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# GENERALIZED ADAMS METHODS FOR THE SOLUTION OF SYSTEMS OF NONLINEAR EQUATIONS

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## 1. Introduction

We consider the problem of solving a system of nonlinear equations

$$f_j(x_1, x_2, \cdots, x_n)=0, \quad j=1, 2, \cdots, n.$$

These may be written more concisely as

$$F(x)=0 \tag{1.1}$$

where $x$ is the column vector of variables $x_i$ and $F$ is the column vector of functions $f_j$. Then the Newton's method is defined by

$$x_{n+1}=x_n - J_n^{-1}F_n$$

where $x_n$ is the n-th approximation to the solution of (1.1), $F_n=F(x_n)$, and $J_n$ is the Jacobian matrix evaluated at $x_n$.

Newton's method, in solving a system of nonlinear equations, is the best-known method, and it is mathematically the most preferable of the several known methods because of its quadratic convergence. However, it fails very often to converge to a solution when only a poor approximation is known.

With a poor initial guess, a damped Newton's method sometimes solves a system of nonlinear equations when the full Newton's method cannot. By considering the Newton's method as an Euler's method applied to the corresponding differential equations, Boggs(1971) applied $A$-stable integration techniques (trapezoidal rules) to solve systems of nonlinear equations. Boggs choose the trapezoidal rule as the basic method and used predictor-corrector algorithms.

The ordinary differential equation (O. D. E.) in which we are interested is such that its solution $x(t) \rightarrow x^*$ as $t \rightarrow \infty$, where $t$ is the independent variable. Thus we are interested only in the asymptote of the solution. The trapezoidal rule, or the Boggs (weakly) $A$-stable method, solves some problems effectively which the Newton's method fails to solve. But the rate of convergence is very slow even when the numerical solution is very close to the root. The report by Boggs (1971) also shows that the weakly $A$-stable trapezoidal rule is too much sensitive to the algorithm.

These facts lead us to develop a more rapidly converging integration technique than the Boggs method. In this paper, a class of Generalized Adams methods is developed. The Boggs method (weakly $A$-stable method), the Gear's method (stiffly stable method) and the Generalized Adams method ($A$-stable method) are compared on some chosen problems. The results show that the newly proposed method is better than other methods for some particular problems.

Throughout this paper, $F(x)=0$ is the equation whose solution is sought. The point $x^*$ will always denote the root of the system of equations, and $x_0$ the initial approximation to $x^*$. The function $F: R^N \to R^N$ is assumed differentiable, and the Jacobian of $F$ at the point $x$ is denoted by $J(x)$.

## 2. The differential equations and $A$-stability

In order to derive the O. D. E., Boggs (1971) introduced the homotopy operator $H(t, x)=0$ which imbeds the real parameter $t$ into the original equation in such a way that $H(0, x)=0$ has a solution $x_0$ and $H(t', x)=F(x)$, where $t'$ may be infinite. In particular we are interested in the homotopy

(2.1) $$H(t, x)=F(x)-\exp(-t)F(x_0).$$

Assume that the curve $x(t)$ is differentiable with respect to $t$ and $H$ is differentiable with respect to $x$. Then, by differentiating (2.1) with respect to $t$, since $H(t, x(t))=0$, we have

(2.2) $$x'(t)=-J^{-1}(x)F(x), \quad x(0)=x_0.$$

As usual, we assume that the Jacobian matrix is nonsingular.

Note that the Euler's method with a step size of one applied to (2.2) is equivalent to the Newton's method applied to the original equation $F(x)=0$. Using the imbedding functions, we are interested only in the asymptote of solutions of (2.2). We are therefore led to consider $A$-stable integration methods which compromise between the accuracy and the rate of convergence while maintaining stability.

The general linear $k$-step method for the numerical solution of a system of O. D. E.

$$x'(t)=f(t, x), \quad x(0)=x_0$$

is defined by

(2.3) $$\sum_{i=0}^{k}\alpha_i x_{n+i}=h\sum_{i=0}^{k}\beta_i f_{n+i},$$

where $f_n=f(t_n, x_n)$ and $h$ is the step size.

Definition (Dahlquist). A $k$-step method is called $A$-stable, if all solutions of (2. 3) tend to zero, as $n\to\infty$, when the method is applied with fixed positive $h$ to any differential equation of the form

$$dx/dt=qx, \tag{2.4}$$

where $q$ is a complex constant with nonnegative real part.

Dahlquist(1963) proved that the maximum order for an $A$-stable linear multistep method is two and the smallest error constant $c^*=1/12$ is obtained for the trapezoidal rule. Boggs introduced the concept of the weakly $A$-stability which is a weaker stability condition than $A$-stability.

DEFINITION (Boggs). A $k$-step method is said to be weakly $A$-stable with respect to the equation (2. 4) if there exists an $h$ depending on $q$ in the equation and on the method such that all solutions of (2. 3) tend to zero as $n\to\infty$ when the method is applied to that equation.

Based on the weakly $A$-stability, Boggs applied the trapezoidal rule with variable step sizes to solve the O. D. E. (2. 2). For the initial value problem (2. 2), the trapezoidal rule becomes

$$x_{n+1}=x_n-(h/2)\ [J_n{}^{-1}F_n+J_{n+1}{}^{-1}F_{n+1}].$$

Boggs used the P(EC)E algorithm based on the following rule:

1) Predict $x_{n+1}$ from $x_n$ using the explicit Euler's method.

2) Evaluate $F$ and $J^{-1}$, and then correct $x_{n+1}$ using the trapezoidal rule.

## 3. Generalized Adams method

Using the imbedding function (2. 1), we are interested in the asymptote of the solution and not concerned too much with accuracy. The Boggs method sometimes solves systems of nonlinear equations with poor initial guess which the Newton's method or the damped Newton's method fails to solve. But the convergence is too slow. Therefore, we want to develop a more rapidly converging integration method while maintaining $A$-stability.

Lawson(1975) proposed Generalized Runge-Kutta Processes for stiff initial value problems which integrate exactly any particular integral of the initial value problem $y'=Ay+p(t)$, $p(t)$ a polynomial of degree restricted only by the order of the method, and $A$ a real nonsingular matrix. In this paper, we develop a class of Generalized Adams methods which are nonlinear $A$-stable methods, and examine the possibility of using the methods to solve nonlinear simultaneous equations when a good initial estimate of the solution is not available.

Given an O. D. E.

$$y'(t)=f(t,y),$$

we identify $y'$ as

$$y'(t)=Ay(t)+u(t) \tag{3.1}$$

where $u(t)=f(t,y)-Ay(t)$, and $A$ is a real nonsingular matrix. Let $z=hA$. Then we have

$$y(t+h)=\exp(z)y(t)+h\int_0^1 \exp[(1-s)z]u(t+sh)\,ds. \tag{3.2}$$

Now, we want to apply the Adams method to the integration part of (3. 2). We will use the Newton's backward difference formula

$$u(t+sh)=\sum_{i=0}^{m}(-1)^i\binom{-s}{i}\nabla^i u_n+(-1)^{m+1}h^{m+1}\binom{-s}{m+1}u^{(m+1)}(\eta),$$

where $\nabla$ is the backward difference operator, $u_n=u(t+nh)$, and $u^{(m+1)}(\eta)$ is the $(m+1)$st derivative of $u$ evaluated at some point in an interval containing $t+sh$, $t+(n-m)h$, and $t+nh$ (see Gear, 1971, pp. 105-106). Substituting this in (3. 2), we get

$$y(t+h)=\exp(z)y(t)+h\sum_{i=0}^{m}\Gamma_i(z)\nabla^i u_n \tag{3.3}$$

$$+(-1)^{m+1}h^{m+2}\int_0^1 \exp[(1-s)z]\binom{-s}{m+1}u^{(m+1)}(\eta)\,ds,$$

where

$$\Gamma_i(z)=(-1)^i\int_0^1 \exp[(1-s)z]\binom{-s}{i}ds. \tag{3.4}$$

If the last term in (3. 3) is ignored, replacing $z=hA$, we have Generalized Adams methods

$$y_{n+1}=E(hA)y_n+h\sum_{i=0}^{m}\Gamma_i(hA)\nabla^i u_n \tag{3.5}$$

where $E(z)$ is regarded as an approximation to $\exp(z)$.

The method of generating functions can be used to determine the coefficients $\Gamma_i$. Define

$$G(t)=\sum_{i=0}^{\infty}\Gamma_i(z)t^i.$$

The summation is absolutely convergent for $|t|<1$ since $\Gamma_i$ is bounded by $[\exp(z)-1]/z$ from (3. 4). Consequently,

$$G(t)=\int_0^1 \exp[(1-s)z]\sum_{i=0}^{\infty}(-t)^i\binom{-s}{i}ds$$

$$=\int_0^1 \exp[(1-s)z]\,(1-t)^{-s}ds$$

$$=[\exp(z)-(1-t)^{-1}]/[z+\ln(1-t)].$$

Therefore, we have

$$[z+\ln(1-t)]G(t)=\exp(z)-(1-t)^{-1}.$$

Equating the coefficients of $t^i$, we have the recursive formula

$$\Gamma_0(z)=[\exp(z)-1]/z$$

(3.6)

$$z\Gamma_i(z)-\sum_{k=0}^{i}(1/k)\Gamma_{i-k}(z)=-1,\quad i=1,2,\cdots,m.$$

As an example, when the $\langle 3,1\rangle$ Padé approximation

(3.7) $$E_{3,1}(z)=[1-3z/4+z^2/4-z^3/24]^{-1}\,[1+z/4],$$

denoted by $d^{-1}_{3,1}(z)n_{3,1}(z)$, is used for the approximation to $\exp(z)$, we get

$$\Gamma_0(z)=d^{-1}_{3,1}(z)(1-z/4+z^2/24).$$

Given a system of nonlinear equations

(3.8) $$F(x)=Bx+g(x)=0,$$

we use the imbedding function (2.1). Then, the O.D.E. for (3.8) is

(3.9) $$x'=Ax+u.$$

where $A=-J^{-1}B$ and $u=-J^{-1}g$. If we use only the first term in the summation part of (3.5), using the approximation (3.7) to $\exp(z)$, the formula becomes

(3.10) $$d_{3,1}(z)x_{n+1}=n_{3,1}(z)x_n+h(1-z/4+z^2/24)u_n.$$

## 4. Error analysis

We first give a sufficient condition under which the formula (3.5) is $A$-stable.

THEOREM 1. *If* $|E(z)|<1$ *for* $\mathrm{Re}(z)<0$, *then the Generalized Adams method* (3.5) *is A-stable.*

*Proof.* When (3.5) is applied to the initial value problem $y'=qy$, $y(0)=y_0$, the Generalized Adams method generates the approximate solution $y_n=[E(hq)]^n y_0$. Thus, if $q$ is a complex constant with negative real part, $\lim_{n\to\infty} y_n=0$, establishing $A$-stability.

Ehle(1973) proved that the Padé approximations to $\exp(z)$, for which deg(denominator) − deg(numerator) = 0, 1, or 2, satisfy the condition in Theorem 1. Therefore, when (3.7) is used for the approximation to $\exp(z)$, the scheme of (3.5) is $A$-stable.

To demonstrate the good asymptotic properties of the Generalized Adams method, two theorems are presented without proofs. They can be proved in a similar way to those of Theorem 1 and Theorem 2 of Lawson (1975).

THEOREM 2. *Let* $E(z)-\exp(z)=0(z^{m+1})$, $z\to 0$, *and let* $\{\Gamma_i(hA)\}$ *in* (3.5) *be computed from* (3.6). *Then, formula* (3.5) *is exact for any particular integral of* $y'=Ay+u(t)$, *where* $u(t)$ *is a vector polynomial of degree* $m-1$ *or less and* $A$ *is a real nonsigular matrix.*

THEOREM 3. *Let the scheme of* (3.5) *be A-stable and exact for the particular integral of* $y'=By+u(t)$, *where* $B$ *is a stable square constant matrix. Then,*

$$\lim_{n\to\infty}[y_n-y(t_n)]=0,$$

*regardless of step size* $h$.

## 5. Testing procedure and numerical results

The Generalized Adams method (GENADA) is compared with the Boggs' trapezoidal rule method (BOGSUB) and the Gear's stiffly stable method (DIFSUB). Formula (3.10) is used for GENADA. The motivation for the choice of stiffly stable method of Gear (1971) is that it is currently the only stiff equation method whose source listing has had wide distribution. Two cases of Boggs method are considered, one with variable step size and the other one with fixed step size. On each case of Boggs methods, the Jacobian is computed after each iteration and the Broyden's approximation formula is used to computed the inverse Jacobian.

The convergence criteria used in each subroutine are that each component of two succeeding iterates must agree to within a relative error of $10^{-5}$ and each component of the function must be less than $10^{-5}$ in absolute value. For fixed step size cases, firstly $h=1$ is used. If it fails, $h=0.1$ with relative error bound $10^{-3}$ is tried again.

Programmes were written in FORTRAN IV to perform double-precision arithmetic and were compiled and executed on an Honeywell 6000 computer.

Three chosen problems are tested. The first problem is from Boggs (1971) and the second is found in Broyden (1969) and also discussed in Boggs (1971). The last one is due to Freudenstein and Roth (1963), which also can be found in Broyden (1965 and 1969).

PROBLEM 1.

$$F(x)=\begin{bmatrix} x_1 & -1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}+\begin{bmatrix} 1 \\ -\cos[(\pi/2)x_2] \end{bmatrix}$$

with initial guess $x_0=\begin{bmatrix}1\\0\end{bmatrix}$. We seek the solution $x^*=\begin{bmatrix}0\\1\end{bmatrix}$. The Jacobian of the system is

$$J(x)=\begin{bmatrix}2x_1 & -1\\ 1 & (\pi/2)\sin[(\pi/2)x_2]\end{bmatrix}.$$

The Jacobian is singular for

$$\sin[(\pi/2)x_2]=-1/(\pi x_1).$$

Note that there is another root $x^{**}=\begin{bmatrix}-\sqrt{2}/2\\ 1.5\end{bmatrix}$.

PROBLEM 2.

$$F(x)=\begin{bmatrix}-1/2 & -1/(4\pi)\\ -2e & e/\pi\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}+\begin{bmatrix}(1/2)\sin(x_1x_2)\\ [1-1/(4\pi)][\exp(2x_1)-e]\end{bmatrix}$$

with initial guess $x_0=\begin{bmatrix}0.4\\3.0\end{bmatrix}$. According to Boggs' investigation, we seek the solution which is approximately $x^*=\begin{bmatrix}0.30\\2.8\end{bmatrix}$. The Jacobian of the system is

$$J(x)=\begin{bmatrix}(1/2)x_2\cos(x_1x_2)-1/2 & (1/2)x_1\cos(x_1x_2)-1/(4\pi)\\ 2[1-1/(4\pi)]\exp(2x_1)-2e & e/\pi\end{bmatrix}.$$

Note that there is another solution at $x^{**}=\begin{bmatrix}0.5\\ \pi\end{bmatrix}$.

PROBLEM 3.

$$F(x)=\begin{bmatrix}1 & (-x_2+5)x_2-2\\ 1 & (x_2+1)x_2-14\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}+\begin{bmatrix}-13\\-29\end{bmatrix}$$

with initial guess $x_0=\begin{bmatrix}15.0\\-2.0\end{bmatrix}$. Analytic solution of the system gives a real root $x^*=\begin{bmatrix}5\\4\end{bmatrix}$ and two complex roots. Thus, we are seeking the real root $x^*$. The Jacobian of the system is given by

$$J(x)=\begin{bmatrix}1 & (-3x_2+10)x_2-2\\ 1 & (3x_2+2)x_2-14\end{bmatrix}$$

The Jacobian is thus singular for

$$x_2=(2\pm\sqrt{22})/3.$$

The results of the numerical tests are summarized in Table 1 and discussed below. The methods are compared in terms of the number of iteraions and the number of function evaluations. The abbreviations used in the table mean the following:

ITER=number of iterations required to solve problem
FNS=total number of function evaluations
VAR=when variable step size is used, i. e. when accuracy test is given
FIX=when fixed step size is used
(…)=values at second try
$>N$=need more than $N$, but converging to the right root.

TABLE 1

| | | GENADA | BOGSUB | | DIFSUB |
|---|---|---|---|---|---|
| | | | VAR | FIX | |
| PROB. 1 | ITER | 16 | 71 | (55) | 19 |
| | FNS | 16 | 142 | (110) | 52 |
| PROB. 2 | ITER | (66) | >101 | (101) | 34 |
| | FNS | (66) | >202 | (202) | 44 |
| PROB. 3 | ITER | 34 | fail | (fail) | fail |
| | FNS | 34 | | | |

When GENADA was applied to problem 2 with $h=1$, it converged to $x^{**} = \begin{bmatrix} 0.5 \\ \pi \end{bmatrix}$ which is another root, but that is not the solution we are seeking. In problem 3, DIFSUB converged to $\begin{bmatrix} 17.7 \\ -0.887 \end{bmatrix}$ after 30 iterations, but it is not a root of the system. Failures in BOGSUB are because of divergence or singular Jacobian.

## 6. Conclusions

Based on the examples in this paper and several other examples with results similar to those reported here, some conclusions can be given.

GENADA, which is a nonlinear $A$-stable method, performs more effectively than BOGSUB which is a linear $A$-stable method. DIFSUB is also successful. Since no accuracy test was used in GENADA, the results reported here are not enough to compare Generalized Adams methods with the stiffly stable method of Gear in solving systems of nonlinear equations. However, we can say that GENADA is an effective new way of solving nonlinear systems of equations with poor initial approximations. But, algorithm (3.10) is subject to improvement.

To apply the Generalized Adams method in solving "stiff O. D. E. which requires accuracy as well as stability, the first four terms in the summation part of (3.5) are suggested when $\langle 3, 1\rangle$ Padé approximation is used. Implicit Generalized Adams methods may have better performance in this case.

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