THE DEFERRED CORRECTION PROCEDURE FOR LINEAR MULTISTEP FORMULAS*

SUN GENG (孙 耿)

(Institute of Mathematics, Academia Sinica, Beijing, China)

Abstract

A general approach of deferred correction procedure based on linear multistep formulas is proposed. Several deferred correction procedures based on backward differentiation formulas (Gear's method), which allow us to develop L-stable algorithms of order up to 4 and $L(\alpha)$-stable algorithms of order up to 7, are derived. Preliminary numerical results indicate that this approach is indeed efficient.

1. Introduction

The original idea of deferred correction was first proposed by Fox[4] to improve the accuracy of the basic solution. Significant improvements and extensions have been made since then. The concept of deferred correction now has a much wider meaning than the original idea of Fox. The various techniques of deferred correction have been widely used to obtain solutions of ordinary differential equations with improved orders of accuracy (see [5]—[8], [1]). The main reason why the technique of deferred correction arouses so much interest is that it often has more computational advantages than that of Richardson extrapolation. Particularly, in dealing with stiff systems, a deferred correction procedure or a local extrapolation one based on an underlying method that is usually of a low order and a high stability should preserve the good stability properties of this method. In this connection it is well known that local extrapolation is not praiseworthy.

In this paper we consider the problem of deriving an efficient deferred correction procedure based on linear multistep formulas. The key to the settlement of the question lies in choosing an appropriate correction term such that when the procedure is applied to the usual scalar test equation $y'=\lambda y$, with a constant step size h, the correction term is a rational function of λh, not a polynomial in λh as is usually the case. The procedures proposed in this paper can not only raise the order of accuracy of the basic solution but also improve the stability properties of the underlying formulas.

In Section 2 we explain our general approach and give some examples for simple deferred correction. In Section 3 we derive several deferred correction procedures based on BDF, which allow us to develop L-stable algorithms of order up to 4 and $L(\alpha)$-stable algorithms of order up to 7. Finally in Section 4 we present preliminary numerical results which will indicate that these algorithms

* Received April 2, 1984.

are indeed efficient.

2. The General Approach

In this section we shall be concerned with the numerical solution of the initial value problem

$$y' = f(t, y), \qquad y(t_0) = y_0, \tag{2.1}$$

obtained by using linear multistep formula

$$LM(h, p, y_{n+k}) = \sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f_{n+j} = 0 \tag{2.2}$$

with $\alpha_k = 1$ and the local truncation error (LTE)

$$T_k = C_{p+1} h^{p+1} y^{(p+1)}(t_n) + O(h^{p+2}). \tag{2.3}$$

The basic idea of deferred correction is to compute another improved numerical solution y_{n+k} by adding in a correction term computed from the numerical solution $\bar{y}_{n+k}$ of

$$LM(h, p, \bar{y}_{n+k}) = 0.$$

For this purpose we choose a formula

$$LC(h, q, y_{n+k}) = \sum_{j=0}^{k} \bar{\alpha}_j y_{n+j} - h \sum_{j=0}^{k} \bar{\beta}_j f_{n+j} = 0, \quad q > p, \ \bar{\alpha}_k = 1, \tag{2.4}$$

with an order higher than that of $LM(h, p, \bar{y}_{n+k}) = 0$ such that LC can be split into two parts, namely

$$LC(h, q, y_{n+k}) = LM(h, p, y_{n+k}) + L\varepsilon(h, p, y_{n+k}).$$

Obviously the LTE associated with

$$L\varepsilon(h, p, y_{n+k}) = 0 \tag{2.5}$$

is $(-T_k)$. Therefore $L\varepsilon$ may serve as the deferred correction term which is to be found and the solution $\bar{y}_{n+k}$ of $LM(h, p, \bar{y}_{n+k}) = 0$ can be improved to y_{n+k} by means of the correction formula

$$LM(h, p, y_{n+k}) = -L\varepsilon(h, p, \bar{y}_{n+k}). \tag{2.6}$$

As we shall see in the following such a choice of correction term (2.5) is often unsatisfactory for solving stiff systems since this form of deferred correction procedure usually destroys the good stability properties of the underlying formula.

However, this choice of (2.5) (called simple correction term) unifies the deferred correction procedure and the popular predictor corrector into one procedure and makes it easy to derive some implicit multistep formulas.

As an alternative, in dealing with stiff systems we consider a rational deferred correction procedure (see [1])

$$LM(h, p, \bar{y}_{n+k}) = 0, \tag{2.7a}$$

$$LM(h, p, y_{n+k}) = -P_l(hJ)(I - h\beta_k J)^{-m} L\varepsilon(h, p, \bar{y}_{n+k}), \tag{2.7b}$$

where J is an approximation to the Jacobian matrix $\frac{\partial f}{\partial y}$, P_l is a polynomial of degree l and l, m are integers.

As we shall see in Section 3, if the following conditions

(i) $$m>l\geqslant 0, \tag{2.8a}$$

(ii) $$P_l(q)(I-\beta_k q)^{-m}=1+O(q) \tag{2.8b}$$

are satisfied, then the deferred correction procedure obtained with (2.7) not only raises the order of accuracy of solution $\bar{y}_{n+k}$ but also improves the stability properties of the underlying formula (2.7a).

Assume that the solution values $y_n, y_{n+1}, \cdots, y_{n+k-1}$ are available. The deferred correction procedure used in practice is to carry out the following steps:

(1) Compute $\bar{y}_{n+k}$ from the underlying formula $LM(h, p, \bar{y}_{n+k})=0$ or some other appropriate one.

(2) Compute the correction term

$$\varepsilon=-P_l(hJ)(I-h\beta_k J)^{-m}L\varepsilon(h, p, \bar{y}_{n+k}).$$

Note that $(I-h\beta_k J)$ has already been computed and LU decomposed. So this only requires multiple back substitutions.

(3) Compute y_{n+k} from the correction equation

$$LM(h, p, y_{n+k})=\varepsilon.$$

Let's consider now the LTE associated with such a procedure ((1)—(3)).

First of all we have

$$y(t_{n+k})-\bar{y}_{n+k}=C_{p+1}h^{p+1}y^{(p+1)}(t_n)+O(h^{p+2})$$

from (1) and

$$f(t_{n+k}, y(t_{n+k}))-f(t_{n+k}, y_{n+k})=\frac{\partial f}{\partial y}(y(t_{n+k})-\bar{y}_{n+k})+\cdots=O(h^{p+1}),$$

where $y(t)$ is the exact solution of (2.1).

Further we have

$$\begin{aligned}\varepsilon=&-(1+O(h))\{-C_{p+1}h^{p+1}y^{(p+1)}_{(t_n)}+O(h^{(p+2)})\\&+(\bar{\beta}_k-\beta_k)h[f(t_{n+k}, y(t_{n+k}))-f(t_{n+k}, y_{n+k})]\}\\=&C_{p+1}h^{p+1}y^{(p+1)}_{(t_n)}+O(h^{p+2})\end{aligned}$$

from (2) and condition (2.8b). It follows that the correction formula (2.7b) has an order at least $(p+1)$.

Some examples of the simple deferred correction procedure are given as follows:

Example 1. Consider the Adams-Bashforth formula in the form of backward difference operator

$$LM(h, k, y_{n+1})=y_{n+1}-y_n-h\sum_{j=0}^{k-1}\gamma_j\nabla^j f_n=0$$

with the LTE

$$T_k=\gamma_k h^{k+1}y^{(k+1)}_{(t_n)}+O(h^{k+2}).$$

We choose the correction term

$$L\varepsilon(h, k, y_{n+1})=-\gamma_k h\cdot\nabla^k f_{n+1}.$$

Obviously the LTE associated with $L\varepsilon(h, k, y_{n+1})=0$ is $(-T_k)$, then the deferred correction procedure

$$LM(h, k, \bar{y}_{n+1})=0, \tag{2.9a}$$

$$LM(h, k, y_{n+b})=-L\varepsilon(h, k, \bar{y}_{n+1}) \tag{2.9b}$$

has an order at least $(k+1)$. In fact (2.9) is the predictor corrector procedure of

Adams–Bashforth–Moulton formula. This means that

$$y_{n+1}-y_n-h\sum_{j=0}^{k-1}\gamma_j\nabla^j f_n-h\gamma_k\nabla^k f_{n+1}=0$$

is Adams-Moulton formula. The latter can be easily proved.

Example 2. Consider the Nyström formula in the form of backward difference operator

$$LM(h,\ p,\ y_{n+1})=y_{n+1}-y_n-h\sum_{j=0}^{k-1}k_j\cdot\nabla^j f_n=0.$$

If we choose

$$L\varepsilon(h,\ k,\ y_{n+1})=-k_k h\nabla^k f_{n+1}$$

as our correction term, then the Milne–Simpson formula can be written as

$$y_{n+1}-y_{n-1}-h\sum_{j=0}^{k-1}k_j\cdot\nabla^j f_n-hk_k\cdot\nabla^k f_{n+1}=0.$$

Example 3. Consider the simple deferred correction procedure based on BDF in the form of multistep formula.

For the underlying formula

$$LM(h,\ k,\ y_{n+k})=y_{n+k}-GR_k-h\beta_k f_{n+k}=0 \tag{2.10}$$

with the LTE

$$T_{G_k}=-\frac{\beta_k}{(k+1)}h^{k+1}y_{(t_n)}^{(k+1)}+O(h^{k+2}), \tag{2.11}$$

where $GR_k=-\sum_{j=0}^{k-1}\alpha_j y_{n+j}$, we choose

$$L\varepsilon(h,\ k,\ y_{n+k})=\frac{\beta_k}{(k+1)}h\Delta^k f_n \tag{2.12}$$

as our correction term, where Δ is the forward difference operator, then the simple deferred correction procedure

$$LM(h,\ k,\ \bar{y}_{n+k})=0, \tag{2.13a}$$

$$LM(h,\ k,\ y_{n+k})=-L\varepsilon(h,\ k,\ \bar{y}_{n+k}) \tag{2.13b}$$

is of order $(k+1)$.

We now examine the stability of this procedure.

To this end we apply the procedure to the scalar test equation $y'=\lambda y$, Re $\lambda<0$. Applying (2.13a) to the test equation, we obtain

$$y_{n+k}=(1-\beta_k q)^{-1}GR_k,\qquad q=\lambda h. \tag{i}$$

Using (i) to compute the correction term $L\varepsilon(h,\ k,\ \bar{y}_{n+k})$ we have

$$L\varepsilon(h,\ k,\ y_{n+k})=\frac{\beta_k q}{(k+1)}\left\{(1-\beta_k q)^{-1}GR_k+\sum_{j=1}^{k}(-1)^j C_k^j y_{n+k-j}\right\}. \tag{ii}$$

Finally, applying (2.13b) to the same scalar test equation and using (ii) we obtain

$$(1-\beta_k q)^2 y_{n+k}+\frac{\beta_k q}{(k+1)}(1-\beta_k q)\sum_{j=1}^{k}(-1)^j C_k^j y_{n+k-j}+\left[\frac{\beta_k q}{(k+1)}(1-\beta_k q)\right]GR_k=0.$$

This may in turn be rewritten in the form

$$\sum_{j=0}^{k}C_j(q)y_{n+j}=0.$$

The characteristic equation associated with this k^{th} order difference equation is

$$\sum_{j=0}^{k} C_j(q) r^j = 0, \qquad (2.14)$$

where $C_j(q)$ is a polynomial of degree 2.

The conditions for the roots of this polynomial are that all of them must be less than 1 in modulus according to Schur's theorem (see [3], p. 82) and these conditions may easily be tested using an entirely numerical approach. In Figure 1 these stability regions are drawn. As can be seen, this procedure destroys the good stability properties of BDF, hence it is unsatisfactory for solving stiff systems.

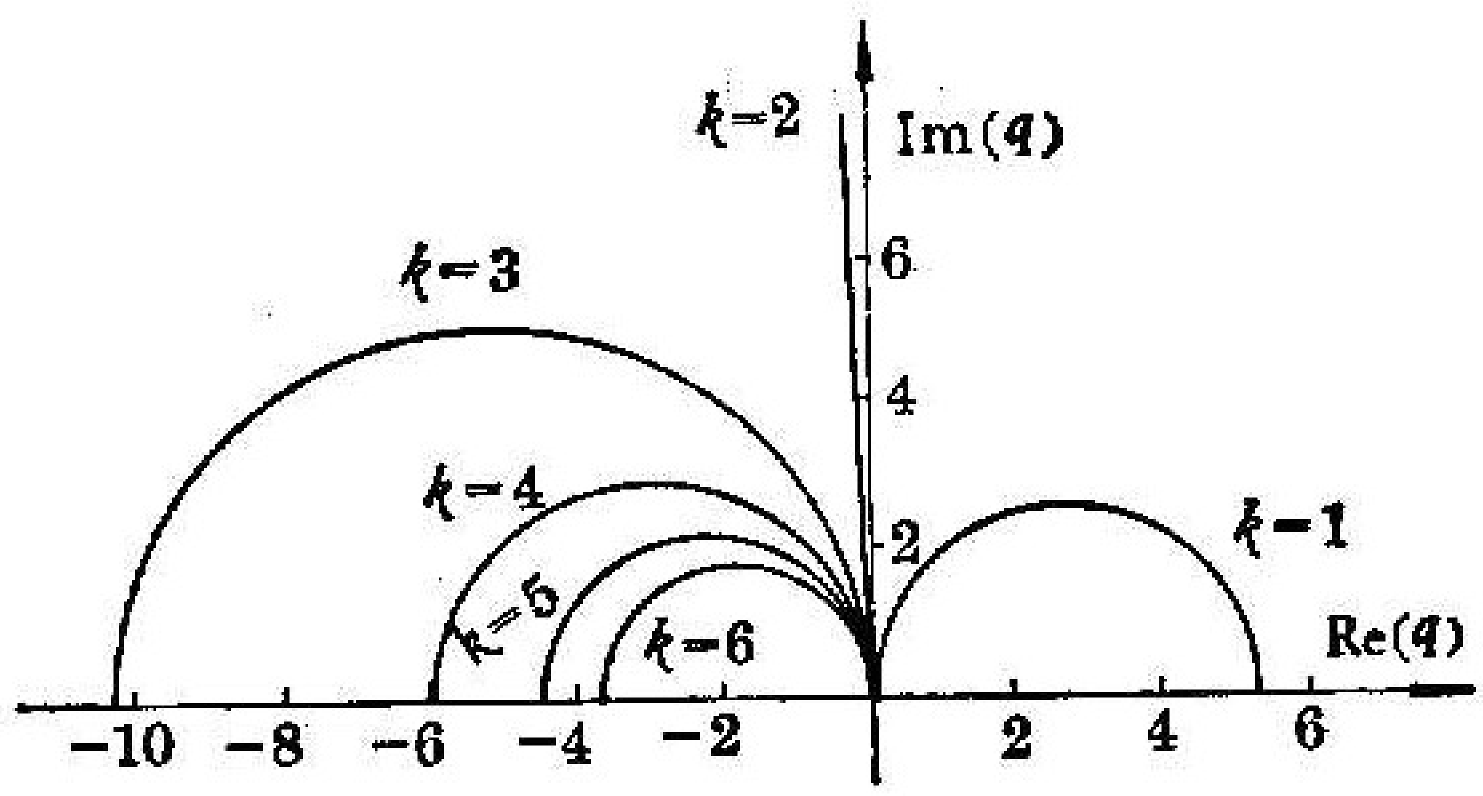

Fig. 1 Regions of absolute stability of the simple deferred correction procedures based on BDFs for $k=1$—6. In each case the region of stability is to the left of the dividing line from origin to end and is symmetric about the real axis.

3. Case Studies on Deferred Correction Procedure

The purpose of this section is to derive six deferred correction procedures based on BDF. All these procedures have L-stable algorithms of order up to 4 and $L(\alpha)$-stable algorithms of order up to 7 and the same stability regions for each value of k. Just like Gear's method, each of our algorithms associated with these procedures requires that the coefficient matrix $(I-\beta_k hJ)$ and LU decomposition be evaluated at most once per unit step.

Procedure 1. The BDF serves as the underlying formula

$$LM(h,\ k,\ y_{n+k}) = y_{n+k} - GR_k - h\beta_k f_{n+k} = 0 \qquad (3.1a)$$

with the basic correction term

$$Le(h,\ k,\ y_{n+k}) = \frac{1}{(k+1)} \beta_k h \Delta^k f_n \qquad (3.1b)$$

and the correction formula

$$LM(h,\ k,\ y_{n+k}) = -(I-h\beta_k J)^{-1} Le(h,\ k,\ y_{n+k}). \qquad (3.1c)$$

Then the deferred correction procedure (the algorithm)

$$\begin{aligned} &LM(h,\ k,\ \bar{y}_{n+k}) = 0, \\ &LM(h,\ k,\ y_{n+k}) = -(I-h\beta_k J)^{-1} Le(h,\ k,\ \bar{y}_{n+k}) \end{aligned} \qquad (3.1)$$

has order $(k+1)$.

The cost of carrying out this algorithm is determined by the following steps:

1. compute $\bar{y}_{n+k}$ using Gear's method,
2. make a back substitution and
3. compute y_{n+k} using the correction formula (3.1c).

Practical experience has shown that, since $\bar{y}_{n+k}$ often serves as a very good initial approximation to y_{n+k}, this quasi-Newton scheme usually converges rapidly. Therefore this algorithm requires roughly double number of iteration of Gear's method if a back substitution is thought to be an iteration.

Procedure 2. The underlying formula of procedure 1 is only used to derive the correction formula. However, we compute $\bar{y}_{n+k}$ using the explicit multistep formula (see [2])

$$ELM(h,\ k,\ y_{n+k})=y_{n+k}-GR_k-h\beta_k[f_{n+k}-\Delta^k f_n]=0. \tag{3.2a}$$

We can also take

$$Le(h,\ k,\ y_{n+k})=\frac{1}{(k+1)}h\beta_k\Delta^k f_n \tag{3.2b}$$

as the basic correction term; the correction formula will be

$$LM(h,\ k,\ y_{n+k})=-(I-h\beta_k J)^{-2}Le(h,\ k,\ \bar{y}_{n+k}) \tag{3.2c}$$

and the algorithm

$$\begin{aligned}&ELM(h,\ k,\ \bar{y}_{n+k})=0,\\&LM(h,\ k,\ y_{n+k})=-(I-h\beta_k J)^{-2}Le(h,\ k,\ \bar{y}_{n+k})\end{aligned} \tag{3.2}$$

has order $(k+1)$.

The cost of carrying out this algorithm is equivalent to that of Gear's method with two additional back substitutions.

Procedure 3. We take linearly implicit multistep formula[2]

$$LI_1(h,\ k,\ y_{n+k})=y_{n+k}-GR_k-h\beta_k\Big[f_{n+k}+\frac{\partial f}{\partial y}\Delta^k y_n-\Delta^k f_n\Big]=0 \tag{3.3a}$$

with the LTE

$$T_k=\frac{k}{(k+1)}\beta_k h^{k+1}y^{(k+1)}_{(t_n)}-\beta_k h^{k+1}\frac{\partial f}{\partial y}y^{(k)}_{(t_n)}+O(h^{k+2})$$

as the underlying formula. The basic correction term will then be

$$Le_1(h,\ k,\ y_{n+k})=\beta_k h\Big(\frac{\partial f}{\partial y}\Delta^k y_n-\frac{k}{(k+1)}\Delta^k f_n\Big) \tag{3.3b}$$

and the correction formula is

$$LI_1(h,\ k,\ \bar{y}_{n+k})=-(I-h\beta_k J)^{-1}Le_1(h,\ k,\ \bar{y}_{n+k}). \tag{3.3c}$$

Then the algorithm

$$\begin{aligned}&LI_1(h,\ k,\ \bar{y}_{n+k})=0,\\&LI_1(h,\ k,\ y_{n+k})=-(I-h\beta_k J)^{-1}Le_1(h,\ k,\ \bar{y}_{n+k})\end{aligned} \tag{3.3}$$

has order $(k+1)$.

The cost of carrying out this algorithm only comprises three back substitutions.

Procedure 4. We take the linearly implicit one-leg formula[2]

$$LI_2(h,\ k,\ y_{n+k})=y_{n+k}-GR_k-h\beta_k\Big[f(t_{n+k},\ y_{n+k}-\Delta^k y_n)+\frac{\partial f}{\partial y}\Delta^k y_n\Big]=0 \tag{3.4a}$$

with the LTE

$$T_k=T_{G_k}+\frac{1}{2}\beta_k h^{2k+1}\frac{\partial^2 f}{\partial y^2}(y^{(k)}_{(t_n)})^2+O(h^{3k+1})$$

as the underlying formula and

$$Le(h,\ k,\ y_{n+k})=\frac{1}{(k+1)}h\beta_k\Delta^k f_n \tag{3.4b}$$

as the basic correction term. The correction formula is

$$LI_2(h,\ k,\ y_{n+k}) = -(I-\beta_k hJ)^{-1}L\varepsilon(h,\ k,\ \bar{y}_{n+k}). \tag{3.4c}$$

Then the algorithm

$$\begin{aligned} &LI_2(h,\ k,\ \bar{y}_{n+k}) = 0, \\ &LI_2(h,\ k,\ y_{n+k}) = -(I-\beta_k hJ)^{-1}L\varepsilon(h,\ k,\ \bar{y}_{n+k}) \end{aligned} \tag{3.4}$$

has order $(k+1)$. The cost of carrying out it is about the same as in procedure 3.

Procedure 5. Same as procedure 1 except that we use (3.3a), rather than (3.1a), to compute $\bar{y}_{n+k}$.

Procedure 6. Same as procedure 1 except that we use (3.4a), rather than (3.1a) to compute $\bar{y}_{n+k}$.

The cost of carrying out each algorithm of procedures 5 and 6 is equivalent to that of Gear's method with one or two additional back substitutions.

Of course, we can give still more procedures with similar properties as indicated above; they are omitted here due to lack of place.

We now examine the stability of these procedures. Just like Example 3 in Section 2 we apply these procedures to the test equation $y' = \lambda y$; finally we obtain similarly the k^{th} order difference equation for each of these procedures

$$\sum_{j=0}^{k} \bar{C}_j(q) y_{n+j} = 0, \tag{3.7}$$

where $\bar{C}_j(q)$ $(j \leqslant k-1)$ and $\bar{C}_k(q)$ are polynomials of degree 2 and 3 respectively. This shows that these algorithms are stable at infinity.

The characteristic equation associated with (3.7) is

$$\sum_{j=0}^{k} \bar{C}_j(q) r^j = 0. \tag{3.8}$$

The regions of absolute stability of our algorithms are found for each value of k using Schur's theorem just like Example 3 in Section 2. These stability regions are drawn in Figure 2 and two parameters for assessing the stability properties are given in Table 1. As can be seen, these algorithms have better stability properties than Gear's method.

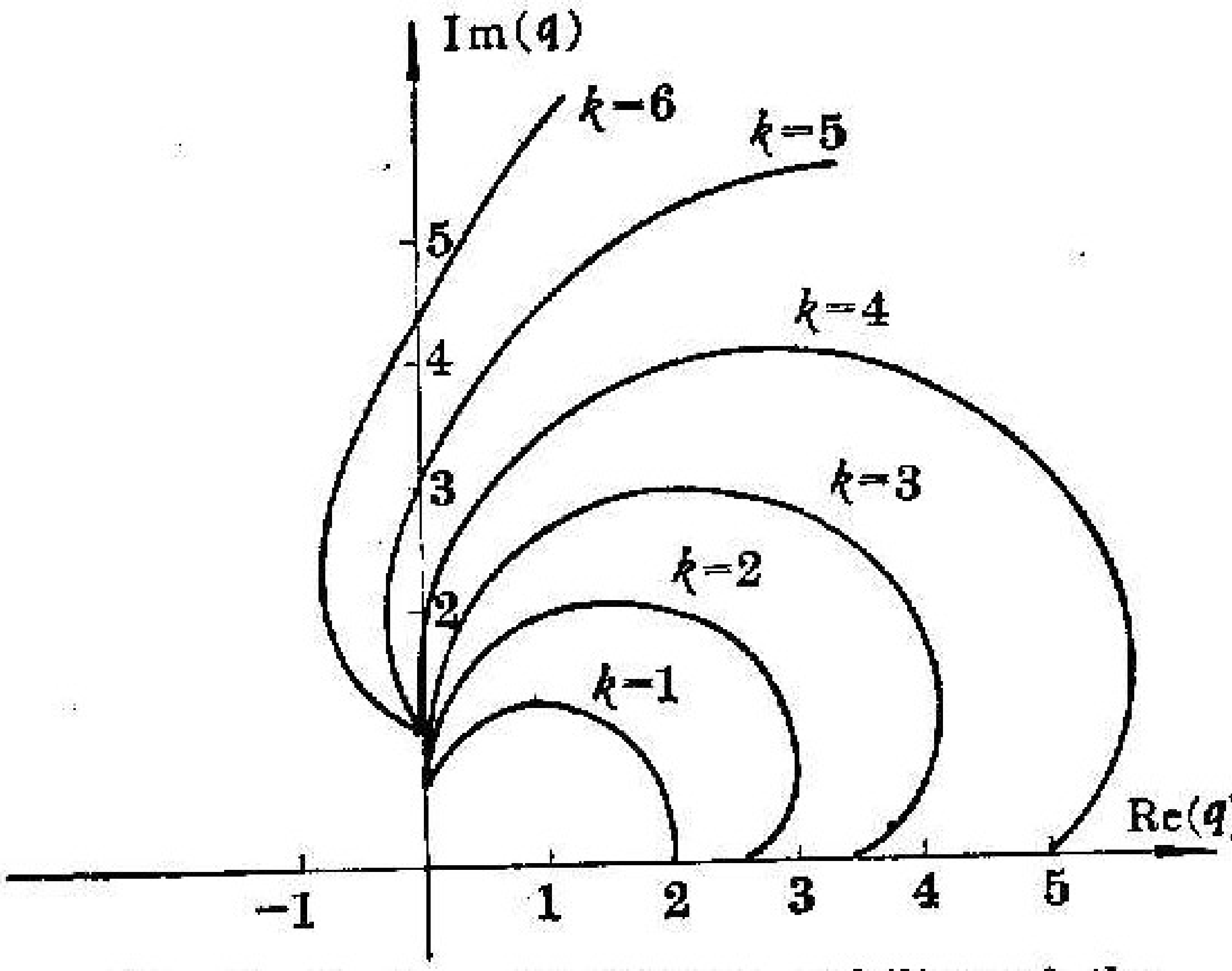

Fig. 2 Regions of absolute stability of the deferred correction algorithms based on BDFs for $k=1-6$. In each case the region of stability is to the left of the dividing line and is symmetric about the real axis.

Table 1

k	BDFs			Deferred correction		
	order	$D_{\min}$	$\alpha_{\max}$	order	$D_{\min}$	$\alpha_{\max}$
3	3	0.1	80°	4		L-stable
4	4	0.7	73°	5	0.04	88°
5	5	2.4	51°	6	0.27	81°
6	6	6.1	18°	7	0.79	67°

4. Numerical Results

In this section we present some preliminary numerical results which can be used to make a comparison between deferred correction procedure and BDF. The aim of this investigation is to demonstrate numerically the superior performance of our deferred correction procedure for each given fixed steplength over that of BDF with the same steplength, for a small selection of test problems. Of course we can not yet claim that these numerical results demonstrate the superiority of our algorithm over Gear's method, but they at least tell us that the deferred correction procedure based on BDF is worth further investigation and examination.

All numerical experiments have been run on the FELIX-512 machine in FORTRAN double precision. The formulas which we considered are respectively

(i) BDF($k=3$),

(ii) Procedure 4 ($k=3$) ($P_4(k=3)$),

(iii) Procedure 6 ($k=3$) ($P_6(k=3)$).

These formulas were implemented with the fixed steplength $h=0.1$.

The two test problems ([g] E_2 and D_5) are respectively

(P_1): $$y_1'=y_2, \quad y_1(0)=2,$$

$$y'=5(1-y_1^2)y_2-y_1, \quad y_2(0)=0, \quad t_f=1.$$

The exact solution $y_1(1)=1.869409210$, $y_2(1)=-0.148239937$.

(P_2): $$y'=0.01-[1+(y_1+1000)(y_1+1)]\cdot(0.01+y_1+y_2), \quad y_1(0)=0,$$

$$y_2'=0.01-(1+y_2^2)(0.01+y_1+y_2), \quad y_2(0)=0, \quad t_f=100.$$

The exact solution $y_1(100)=-0.99164207$, $y_2(100)=0.98333636$.

In Tables 2 and 3 we give the maximal relative errors at t_f of the numerical solution of (P_1) and (P_2) respectively using the formulas (i), (ii) and (iii). L denotes the number of the iteration per step.

Table 2 Maximal relative errors of (P_1)

L	BDF($k=3$)	$P_4(k=3)$	$P_6(k=3)$
2	$4.23*10^{-4}$		
3	$4.23*10^{-4}$	$5.90*10^{-5}$	$2.80*10^{-5}$
4	$4.23*10^{-4}$		$2.30*10^{-5}$

Table 3 Maximal relative errors of (P_2)

L	BDF($k=3$)	$P_4(k=3)$	$P_6(k=3)$
3	$7.5*10^{-3}$	$7.7*10^{-6}$	$1.1*10^{-5}$
4	$2.1*10^{-4}$		$6.8*10^{-7}$
5	$9.6*10^{-6}$		$1.0*10^{-6}$

As can be seen from the two tables, our numerical results are consistent with the conclusions obtained in the previous section. This indicates that a properly implemented version of our algorithm can be useful for numerical integration of stiff systems and at least the deferred correction procedure which we have derived can improve Gear's method such that the resultant code can deal with a wider range of stiff systems than Gear's method does.

References

[1] J. R. Cash, On improving the absolute stability of local extrapolation, *Numer. Math.*, **40** (1982), 329—337.

[2] 孙耿，毛祖范，两类线性隐式方法，计算数学，**3** (1981), 169—174.

[3] J. D. Lambert, Computational Methods in ODEs, 1973.

[4] L. Fox, Some improvements in the use of relaxation methods for the soluti n of ordinary and partial differential equations, *Proc. Royal Soc. London Ser.*, A. 190 (1947), 31—59.

[5] R. Frank, C. W. Ueberhuber, Iterated defect correction for the efficient solution of stiff systems of ODEs, *BIT*, **17** (1977), 146—159.

[6] H. J. Stetter, The defect correction principle and discretization methods, *Numer. Math.*, **29** (1978), 425—443.

[7] B. Lindberg, Error estimation and iterative improvement for discretization algorithms, *BIT*, **20** (1980), 486—500.

[8] R. D. Skell, A theoretical framework for proving accuracy results for deferred correction, *SIAM J. Numer. Anal.*, **19** (1982), 171—196.

[9] W. H. Enright, T. E. Hull, B. Lindberg, Comparing numerical methods for stiff systems of ODEs, *BIT*, **15** (1975), 10—48.