A CLASS OF NONLINEAR METHODS FOR ORDINARY DIFFERENTIAL EQUATIONS*

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Consider the initial value problem

$$\frac{dy}{dx}=f(x, y), \quad y(x^{(0)})=y^{(0)}, \tag{1}$$

where $x\in R$, $y, f\in R^n$. If the solution of the differential equation is approximated by polynomials, then general linear methods, such as linear multistep methods and Runge–Kutta methods, can be constructed. When one approximates the solution by rational fractions, there are some nonlinear methods[1,2].

In this paper, we propose a new class of nonlinear methods. Set

$$y_0=x, \quad f_0(y_0, y_1, \cdots, y_n)\equiv 1, \tag{2}$$

$$Y=(y_0, y_1, \cdots, y_n)^T, \quad F=(f_0, f_1, \cdots, f_n)^T.$$

Then (1) is converted to the following initial value problem

$$\frac{dY}{dx}=F(Y), \quad Y(x^{(0)})=Y^{(0)}. \tag{3}$$

Obviously, the solution $Y(x)$ is a curve in R^{n+1}. By means of Frenet frame and the normal representation of curves, we construct a class of one-step multistage nonlinear methods. According to the absolute stability, a stepsize criterion is obtained. It shows that the stepsize should be in inverse proportion to the curvature of the solution curve. It reflects the geometric nature of the solution curve computed. The stepsize criterion applies to nonstiff problems, especially to stiff problems. Numerical experiments for a stiff problem in reaction dynamics have demonstrated the efficiency of this class of nonlinear methods.

§ 1. Normal Representation of Curves

As in differential geometry, the normal representation of curves usually does not exceed the third order[3]. To obtain fourth order nonlinear methods, one must expand the curves further. Let the curve Y be parametrized by the arc length s: $Y(x)=Y(x(s))$, which will be denoted as $Y(s)$ too. Let the arc start from the point where the Frenet frame is established. Then, in the neighborhood of the starting point of the arc, we have

$$Y(s)=Y(0)+s\dot{Y}(0)+\frac{s^2}{2}\ddot{Y}(0)+\frac{s^3}{6}\dddot{Y}(0)+\frac{s^4}{24}\ddddot{Y}(0)+O(s^5). \tag{4}$$

By the Frenet equation

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$$\begin{bmatrix} \dot{e}_1 \\ \dot{e}_2 \\ \dot{e}_3 \\ \dot{e}_4 \end{bmatrix} = \begin{bmatrix} 0 & \varkappa & 0 & 0 \\ -\varkappa & 0 & \tau & 0 \\ 0 & -\tau & 0 & \sigma \\ 0 & 0 & -\sigma & 0 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{bmatrix},$$

the unit tangent vector

$$e_1 = \dot{Y} = \frac{dY}{dx}\,\frac{dx}{ds} = \frac{1}{l}F,$$

where

$$l = \left\{\sum_{j=0}^{n} f_j^2\right\}^{1/2}; \tag{5}$$

the unit principal normal vector satisfies

$$\varkappa e_2 = \dot{e}_1 = \frac{1}{l^2}\left\{U - \frac{q}{l^2}F\right\},$$

where

$$u_i = \sum_{j=0}^{n} \frac{\partial f_i}{\partial y_j} f_j, \quad U = (u_0, u_1, \cdots, u_n)^T,$$

$$p = \left\{\sum_{j=0}^{n} u_j^2\right\}^{1/2}, \quad q = \sum_{i=0}^{n} f_i u_i,$$

$$\varkappa = \sqrt{l^2p^2 - q^2}/l^3. \tag{6}$$

The expresions for unit vectors e_3 and e_4 are not listed here as τ and σ do not appear in the ensuing computations. Thus,

$$-\varkappa e_1 + \tau e_3 = \dot{e}_2 = -\dot{\varkappa}/\varkappa\, e_2 + 1/\varkappa\, \dddot{Y}$$

and

$$-\tau e_2 + \sigma e_4 = \dot{e}_3 = \frac{1}{\varkappa\tau}\{\ddddot{Y} + 3\varkappa\dot{\varkappa}e_1 + (\varkappa^3 - \ddot{\varkappa})e_2 - (2\dot{\varkappa}\tau + \varkappa\dot{\tau})e_3\}.$$

Substituting the above expressions into (4) we obtain the following result.

Theorem 1. *Let $Y(s)$ be a curve in $R^{n+1}(n \geqslant 3)$, parametrized by arc length s. Then, in the neighborhood of $s=0$, the curve has the following normal representation*

$$Y(s) = Y(0) + \left[s - \frac{s^3}{6}\varkappa^2 - \frac{s^4}{8}\varkappa\dot{\varkappa}\right]e_1 + \left[\frac{s^2}{2}\varkappa + \frac{s^3}{6}\dot{\varkappa} + \frac{s^4}{24}(\ddot{\varkappa} - \varkappa^3 - \varkappa\tau^2)\right]e_2$$
$$+ \left[\frac{s^3}{6}\varkappa\tau + \frac{s^4}{24}(2\dot{\varkappa}\tau + \varkappa\dot{\tau})\right]e_3 + \frac{s^4}{24}\varkappa\tau\sigma e_4 + O(s^5). \tag{7}$$

§ 2. First to Third Order Schemes

1) Omitting s^2 and higher order terms in (7) and substituting h for s, one gets the first order scheme

$$\begin{bmatrix} y_0 + \Delta y_0 \\ y_1 + \Delta y_1 \\ \vdots \\ y_n + \Delta y_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix} + \frac{h}{\sqrt{f_0^2 + f_1^2 + \cdots + f_n^2}} \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{bmatrix}. \tag{8}$$

This is an analogue of the Euler polygon method, but here h, instead of being an increment in x as usual, is the stepsize of movement along the tangent to the solution curve. It is an one-step nonlinear explicit scheme because the right-hand functions $f_j (j=1, 2, \cdots, n)$ appear in the denominator as summands within a radical sign.

2) Naturally, by neglecting s^3 and higher terms in (7) one gets the second order scheme

$$Y+\Delta Y=Y+\frac{h}{l}F+\frac{h^2}{2l^2}\left\{U-\frac{q}{l^2}F\right\}. \tag{9}$$

It could be geometrically summarized as "go along the tangent and correct along the normal". This is a one-step nonlinear second order explicit scheme with derivatives because it involves not only the right-hand functions but also their derivatives.

Furthermore, on the basis of (8) we could construct the following two-stage scheme

$$\begin{bmatrix} y_0+\Delta y_0 \\ y_1+\Delta y_1 \\ \vdots \\ y_n+\Delta y_n \end{bmatrix}=\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}+\frac{h}{2}\left\{\frac{1}{l}\begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{bmatrix}+\frac{1}{l^*}\begin{bmatrix} f_0^* \\ f_1^* \\ \vdots \\ f_n^* \end{bmatrix}\right\}, \tag{10}$$

where

$$f_j^*=f_j\left(y_0+h\frac{f_0}{l},\ y_1+h\frac{f_1}{l},\ \cdots,\ y_n+h\frac{f_n}{l}\right),$$

$$l^*=\left\{\sum_{j=0}^{n} f_j^{*2}\right\}^{1/2}.$$

Theorem 2. *The one-step two-stage nonlinear explicit scheme* (10) *is a second order scheme for the initial value problem* (3).

In fact, (10) can be written in vector form as

$$\Delta Y=\frac{s}{2}\left\{\frac{1}{l}F+\frac{1}{l^*}F^*\right\},$$

where

$$F^*=F(Y(0)+se_1),\quad l^*=l(Y(0)+se_1).$$

By (7),

$$F^*=F+\frac{s}{l}U+O(s^2)$$

and

$$\frac{1}{l^*}=\frac{1}{l}-s\frac{q}{l^3}+O(s^2).$$

Hence

$$\frac{1}{l^*}F^*=\frac{1}{l}F+s\left\{\frac{1}{l^2}U-\frac{q}{l^4}F\right\}+O(s^2).$$

Thus

$$\Delta y=se_1+\frac{s^2}{2}\varkappa e_2+O(s^3),$$

and (10) is a second order scheme.

3) On the basis of (9), we construct the two-stage scheme

$$Y+\Delta Y=Y+\frac{h}{l}F+\frac{h^2}{6}\left\{2\left[\frac{1}{l^2}U-\frac{q}{l^4}F\right]-\frac{1}{l^{*2}}\left[U^*-\frac{q^*}{l^{*4}}F^*\right]\right\}, \tag{11}$$

where the evaluation points are chosen as in (10):

$$u_j^*=u_j\left(y_0+h\frac{f_0}{l},\ y_1+h\frac{f_1}{l},\ \cdots,\ y_n+h\frac{f_n}{l}\right),$$

$$q^*=\sum_{j=0}^{n} f_j^* u_j^*.$$

Theorem 3. *The one-step two-stage nonlinear explicit scheme with derivatives* (11) *is a third order scheme for the initial value problem* (3).

By arguments similar to those used in the proof of Theorem 2,

$$\frac{1}{l^{*2}}U^*-\frac{q^*}{l^{*4}}F^*=\varkappa^* e_2^*.$$

Moreover,

$$\varkappa^*=\varkappa+s\dot{\varkappa}+O(s^2) \quad \text{and} \quad e_2^*=e_2+s(-\varkappa e_1+\tau e_3)+O(s^2),$$

so that

$$\varkappa^* e_2^*=\varkappa e_2+s\{-\varkappa^2 e_1+\dot{\varkappa} e_2+\varkappa\tau e_3\}+O(s^2).$$

Hence

$$\Delta y=se_1+\frac{s^2}{6}\{2\varkappa e_2+\varkappa^* e_2^*\}=\left(s-\frac{s^3}{6}\varkappa^2\right)e_1+\left(\frac{s^2}{2}\varkappa+\frac{s^3}{6}\dot{\varkappa}\right)e_2+\frac{s^3}{6}\varkappa\tau e_3+O(s^4),$$

and (11) is a third order scheme.

§ 3. Fourth Order Schemes

In order to derive fourth order schemes, we approach the problem by extending to the one-step three-stage schemes and by refining the evaluation points to

$$Y+pse_1+\frac{(ps)^2}{2}\varkappa e_2, \quad 0\leqslant p\leqslant 1.$$

1) Let α, β, γ be three combinational coefficients, and construct the three-stage scheme

$$\Delta y=se_1+\frac{s^2}{2}\{\alpha\varkappa^{(1)}e_2^{(1)}+\beta\varkappa^{(2)}e_2^{(2)}+\gamma\varkappa^{(3)}e_2^{(3)}\}, \tag{12}$$

where

$$\varkappa=\varkappa(Y(0)), \quad e_2=e_2(Y(0)),$$

and

$$\varkappa^{(i)}=\varkappa\left(Y(0)+p_i se_1+\frac{(p_i s)^2}{2}\varkappa e_2\right),$$

$$e_2^{(i)}=e_2\left(Y(0)+p_i se_1+\frac{(p_i s)^2}{2}\varkappa e_2\right), \quad i=1, 2, 3.$$

Because

$$\varkappa^{(i)}e_2^{(i)}=\varkappa e_2+p_i s(-\varkappa^2 e_1+\dot{\varkappa} e_2+\varkappa\tau e_3)$$
$$+\frac{(p_i s)^2}{2}\{-3\varkappa\dot{\varkappa} e_1+(\ddot{\varkappa}-\varkappa^3-\varkappa\tau^2)e_2+(2\dot{\varkappa}\tau+\varkappa\dot{\tau})e_3+\varkappa\tau\sigma e_4\},$$

by comparing $\frac{s^2}{2}\{\alpha\varkappa^{(1)}e_2^{(1)}+\beta\varkappa^{(2)}e_2^{(2)}+\gamma\varkappa^{(3)}e_2^{(3)}\}$ and the expression

$$\frac{s^2}{2}\ddot{Y}(0)+\frac{s^3}{6}\dddot{Y}(0)+\frac{s^4}{24}\ddddot{Y}(0),$$

we get the following relations:

$$\begin{aligned} &\alpha+\beta+\gamma=1, \\ &\lambda\alpha+\mu\beta+\nu\gamma=\frac{1}{3}, \\ &\lambda^2\alpha+\mu^2\beta+\nu^2\gamma=\frac{1}{6} \end{aligned} \tag{13}$$

with $\lambda=p_1$, $\mu=p_2$, $\nu=p_3$.

Theorem 4. *The one-step three-stage nonlinear explicit scheme with derivatives* (12) *is a fourth order scheme for the initial value problem* (3), *if and only if the coefficients* α, β, γ *and* λ, μ, ν *satisfy* (13), *that is*

$$\begin{aligned} &\alpha=\frac{\frac{1}{3}(\mu+\nu)-\mu\nu-\frac{1}{6}}{(\lambda-\mu)(\nu-\lambda)}, \\ &\beta=\frac{\frac{1}{3}(\nu+\lambda)-\nu\lambda-\frac{1}{6}}{(\lambda-\mu)(\mu-\nu)}, \\ &\gamma=\frac{\frac{1}{3}(\lambda+\mu)-\lambda\mu-\frac{1}{6}}{(\mu-\nu)(\nu-\lambda)}. \end{aligned} \tag{14}$$

2) We have found that by setting $\lambda=0$, $\mu=1/2$, $\nu=1$ in (14), one gets $\alpha=1/3$, $\beta=2/3$ and $\gamma=0$, which is a special one-step two-stage nonlinear fourth order explicit scheme with derivatives:

$$\begin{bmatrix} y_0+\Delta y_0 \\ y_1+\Delta y_1 \\ \vdots \\ y_n+\Delta y_n \end{bmatrix}=\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}+\frac{h}{l}\begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{bmatrix}$$

$$+\frac{h^2}{6}\left\{\left[\frac{1}{l^2}\begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_n \end{bmatrix}-\frac{q}{l^4}\begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{bmatrix}\right]+2\left[\frac{1}{\bar{l}^2}\begin{bmatrix} \bar{u}_0 \\ \bar{u}_1 \\ \vdots \\ \bar{u}_n \end{bmatrix}-\frac{\bar{q}}{\bar{l}^4}\begin{bmatrix} \bar{f}_0 \\ \bar{f}_1 \\ \vdots \\ \bar{f}_n \end{bmatrix}\right]\right\}. \tag{15}$$

where $\bar{f}_j$ and $\bar{u}_j$ are evaluated at point

$$\left(y_0+\frac{h}{2}\frac{f_0}{l}+\frac{h^2}{8}\left(\frac{u_0}{l^2}-\frac{q}{l^4}f_0\right),\ y_1+\frac{h}{2}\frac{f_1}{l}+\frac{h^2}{8}\left(\frac{u_1}{l^2}-\frac{q}{l^4}f_1\right),\ \cdots,\ y_n+\frac{h}{2}\frac{f_n}{l}+\frac{h^2}{8}\left(\frac{u_n}{l^2}-\frac{q}{l^4}f_n\right)\right),$$

$$\bar{l}=\left\{\sum_{j=0}^{n}\bar{f}_j^2\right\}^{1/2},\quad \bar{q}=\sum_{j=0}^{n}\bar{f}_j\bar{u}_j.$$

We propose that this fourth order scheme be used in actual computations.

§ 4. Stepsize Criterion

Now, we shall derive a stepsize criterion for (10) and (15) according to the absolute stability. For this purpose, consider the test equations

$$\begin{cases} \dfrac{dy_0}{dx}=1, \\ \dfrac{dy_1}{dx}=-\alpha y_1-\beta y_2, \\ \dfrac{dy_2}{dx}=\beta y_1-\alpha y_2, \end{cases} \tag{16}$$

where $\alpha>0$. For convenience, denote $y_0=x$, $y_1=y$, $y_2=z$. According to (10), after the k-th step we compute

$$\begin{bmatrix} x^* \\ y^* \\ z^* \end{bmatrix}=\begin{bmatrix} x_k \\ y_k \\ z_k \end{bmatrix}+\frac{h}{\sqrt{1+(\alpha^2+\beta^2)(y_k^2+z_k^2)}}\begin{bmatrix} 1 \\ -\alpha y_k-\beta z_k \\ \beta y_k-\alpha z_k \end{bmatrix},$$

and obtain

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \\ z_{k+1} \end{bmatrix}=\begin{bmatrix} x_k \\ y_k \\ z_k \end{bmatrix}+\frac{h}{2}\left\{\frac{h}{\sqrt{1+(\alpha^2+\beta^2)(y_k^2+z_k^2)}}\begin{bmatrix} 1 \\ -\alpha y_k-\beta z_k \\ \beta y_k-\alpha z_k \end{bmatrix}\right.$$
$$\left.+\frac{h}{\sqrt{1+(\alpha^2+\beta^2)(y^{*2}+z^{*2})}}\begin{bmatrix} 1 \\ -\alpha y^*-\beta z^* \\ \beta y^*-\alpha z^* \end{bmatrix}\right\}.$$

Absolute stability can be reduced to the requirement:

$$y_{k+1}^2+z_{k+1}^2\leqslant y_k^2+z_k^2. \tag{17}$$

Presently,

$$y_{k+1}^2+z_{k+1}^2=(y_k^2+z_k^2)\left\{1-\frac{2\alpha}{l}h+\frac{\alpha^2(l^2+1)}{l^4}h^2\right\}+O(h^3),$$

where

$$l=\sqrt{1+(\alpha^2+\beta^2)(y_k^2+z_k^2)}.$$

To ensure the validity of (17), the stepsize h must be restricted: $h<\dfrac{2l^3}{\alpha(l^2+1)}$. Making use of the inequality between the harmonic mean and the geometric mean, we find that the curvature of the curve at point (x_k, y_k, z_k)

$$\varkappa=\frac{\alpha^2+\beta^2}{l^3}\sqrt{y_k^2+z_k^2}\sqrt{1+\beta^2(y_k^2+z_k^2)}\geqslant\frac{2\alpha(l^2-1)}{l^3\cdot l^2}.$$

Thus we obtain a criterion for selecting stepsize (a stepsize criterion): The permissible stepsize

$$h_{\text{perm}}=\frac{4(l^2-1)}{\varkappa l^2(l^2+1)}. \tag{18}$$

For scheme (15), the same stepsize criterion is derived.

Theorem 5. *By the absolute stability, the one-step nonlinear second order scheme without derivatives* (10) *and the one-step two-stage nonlinear fourth order scheme with derivatives* (15) *must satisfy the stepsize criterion* (18).

From (18), the stepsize should be in inverse proportion to the curvature of the curve. Being a manifestation of the geometric nature of solution curves, this criterion applies to both stiff and nonstiff problems. This approach is more natural than the variable stepsize strategy adopted so far for stiff problems. Also, the one-step methods are especially flexible in variable stepsize procedures.

§ 5. Numerical Experiments

Examine the following stiff problem in reaction dynamics:

$$\begin{cases} \dfrac{du}{dt}=0.01-(0.01+u+v)[1+(u+1000)(u+1)], \\ \dfrac{dv}{dt}=0.01-(0.01+u+v)(1+v^2), \end{cases}$$

$$u(0)=v(0)=0, \quad 0\leqslant t\leqslant 100.$$

The system is fairly stiff at the very beginning of the process with a stiffness ratio $S\approx 10^5$, which is later reduced to approximately 10^2. When the problem was solved by using the classical Runge-Kutta method, the computation blew up after two steps with a fixed stepsize $h_{fix}=0.005$. The results of the computation are tabulated in Table 1, with $h_{fix}=0.0005$, 0.001, 0.002 and 0.0025 respectively[4].

Table 1 Results using Runge-Kutta method

h_{fix}	$u(100)$	$v(100)$
0.0005	−0.99164207	0.98333636
0.001	−0.99164207	0.98333636
0.002	−0.99164213	0.98333643
0.0025	−0.99164243	0.98333677

On applying the fourth order nonlinear method proposed in this paper, the permissible stepsize determined by the stepsize criterion might be quite large. Therefore, in order to ensure the accuracy, the working stepsize was constrained by the maximum stepsize, $h_{working}=\min\{h_{max}, h_{perm}\}$. Satisfactory results were obtained when computation was carried out with $h_{max}=0.001$, 0.005, 0.01 and 0.02 respectively (see Table 2).

Table 2 Results using nonlinear method

h_{max}	$u(100)$	$v(100)$
0.001	−0.99164207	0.98333636
0.005	−0.99164206	0.98333635
0.01	−0.99164204	0.98333634
0.02	−0.99164196	0.98333627

The numerical experiment[5,6] showed that except for a small starting interval this stiff problem could be solved with h_{perm} as wide as 0.05 in an extensive range. But in the small starting interval, high stiffness goes with large curvature, for instance, $h_{perm}=0.0001$ when $t=0.0072$. If the computation should be carried out at these places by a stepsize greater than h_{perm}, the previous errors would be "amplified" and propagated, affecting the accuracy of the outcome. By means of the stepsize criterion, this shortcoming of the fixed stepsize approach has turned out clearly. Although $h_{fix}=0.002$ or 0.0025 is very small globally, it is still inappropriate to the starting interval with high stiffness, resulting in certain errors. In fact, adopting the variable stepsize strategy defined by the stepsize criterion in the starting interval and using $h_{max}=0.001$—0.02, which was much larger than 0.0025, over the remaining wide range, we were able to obtain fairly good results. This class of nonlinear methods based on Frenet frame is very effective.

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