A THIRD ORDER SMALL PARAMETER METHOD AND ITS NORDSIECK EXPRESSION*

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Abstract

A third order small parameter method and its Nordsieck expression are given in this paper. It is based on Gear's method of order 2 and order 3. For moderate stiff problems this method is suitable.

In [1] we proposed a second order numerical method for stiff ODEs. The purpose of this paper is to raise the order from 2 to 3 and give its Nordsieck expression, making it automatically suit varying stepsize calculation.

§ 1. Derivation of the Method and the Truncation Error

For the differential equation

$$y'=f(t, y), \tag{1.1}$$

from the second order Gear formula

$$y_{n+1}=\frac{4}{3}y_n-\frac{1}{3}y_{n-1}+\frac{2}{3}hf_{n+1}, \tag{1.2}$$

we have

$$\frac{2}{3}hy'_{n+1}=y_{n+1}-\frac{4}{3}y_n+\frac{1}{3}y_{n-1} \tag{1.3}$$

and from (1.1) we have

$$\varepsilon y'_{n+1}=\varepsilon f_{n+1}, \tag{1.4}$$

where $\varepsilon>0$ is a small parameter.

(1.3) + (1.4) yields

$$\frac{2}{3}hy'_{n+1}=p\left[\varepsilon f_{n+1}+y_{n+1}-\frac{4}{3}y_n+\frac{1}{3}y_{n-1}\right], \tag{1.5}$$

where

$$p=\frac{h}{h+\frac{3}{2}\varepsilon},\quad 0<p<1.$$

We rewrite the third order Gear formula as follows:

$$y_{n+1}=\frac{18}{11}y_n-\frac{9}{11}y_{n-1}+\frac{2}{11}y_{n-2}+\frac{6}{11}\cdot\frac{3}{2}\left(\frac{2}{3}hy'_{n+1}\right). \tag{1.6}$$

From (1.5) and (1.6), we have

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$$y_{n+1}=\frac{18}{11}y_n-\frac{9}{11}y_{n-1}+\frac{2}{11}y_{n-2}+\frac{9}{11}p\Big[\varepsilon f_{n+1}+y_{n+1}-\frac{4}{3}y_n+\frac{1}{3}y_{n-1}\Big]. \tag{1.7}$$

Expanding both sides of (1.7) in the Taylor expression form, we get

$$y'_n=f_n-\frac{4}{3}\frac{1}{\varepsilon}\cdot\frac{h^3}{6}y'''_n+O(h^4). \tag{1.8}$$

Then the local truncation error is

$$\frac{2}{9}\frac{h^4}{\varepsilon}y_n^{(IV)}. \tag{1.9}$$

§ 2. The Stability Region

For the model equation

$$y'=\lambda y, \tag{2.1}$$

the eigenequation of scheme (1.7) is

$$\Big(1-\frac{9}{11}p-\frac{9}{11}p\varepsilon\lambda\Big)\mu^3-\Big(\frac{18}{11}-\frac{12}{11}p\Big)\mu^2+\Big(\frac{9}{11}-\frac{3}{11}p\Big)\mu-\frac{2}{11}=0. \tag{2.2}$$

The stability region in the $\varepsilon\lambda$-plane is the outside part of the following curve ($\mu=e^{i\theta}$, $\theta=0°-360°$):

$$\varepsilon\lambda=\frac{\Big(1-\frac{9}{11}p\Big)\mu^3-\Big(\frac{18}{11}-\frac{12}{11}p\Big)\mu^2+\Big(\frac{9}{11}-\frac{3}{11}p\Big)\mu-\frac{2}{11}}{\frac{9}{11}p\mu^3}. \tag{2.3}$$

The outlines for $p=1.0$, 0.9, 0.8, 0.5 are given in Figs. 1 to 4, where $p=1.0$ means $h\to\infty$. Because of the symmetry we only give the upper half part.

Unfortunately, when $p=1$ the unstability region includes a section of negative real axis, and this will cause some trouble in practice. Therefore, we need to find a value p_0 so that when $p<p_0$ the stability region includes the whole negative real axis. We introduce a lemma as follows ([2]):

Lemma. The roots μ_i ($i=1, 2, 3$) of a real coefficient cubic polynomial

$$\mu^3+\tilde{p}\mu^2+\tilde{q}\mu+\tilde{r}$$

satisfy $|\mu_i|\leqslant 1$, if and only if

(i) $1+\tilde{r}>0$, $1-\tilde{r}>0$;

(ii) $1+\tilde{p}+\tilde{q}+\tilde{r}>0$, $1-\tilde{p}+\tilde{q}-\tilde{r}>0$;

(iii) $1-\tilde{q}+\tilde{p}\tilde{r}-\tilde{r}^2>0$.

It is easy to check that the left-hand side of (2.2) satisfies (i) and (ii) of the lemma for any real $\varepsilon\lambda<0$ and $0<p\leqslant 1$. As for (iii), we have

$$\Big(1-\frac{9}{11}p-\frac{9}{11}p\varepsilon\lambda\Big)^2(1-\tilde{q}+\tilde{p}\tilde{r}-\tilde{r}^2)$$
$$=\frac{54}{121}(1-p)^2+\frac{135p^2-117p}{121}\varepsilon\lambda+\frac{81p^2}{121}(\varepsilon\lambda)^2.$$

If $\varepsilon\lambda$ is real negative, it no longer satisfies (iii) for any $0<p\leqslant 1$. But we see that, if $p\to 0$, (iii) is satisfied for any $\varepsilon\lambda<0$, so there exists a value p_0, for which if $p<p_0$, (iii) holds for any $\varepsilon\lambda<0$. In order to find p_0 we regard it as a quadratic equation of $\varepsilon\lambda$, and from the discriminant we get

$$p_0=0.932653$$

i.e. if $p<p_0$, the stability region includes the whole negative real axis.

§ 3. Nordsieck Expression

Because $\varepsilon p=\frac{2}{3}h(1-p)$, we get the matrix form of (1.7) as follows:

$$Y_{n+1}=BY_n+p(\varepsilon f_{n+1}+y_{n+1})C, \tag{3.1}$$

where

$$Y_n=\left(y_n,\ \frac{2}{3}h(1-p)y'_n+py_n,\ y_{n-1},\ y_{n-2}\right)^T,$$

$$C=\left(\frac{9}{11},\ 1,\ 0,\ 0\right)^T,$$

$$B=\begin{pmatrix} \frac{18-12p}{11} & 0 & \frac{-9+3p}{11} & \frac{2}{11} \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

In order to find the Nordsieck expression, we consider the cubic interpolation polynomial, which passes through y_n, f_n, y_{n-1}, y_{n-2}:

$$p(t)=y_n+f_n(t-nh)+\frac{\left(-\frac{7}{4}y_n+\frac{3}{2}hf_n+2y_{n-1}-\frac{1}{4}y_{n-2}\right)}{h^2}(t-nh)^2$$

$$+\frac{\left(-\frac{3}{4}y_n+\frac{h}{2}f_n+y_{n-1}-\frac{1}{4}y_{n-2}\right)}{h^3}(t-nh)^3.$$

On the other hand

$$p(t)=p(nh)+p'(nh)(t-nh)+\frac{1}{2}p''(nh)(t-nh)^2+\frac{1}{6}p'''(nh)(t-nh)^3.$$

Therefore

$$a_n=\frac{h^2}{2!}p''(nh)=-\frac{7}{4}y_n+\frac{3}{2}hf_n+2y_{n-1}-\frac{1}{4}y_{n-2},$$

$$b_n=\frac{h^3}{3!}p'''(nh)=-\frac{3}{4}y_n+\frac{1}{2}hf_n+y_{n-1}-\frac{1}{4}y_{n-2}.$$

(Here the notation a_n and b_n differ from Nordsieck's original by a factor h).

In this way we establish the relation

$$Z_n=RX_n,$$

where

$$Z_n=(y_n,\ hf_n,\ a_n,\ b_n)^T,$$

$$X_n=(y_n,\ hf_n,\ y_{n-1},\ y_{n-2})^T$$

and

$$R=\begin{pmatrix}1&0&0&0\\0&1&0&0\\-\frac{7}{4}&\frac{3}{2}&2&-\frac{1}{4}\\-\frac{3}{4}&\frac{1}{2}&1&-\frac{1}{4}\end{pmatrix}.$$

The vectors X_n and Y_n are connected in the form

$$Y_n=SX_n,$$

where

$$S=\begin{pmatrix}1&0&0&0\\p&\frac{2}{3}(1-p)&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},$$

the inverse

$$S^{-1}=\begin{pmatrix}1&0&0&0\\-\frac{h}{\varepsilon}&\left(\frac{3}{2}+\frac{h}{\varepsilon}\right)&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}.$$

Finally we get the relation of Z_n and Y_n:

$$Z_n=RX_n=RS^{-1}Y_n=TY_n, \tag{3.2}$$

$$T=RS^{-1}=\begin{pmatrix}1&0&0&0\\-\frac{h}{\varepsilon}&\left(\frac{3}{2}+\frac{h}{\varepsilon}\right)&0&0\\\left(-\frac{7}{4}-\frac{3}{2}\frac{h}{\varepsilon}\right)&\left(\frac{9}{4}+\frac{3}{2}\frac{h}{\varepsilon}\right)&2&-\frac{1}{4}\\\left(-\frac{3}{4}-\frac{1}{2}\frac{h}{\varepsilon}\right)&\left(\frac{3}{4}+\frac{1}{2}\frac{h}{\varepsilon}\right)&1&-\frac{1}{4}\end{pmatrix}.$$

Premultiplying both sides of equation (3.1) by the matrix T, and noticing (3.2), then we have

$$Z_{n+1}=TBT^{-1}Z_n+p(\varepsilon f_{n+1}+y_{n+1})TC \tag{3.3}$$

or

$$Z_{n+1}=AZ_n+p(\varepsilon f_{n+1}+y_{n+1})L, \tag{3.4}$$

where

$$A=TBT^{-1}$$

$$=\frac{1}{11\varepsilon}\begin{pmatrix}\varepsilon(11-9p)&\varepsilon(5-3p)&\varepsilon(-1+3p)&\varepsilon(-7-3p)\\(-11h+9hp)&(-5h+3hp)&(h-3hp)&(7h+3hp)\\(-6h+3hp)&(-6\varepsilon-4h+hp)&(-\varepsilon-2h-hp)&(15\varepsilon+14h+hp)\\-h&(-\varepsilon-h)&(-2\varepsilon-h)&(8\varepsilon+5h)\end{pmatrix},$$

$$L=\begin{pmatrix} \frac{9}{11} \\ \frac{3}{2}+\frac{2}{11}\frac{h}{\varepsilon} \\ \frac{9}{11}+\frac{3}{11}\frac{h}{\varepsilon} \\ \frac{3}{22}+\frac{1}{11}\frac{h}{\varepsilon} \end{pmatrix}.$$

We rewrite (3.4) in iterative form:

$$Z_{n+1}=Z_{n+1}^{(0)}+\mathrm{CORT} \tag{3.5}$$

and call CORT the correction vector and $Z_{n+1}^{(0)}$ the initial iteration vector.

Choose

$$Z_{n+1}^{(0)}=PZ_n,$$

where P is the Pascal matrix, namely,

$$P=\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

According to matrix A and $Z_{n+1}^{(0)}$ we can determine the correction vector. Put

$$c=py_n+\left(\frac{2}{3}+\frac{p}{3}\right)hf_n+\left(\frac{4}{3}-\frac{p}{3}\right)a_n+\left(2+\frac{p}{3}\right)b_n.$$

Then

$$\mathrm{CORT}=\begin{pmatrix} 0 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix} b_n+L[p(\varepsilon f_{n+1}+y_{n+1})-C],$$

where $C_2=\frac{4}{3}\frac{h}{\varepsilon}$, $C_3=2\frac{h}{\varepsilon}$, $C_4=\frac{2}{3}\frac{h}{\varepsilon}$.

We can rewrite C in the following form:

$$C=p\left(y_{n+1}^{(0)}+\frac{4}{3}b_{n+1}^{(0)}\right)+\frac{2}{3}(1-p)hf_{n+1}^{(0)}$$

(Notice in the above expression of $Chf_{n+1}^{(0)}=hf_n+2a_n+3b_n\neq hf(t_0, y_{n+1}^{(0)})$).

Finally, we get the Nordsieck expression of this method as follows:

$$Z_{n+1}=PZ_n+L[p(\varepsilon f_{n+1}+y_{n+1})-C]+\begin{pmatrix} 0 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix} b_n.$$

We use simple iteration to solve the implicit equation. For the equation $y'=\lambda y$, the iterative convergence rate is determined by the factor $\frac{9}{11}P(\varepsilon\lambda+1)$. Choosing $P=0.93$ (in this case the stability region includes the whole negative real axis), we have $h=\frac{279}{14}\varepsilon$. If we choose $\varepsilon\leqslant\frac{2}{|\lambda|}(|1+\varepsilon\lambda|<1)$, then we have $|h\lambda|\leqslant\frac{279}{7}\approx 40$.

Similarly, choosing $P=0.7, 0.8$, we have $|h\lambda|\leqslant 7$, $|h\lambda|\leqslant 12$ and convergence factor $\frac{9}{11}P(\varepsilon\lambda+1)\leqslant 0.58, 0.66$. In practice we choose $0.7\leqslant P\leqslant 0.8$. We can see the scheme is very suitable for mild stiff problems.

§ 4. Numerical Experiment

We test an example from [4]:

$$u'=998u+1998v,$$
$$v'=-999u-1999v.$$

The initial values are $u(0)=1$ and $v(0)=0$ and the analytical solution is

$$u=2e^{-t}-e^{-1000t},$$
$$v=-e^{-t}+e^{-1000t}.$$

We start from $t_0=1$ and take $h=0.04$. The values of u and v at $t=1, (1-h), (1-2h)$ are given by the analytical solution. According to

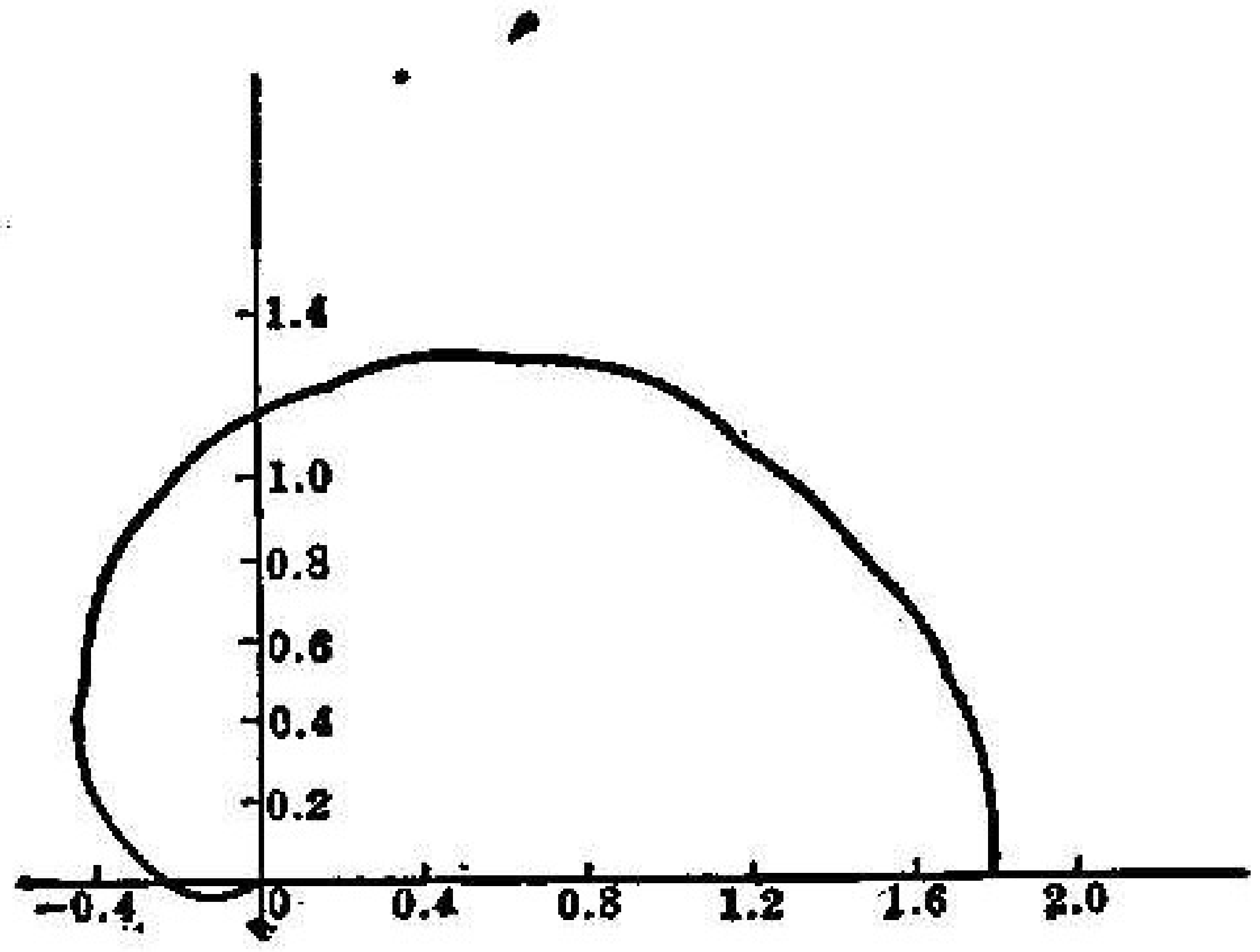

Fig. 1 Stability region in $\varepsilon\lambda$-plane for $p=1$ $(h\to\infty)$. Method is stable outside region indicated

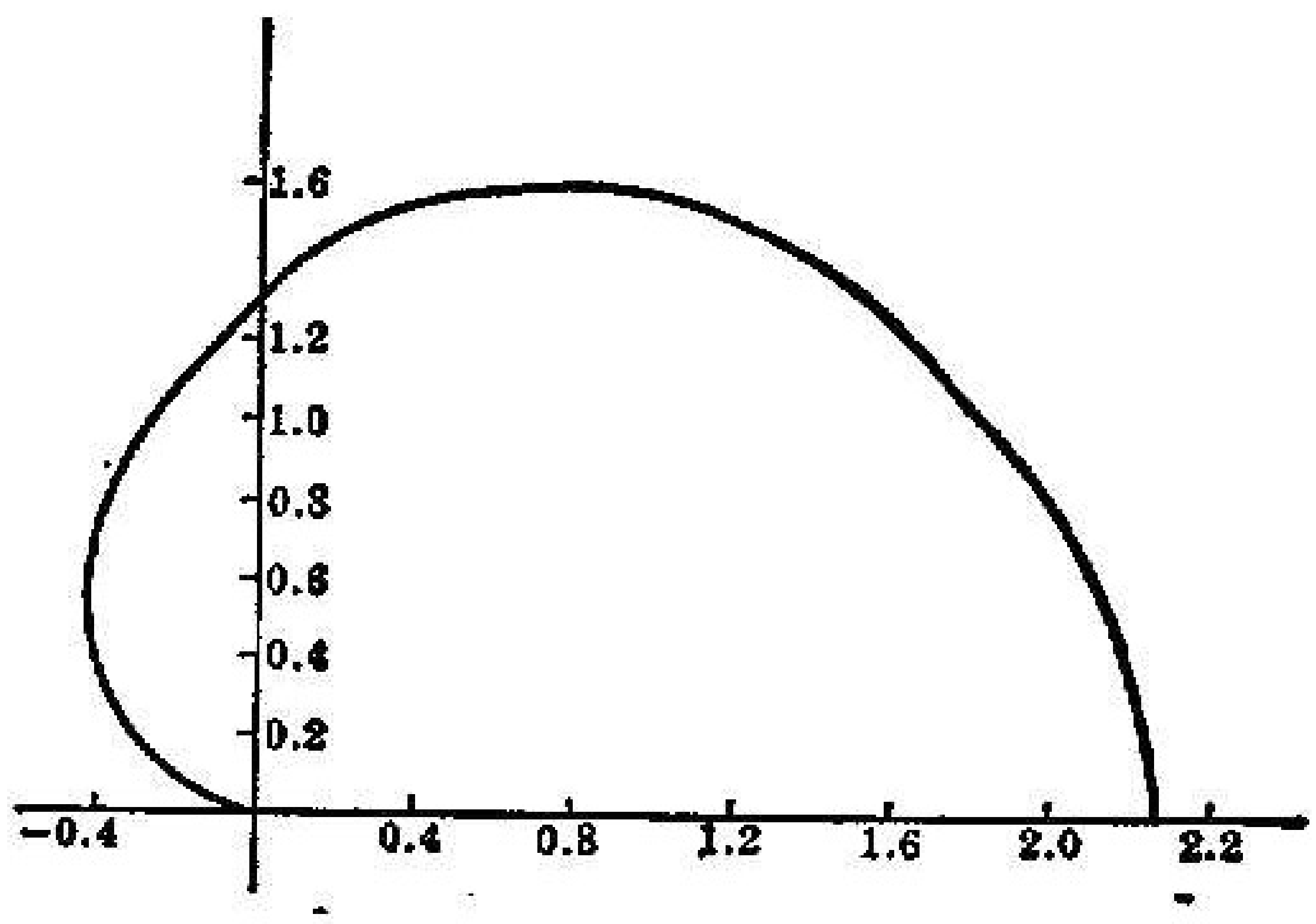

Fig. 2 Stability region in $\varepsilon\lambda$-plane for $p=0.9$. Method is stable outside region indicated

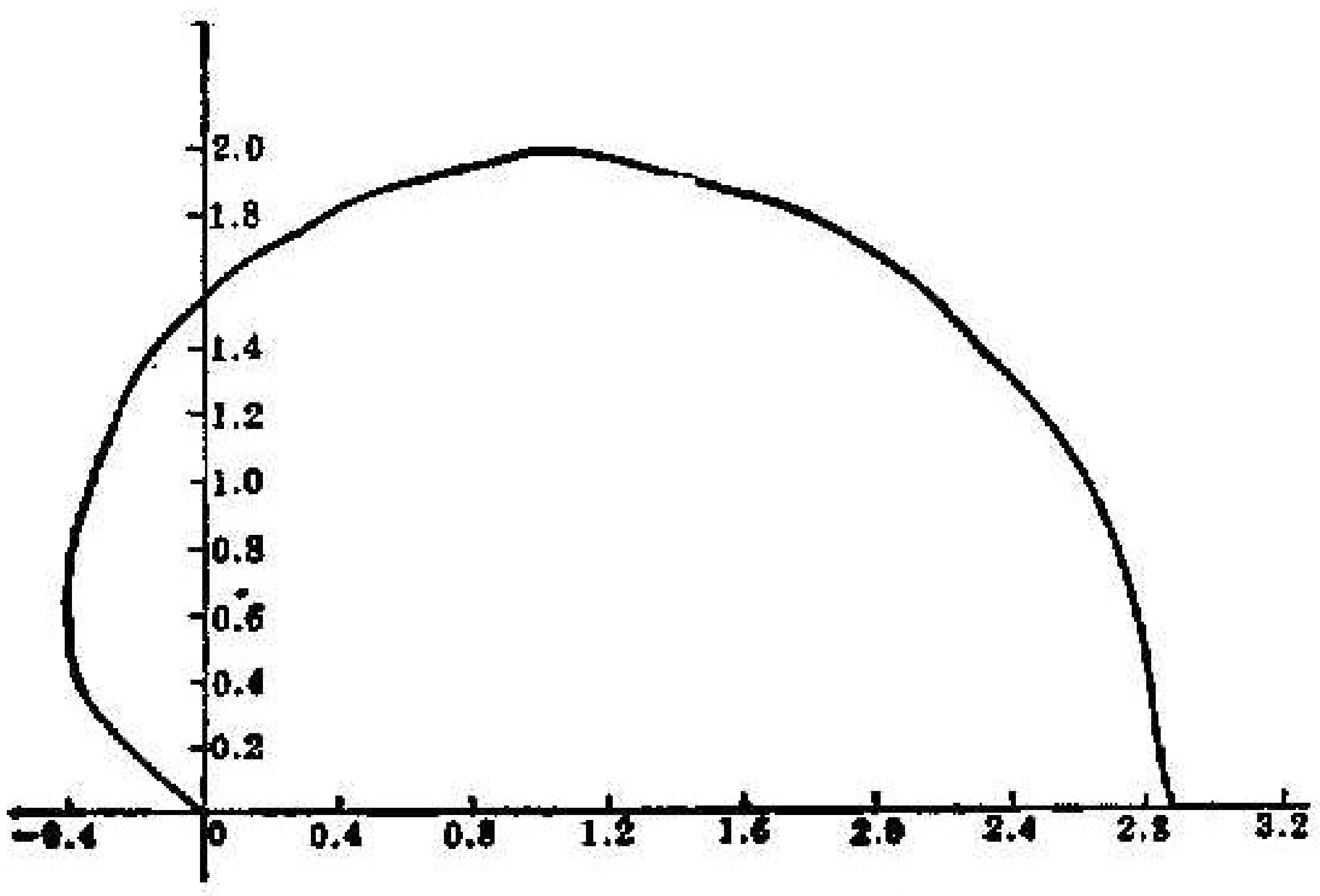

Fig. 3 Stability region in $\varepsilon\lambda$-plane for $p=0.8$. Method is stable outside region indicated

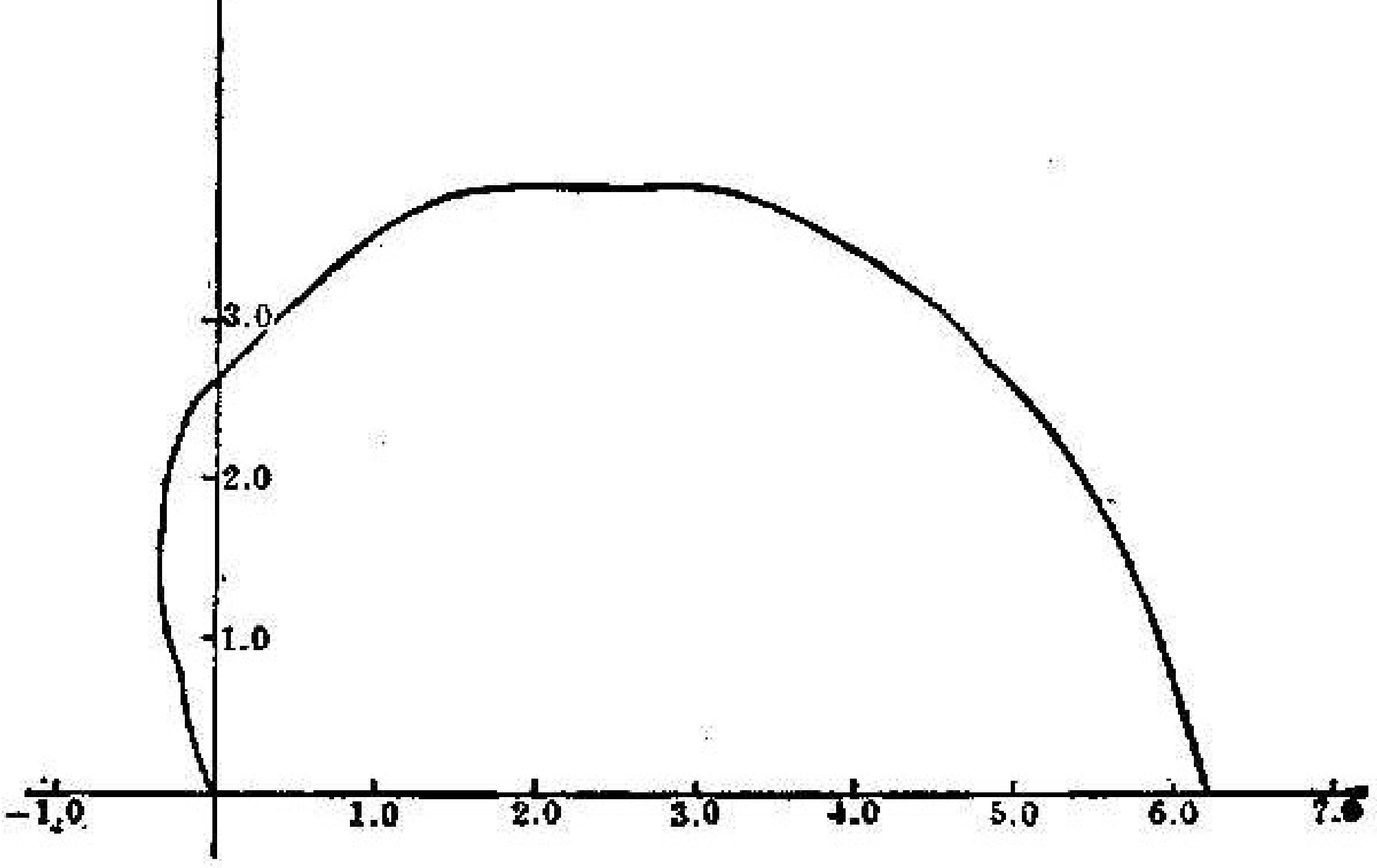

Fig. 4 Stability region in $\varepsilon\lambda$-plane for $p=0.5$. Method is stable outside region indicated

$$a_n = -\frac{7}{4} y_n + \frac{3}{2} h f_n + 2y_{n-1} - \frac{1}{4} y_{n-2},$$

$$b_n = -\frac{3}{4} y_n + \frac{1}{2} h f_n + y_{n-1} - \frac{1}{4} y_{n-2}.$$

we can yield a_0 and b_0 (a_0 and b_0 corresponding to $t_0=1$). Control the iteration by the relative error 10^{-4} and the integration interval is [1, 20]. At $t=20$ the absolute errors of u and v are 0.16×10^{-9} and 0.81×10^{-10} respectively. The number of function evaluation is equal to 5839.

References

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