not complete; the phenomenon occurs only for $f_y < 0$; there is nothing to be apprehensive of for $f_y \geqq 0$ which is very important particularly in regard to the ordinary Simpson's integration rule $\left(f_y \equiv 0\right)$.

(b) Integration According to Runge-Kutta and Similar Methods

Since these methods calculate y_{k+1} from y_k according to a prescribed rule and without use of the preceding values $y_{k-1}, y_{k-2}, \ldots,$

the order remains unchanged in the transition from the differential equation to the difference equation; thus no foreign solutions are brought in, and no instability is to be feared.

The same property can be found in a method indicated by W. E. Milne (ref. 3).

(c) Integration According to Adams

We consider a four-point formula

$$y_{k+1} = y_k + \frac{h}{24}\left(9y'_{k+1} + 19y'_k - 5y'_{k-1} + y'_{k-2}\right) + h^5 \ldots \qquad (2)$$

This again yields, together with the differential equation, two equations for the unknown quantities y_{k+1} and y'_{k+1} which are mostly solved by iteration.

The difference variation equation pertaining to (2) becomes

$$\left(1 - \frac{3h}{8} f_{y,k+1}\right)\eta_{k+1} - \left(1 + \frac{19h}{24} f_{y,k}\right)\eta_k + \frac{5h}{24} f_{y,k-1}\eta_{k-1} - \frac{h}{24} f_{y,k-2}\eta_{k-2} = 0$$

If one again considers f_y as constant, the expression $\eta_k = \lambda^k$ yields an equation of the third order for λ. A solution λ_1 of this equation lies very close to e^{hf_y}, therefore $\eta_{1,k} = \lambda_1{}^k$ corresponds to the solution of the differential variation equation whereas $\lambda_2{}^k$ and $\lambda_3{}^k$ are extraneous solutions.

However, the equation for λ is reduced to $\lambda^3 - \lambda^2 = 0$ when h tends toward 0 so that, for a sufficiently small h, one will have at any rate small λ_2 and λ_3, namely $\sim \pm\sqrt{-hf_y/24}$. The extraneous solutions $\eta_{2,k} = \lambda_2{}^k$ and $\eta_{3,k} = \lambda_3{}^k$ thus converge rapidly. For a sufficiently small h, Adams' method is therefore stable.

(d) Variants of (c)

In order to improve the accuracy of Adams' method, one may use also other expressions for the corrector instead of (2). As long as the corresponding five- or six-point formulas are involved, there are no objections, but one has to be careful when y_{k+1} is not calculated from y_k and the derivatives as in (2) but perhaps from y_{k-1} or y_{k-3} and the derivatives, as for instance in

$$y_{k+1} = y_{k-3} + \frac{2h}{45}\left(7y'_{k+1} + 32y'_k + 12y'_{k-1} + 32y'_{k-2} + 7y'_{k-3}\right) + h^7 \ . \ . \ .$$

In fact the pertinent difference variation equation has a solution

$$\eta_k = \lambda^k \quad \text{with} \quad \lambda = -\left(1 - \frac{19h}{45} f_y + \ . \ . \ .\right)$$

so that the method is unstable for $f_y < 0$.

DIFFERENTIAL EQUATIONS OF THE SECOND ORDER

$$y'' = f(x,y,y')$$

Insofar as these equations are solved by separation into a system of two equations of the first order, what was said so far is valid. Particularly in the case of numerical integration of damped oscillations we must caution against the methods (a) and (d).

However, there exist also methods which solve an equation of the second order without transformation into a system:

(e) The Method of Central Differences[5]

The formulas on which this method is based are (especially for second order)

$$y_{k+1} = 2y_k - y_{k-1} + \frac{h^2}{12}\left(y''_{k+1} + 10y''_k + y''_{k-1}\right) \tag{4}$$

$$y'_{k+1} = y'_{k-1} + \frac{h}{3}\left(y''_{k+1} + 4y''_k + y''_{k-1}\right) \tag{5}$$

[5]Compare reference 2, p. 80.

They yield, together with the differential equation, three equations for the unknown quantities y_{k+1}, y'_{k+1}, and y''_{k+1}. The two simultaneous difference variation equations pertinent to (4) and (5) are solved with the expression $\eta_k = p\lambda^k$, $\eta'_k = q\lambda^k$, under the assumption of a constant f_y and $f_{y'}$; because of

$$\eta''_{k+1} = f_y \eta_{k+1} + f_{y'} \eta'_{k+1}$$

one obtains, with the abbreviations a for $h^2 f_y / 12$ and b for $hf_{y'}/3$, the equations

$$\left.\begin{array}{ll} p\left[(\lambda^2 - 2\lambda + 1) - a(\lambda^2 + 10\lambda + 1)\right] - & \\ q\,\frac{h}{4}\,b(\lambda^2 + 10\lambda + 1) = 0 & \text{[from (4)]} \\ & \\ q\left[(\lambda^2 - 1) - b(\lambda^2 + 4\lambda + 1)\right] - p\,\frac{4}{h}\,a(\lambda^2 + 4\lambda + 1) = 0 & \text{[from (5)]} \end{array}\right\} \quad (6)$$

These equations can exist simultaneously with $(p,q) \neq (0,0)$ only when the determinant of this equation system for p and q vanishes; one obtains after some calculations

$$(\lambda - 1)\left[(\lambda^2 - 1)(\lambda - 1) - a(\lambda + 1)(\lambda^2 + 10\lambda + 1) - b(\lambda - 1)(\lambda^2 + 4\lambda + 1)\right] = 0$$

The four solutions of these equations are

$$\left.\begin{array}{l} \lambda_1 = 1 + \alpha_1 h + \ldots \\ \lambda_2 = 1 + \alpha_2 h + \ldots \end{array}\right\} \quad \text{where } \alpha_1 \text{ and } \alpha_2 \text{ are the solutions of the equation } \alpha^2 - \alpha f_{y'} - f_y = 0$$

$$\lambda_3 = 1$$

$$\lambda_4 = -\left(1 - \frac{h}{3} f_{y'} + \ldots\right)$$

Evidently $\lambda_1{}^k$ and $\lambda_2{}^k$ are the regular solutions of the difference variation equation; they correspond to two fundamental solutions of the differential variation equation; λ_3 and λ_4, in contrast, are extraneous. As long as $f_{y'} \geqq 0$, there is nothing to fear, in particular, the method may be strongly recommended for a y'-free equation, but for $f_{y'} < 0$ (damped oscillations)

$$\eta_{4,k} = \lambda_4{}^k \sim (-1)^k e^{-(kh/3)f_{y'}}$$

increases, and λ_3, too, may still become dangerous because $\lambda_{3,k} \equiv 1$ also becomes finally very large, compared to a function converging toward zero.

The author completely calculated the example $y'' + y' + 1.25y = 0$ with the initial conditions $y_0 = 0$, $y' = 1$ (exact solution: $e^{\frac{-x}{2}} \sin x$) on the sequence-controlled computing machine of the ETH.

There follow a few excerpts from the thus obtained table of functions (we calculated with $h = 0.1$):

x	y	y'
4.8	-0.0903699	0.0531227
4.9	- .0847792	.0584842
5.0	- .0787132	.0626410
5.1	- .0722891	.0656573
5.2	- .0656173	.0676070

In this region nothing conspicuous is noticeable yet, the y-values deviate from the true values approximately by one in the last decimal place, and only formation of the differences for the y'-values reveals a certain irregularity. For $t = 17$, however, the influence of $\lambda_4{}^k$ becomes pronounced for the y'-values and also for the differences of the y-values:

x	y	y'
17.0	-0.00019574	0.00005017
17.1	- .00019061	.00005253
17.2	- .00018366	.00008620
17.3	- .00017524	.00008239
17.4	- .00016548	.00011235
17.5	- .00015475	.00010258

The considerably weaker oscillation of the y-values follows also from the equations (6): for $\lambda = \lambda_4$ one obtains from the first of these equations

$$\frac{p}{q} \sim \frac{h}{4} b \frac{-8}{4} = - \frac{h^2}{6} f_{y'}, \text{ here therefore } p \sim \frac{q}{600}$$

The further course of numerical integration does not require any comment:

x	y	y'
22.8	-0.00000815	0.00005320
22.9	- .00000864	-.00006078
23.0	- .00000862	.00005968
23.1	- .00000887	-.00006247
23.2	- .00000861	.00006601
23.3	- .00000868	-.00006486
29.5	- .00000140	-.00053037
29.6	.00000041	.00054889
29.7	- .00000144	-.00056693
29.8	.00000050	.00058682
29.9	- .00000148	.00060603
30.0	.00000060	-.00062735

The author is well aware that the assumption of a constant f_y and $f_{y'}$ in the above considerations greatly restricts the generality. However, the results show that what matters is only the sign of these quantities, and this sign is indeed invariable in a great many cases. The statements are, therefore, qualitatively almost generally valid. Only when f_y changes its sign, from time to time in the course of the integration, for instance when method (a) is being used, a special case arises since the occurring oscillations alternately increase and are damped again.

GENERAL CONSIDERATIONS

Consideration of the examples suggests the conjecture that instability may occur precisely in the case of integration methods which form y_{k+1} by integration of y' over several intervals (two intervals in method (a), one interval in (b) and (c), four intervals in (d), two intervals in (e)). However, this is not exactly the case and we shall therefore subject a general integration method to an examination.

Almost all known methods use relationships which are contained in the general formula

$$\left.\begin{aligned}
y_{k+1} &= \sum_{-m}^{0} a_{0j}^{(0)} y_{k+j} + h \sum_{-m}^{1} a_{1j}^{(0)} y'_{k+j} + \ldots + \\
&\quad h^{N} \sum_{-m}^{1} a_{1j}^{(0)} y_{k+j}^{(N)} \\
y'_{k+1} &= \sum_{-m}^{0} a_{1j}^{(1)} y'_{k+j} + h \sum_{-m}^{1} a_{2j}^{(1)} y''_{k+j} + \ldots + \\
&\quad h^{N-1} \sum_{-m}^{1} a_{Nj}^{(1)} y_{k+j}^{(N)} \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
y_{k+1}^{n-1} &= \sum_{-m}^{0} a_{n-1,j}^{(n-1)} y_{k+j}^{(n-1)} + h \sum_{-m}^{1} a_{nj}^{(n-1)} y_{k+j}^{(n)} + \ldots + \\
&\quad h^{N-n+1} \sum_{-m}^{1} a_{Nj}^{(n-1)} y_{k+j}^{(N)}
\end{aligned}\right\} \qquad (7)$$

There are, in addition, differential equations

$$\left.\begin{aligned} &F_n\left(x_{k+1}, y_{k+1}, \ldots, y_{k+1}^{(n)}\right) = 0 \\ &F_{n+1}\left(x_{k+1}, y_{k+1}, \ldots, y_{k+1}^{(n+1)}\right) = 0 \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ &F_N\left(x_{k+1}, y_{k+1}, \ldots, y_{k+1}^{(N)}\right) = 0 \end{aligned}\right\} \tag{8}$$

which form, together with the equations (7), $N + 1$ equations for the $N + 1$ unknowns $y_{k+1}, y'_{k+1}, \ldots, y_{k+1}^{(N)}$. Generally, $N = n$; however, W. E. Milne (ref. 3) uses in the method previously mentioned higher derivatives than those appearing in the differential equation. Therefore he differentiates them several times in order to obtain the required number of relationships. One may thus obtain the equations $F_{n+1} \ldots$ to F_N by differentiating the initial equation F_n.

If one, furthermore, brings everything in the equations (7) to one side, the variation equations for the entire system (7) and (8) read evidently $\left(\text{with } a_{i,1}^{(i)} = -1\right)$

$$\sum_{\mu=i}^{N} \sum_{j=-m}^{1} a_{\mu j}^{(i)} h^{\mu-i} \eta_{k+j}^{(\mu)} = 0 \qquad (i = 0, 1, \ldots, n - 1)$$

$$\sum_{0}^{i} \frac{\partial F_i}{\partial y^{(\mu)}} \eta_1^{(\mu)} = 0 \qquad (i = n, n + 1, \ldots, N)$$

If one uses for this the expression $\eta_j^{(\mu)} = p_\mu \lambda^j$, one obtains in substituting a system of $N + 1$ simultaneous equations for the p_μ which can be satisfied only when the determinant of the system disappears

$$\sum_{\mu=i}^{N}\left(\sum_{j=-m}^{l} a_{\mu j}^{(i)}\lambda^{j}\right)h^{\mu-i}p_{\mu} = 0 \qquad (i = 0, 1, \ldots, n - 1)$$

$$\sum_{0}^{i} \frac{\partial F_i}{\partial y^{(\mu)}} p_\mu = 0 \qquad (i = n, n + 1, \ldots, N)$$

If one defines, in addition, with the coefficients $a_{\mu j}^{(i)}$ appearing in the formulas (7) the functions

$$A_{i\mu}(\lambda) = \sum_{j=-m}^{l} a_{\mu j}^{(i)}\lambda^{j+m}$$

wherein $A_{i\mu} \equiv 0$ for $\mu < i$, the characteristic determinant reads as follows

$$D(\lambda) = \begin{vmatrix} A_{00} & hA_{01} & h^2A_{02} & \cdots & & & h^NA_{0N} \\ 0 & A_{11} & hA_{12} & \cdots & & & h^{N-1}A_{1N} \\ \vdots & & \ddots & & & & \vdots \\ 0 & 0 & 0 & A_{n-1,n-1} & & & h^{N-n+1}A_{n-1,N} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ F_{n,y} & F_{n,y'} & & & F_{n,y^{(n)}} & 0 & 0 \\ F_{n+1,y} & F_{n+1,y'} & & & & \ddots & 0 \\ \vdots & & & & & & \vdots \\ F_{N,y} & F_{N,y'} & \cdots & \cdots & \cdots & \cdots & F_{N,y^{(N)}} \end{vmatrix}$$

If the method is to reproduce exactly a polynomial of the ith degree, which is the solution of a differential equation, together with its derivatives - and this one may require - the conditions

$$y_j^{(i)} \equiv 1 \qquad y_j^{(i+1)} \equiv y_j^{(i+2)} \equiv y_j^{(i+3)} \equiv \ldots \equiv y_j^{(N)} \equiv 0$$

must be compatible. Hence follows, however, by substitution into the ith of the equations (7): $\sum_j a_{ij}^{(i)} = 0$, therefore $A_{ii}(1) = 0$.

The equation $D(\lambda) = 0$ which is decisive for the stability of the method must have n solutions in the neighborhood of $\lambda = 1$, corresponding to the n independent solutions of the variation equation. In fact one finds for $h = 0$ where $D(\lambda)$ is, except for one factor, reduced to $A_{00}A_{11} \cdot \cdot \cdot A_{n-1,\, n-1}$, that $\lambda = 1$ is an n-fold zero of $D(\lambda)$, because of $A_{ii}(1) = 0$.

All other zeros of $D(\lambda)$ correspond therefore to extraneous solutions of the difference equation; in order to make the method stable, they must lie, for a sufficiently small h, in the interior or at most on the periphery of the unit circle. This is certainly the case when for $h = 0$ all zeros of $D(\lambda)$ lie in the interior of the unit circle, and certainly not when individual ones are outside it. Therefore:

Sufficient condition for the stability of the method (7) for sufficiently small h:

All functions

$$A_{ii}(\lambda) = \sum_{-m}^{l} a_{ij}^{(i)} \lambda^{j+m}$$

possess, aside from the trivial simple zero $\lambda = 1$ only zeros with $|\lambda| < 1$.

Necessary condition: None of the functions $A_{ii}(\lambda)$ has a zero outside the unit circle.[6]

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[6] J. Todd considered methods which satisfy not even the necessary condition. The solution obtained then becomes completely useless already after a few intervals.

The remaining functions $A_{i\mu}(\lambda)$ can influence the stability only when the necessary condition, but not the sufficient condition, is satisfied.

APPLICATIONS

For the formula (1) there results (one has $N = n = 1$, $m = 1$)

$$A_{00} = -\lambda^2 + 1 \qquad A_{01} = \frac{1}{3}(\lambda^2 + 4\lambda + 1) \qquad F_1 = y' - f(x,y)$$

Therefore

$$D(\lambda) = \begin{vmatrix} 1 - \lambda^2 & \frac{h}{3}(\lambda^2 + 4\lambda + 1) \\ -f_y & 1 \end{vmatrix}$$

The fact that A_{00} has two zeros with $|\lambda| = 1$ already suggests caution, but moreover one reads off imediately that $D(\lambda)$ is positive for $f_y < 0$ and $\lambda = -1$, and negative, in contrast, for $\lambda = -\infty$. Thus a zero lies to the left of -1; the method is unstable.

For the formula 5.42 in the book of Collatz mentioned (p. 81), there is $(N = n = 4, \ m = 1)$

$$\begin{aligned} F_4 &= y^{IV} - f(x,y,y',y'',y''') \\ A_{00} &= A_{22} = -(\lambda - 1)^2 \\ A_{11} &= A_{33} = -\lambda^2 + 1 \\ A_{12} &= 2\lambda \\ A_{34} &= \frac{1}{3}(\lambda^2 + 4\lambda + 1) \end{aligned}$$

All other $A_{i\mu}$ occur only with at least h^2 in the determinant. Thus one has, except for terms with h^2

$$D(\lambda) = \begin{vmatrix} -(\lambda - 1)^2 & 0 & 0 & 0 & 0 \\ 0 & -\lambda^2 + 1 & 2\lambda h & 0 & 0 \\ 0 & 0 & -(\lambda - 1)^2 & 0 & 0 \\ 0 & 0 & 0 & -\lambda^2 + 1 & \frac{h}{3}(\lambda^2 + 4\lambda + 1) \\ -f_y & -f_{y'} & -f_{y''} & -f_{y'''} & 1 \end{vmatrix}$$

For $\lambda = -\infty$, D is positive, for $\lambda = -1 - \epsilon$, D has the sign of

$$-\begin{vmatrix} -\lambda^2 + 1 & \frac{h}{3}(\lambda^2 + 4\lambda + 1) \\ -f_{y'''} & 1 \end{vmatrix}$$

Which for $f_{y'''} < 0$ and a sufficiently small ϵ is negative. Therefore this method is unstable for $f_{y'''} < 0$.

On the other hand it is easy to indicate methods which are always stable. One need only shape the formulas (7) in such a manner that every line begins with

$$'y_{k+1}^{(i)} = y_k^{(i)} + h \sum_{-m}^{1} a_{i+1,j}^{(i)} y_{j+k}^{(i+1)} + h^2 \ . \ . \ . \qquad (i = 0,1, \ . \ . \ ., n-1)$$

Thereby $A_{ii}(\lambda) = -\lambda^{m+1} + \lambda^m$ and has therefore only the trivial zero $\lambda = 1$ on the periphery of the unit circle.

SUMMARY

In the numerical solution of a differential equation as a difference equation, the latter is usually of higher order and therefore has more solutions than the original differential equation. It may well be that some of these "extra" solutions grow faster than any solution of the given equation; in this case the computational solution has the tendency to follow one of these and has after a certain number of integration steps nothing to do with the original differential equation.

The author gives some examples and a criterion for stability of integration methods. This criterion is then applied to some well-known integration formulas.

Translated by Mary L. Mahler
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