A CLASS OF RAPIDLY CONVERGENT INTERATIVE METHODS FOR PROBLEMS IN MATHEMATICAL MODELLING

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Methods with the convergence order $p \geq 2$ (Newton`s, tangent hyperbolas, tangent parabolas etc.) and their approximate variants are studied. Conditions are presented under which the approximate variants preserve their convergence rate intrinsic to these methods and some computational aspects (possibilities to organize parallel computation, globalization of a method, the solution of the linear equations versus the matrix inversion at every iteration etc.) are discussed. Polyalgorithmic computational schemes (hybrid methods) combining the best features of various methods are developed and possibilities of their application to numerical solution of two-point boundary-value problem in ordinary differential equations and decomposition-coordination problem in convex programming are analyzed.

INTRODUCTION

In many scientific and engineering applications the problem of calculating values of mathematical models accurately and rapidly has become greatly acute. On of the central problems in the numerical analysis is the efficient solution of a nonlinear equation

$$F(x)=0, \tag{1}$$

where F is as many times as necessary differentiable operator from one abstract space X into another Y. Generally , the equation (1) may not have any solution in the classical sense or may have several solutions. This report aims mainly at presenting a study of computing an approximate solution of (1) making use of methods with a high order of convergenc, if there exists a solution of (1) in the usual sense. The use of methods with a high convergence order sometimes enables to meet more entirely the above mentioned requirements compared to methods with a lower rate of convergence.

METHODS

For solving (1), if F is a mapping between Banach spaces X and Y, we consider iterative methods of the type

$$X_{k+1} = X_k - Q(X_k, A^i_k), \quad i \leftarrow J = \{1,\ldots,r\}, \quad r \geq 1, \quad k = 0,1,\ldots, \tag{2}$$

where $Q(X, A^i_k)$ is an operator from X into itself and A^i_k are some approximations to inverses occuring in the exact method $X_{k+1} = X_k - Q(X_k, \cdot)$. It is assumed that there exists an "exact method" which is known to be convergent with the convergence order $p \geq 2$ and has a similar form. Calculating on a computer with finite wordlength, F´ cannot be obtained exactly even if it is evaluated by analytical expressions. The investigation of methods with approximate inverse operator gives more realistic impression of convergence properties of methods than the study of the idealized case that F` is computed exactly. Theoretically that is equivalent to solving of the linear subproblems within certain tolerance at each iteration. An approximate variant of the method can also be obtained as a result of a strategy used for solving linear problems, i.e. associated linear equations are solved approximately by taking finitely many steps of an iterative procedure or the inverse operator is approximated by recurrence formula, e.g.

$$A_{k+1} = A_k \sum_{\nu=0}^{q-1} (I - F'(X_{k+1})\, A_k)^{\nu}, \quad q \geq 2, \quad k = 0,1,\ldots, \tag{3}$$

where I denotes the identity mapping.
In special cases, if

$$Q_k = Q(X_k, A_k) = A_k F(X_k), \quad A_k \approx \Gamma_k = [F'(X_k)]^{-1}, \tag{4}$$

$$Q_k = [I - \tfrac{1}{2} A_k F''(X_k)\, A_k F(X_k)]^{-1} A_k F(X_k), \tag{5}$$

$$Q_k = A_k F(X_k) + \tfrac{1}{2} A_k F''(X_k)\, (A_k F(X_k))^2 \tag{6}$$

approximate variants of the Newton, Halley and Chebyshev methods are obtained respectively. Using discretization formulas, the second order derivative can be replaced by an expression containing one additional value of F or F´. If for $-F''(X_k)\, A_k F(X_k)$ to use the approximate expression

$$2\beta\, [F'(X_k - \frac{1}{2\beta} A_k F(X_k)) - F'(X_k)], \quad \beta \neq 0,$$

then (5) yields the method

$$X_{k+1} = X_k - [(1-\beta)\, F'(X_k) + \beta\, F'(X_k - \frac{1}{2\beta}\ A_k\, F(X_k)]^{-1}\, F(X_k). \quad (7)$$

The latter one coincides with the Kogan method provided $\beta = 1$ and $A_k = \Gamma_k$ [1].

As an example of methods with convergence order p = 4 we consider the method

$$X_{k+1} = V_k - 2A_k\, F(V_k) + \frac{1}{\rho}\ \overline{A}_k\, [F(V_k + \rho\, A_k\, F(V_k)) - F(V_k)] \quad (8)$$

$$V_k = X_k - \widetilde{A}_k\, F(X_k),\ \ k = 0,1,\dots\ ,$$

where A_k, $\overline{A}_k$ and $\widetilde{A}_k$ some approximations to Γ_k with

$$\left\|I - F'(x_k)A_k\right\| \le \wp_k < 1, \quad \left\|I - F'(x_k)\overline{A}_k\right\| \le \overline{\wp}_k < 1, \qquad \left\|I - F'(x_k)\widetilde{A}_k\right\| \le \widetilde{\wp}_k < 1$$

and ρ is a nonzero real parameter.

Local convergence theorems are proved for methods (2) [2,3], but they are very technical and therefore omitted here. It is shown that the higher order of convergence, then more accurately, in general, the associated linear subproblems are to be solved and the different methods need different rates of accuracy of approximation. For instance, Γ_k and $[I - ½\ A_k\, F''(X_k)\, A_k\, F(X_k)]^{-1}$ have to be approximated with the accuracy $0\left(\left\|F(x_k)\right\|\right)$ and $0\left(\left\|F(x_k)\right\|^2\right)$ respectively for Halley´s method to obtain the convergence order p = 3 if other reasonable convergence conditions are satisfied. To guarantee the convergence order p = 3 for Chebyshev´s method one has to solve the corresponding linear problems with an accuracy of $0\left(\left\|F(x_k)\right\|^2\right)$ while for its variant

$$X_{k+1} = X_k - A_k\, F(X_k) - A_k\, F(X_k - A_k\, F(X_k)) \quad (9)$$

the approximation rate $0\left(\left\|F(x_k)\right\|\right)$ is sufficient to obtain the same convergence order p = 3.

Assuming that F" is Lipschitz - continuous it follows from these convergence theorems that the convergence order of the methods (8) equals to 4 provided $\wp_k$, $\overline{\wp}_k$ *and* $\widetilde{\wp}_k$ are of the order $0\left(\left\|F(x_k)\right\|\right)$ and $\left\|A - \overline{A}_k\right\| = 0\left(\left\|F(x_k)\right\|^2\right)$.

While only function values are available then inexact methods based on finite difference approximation are greatly useful.

If the evaluation of function values is very labour-consuming it is reasonable to use the approximate variant of (9)

$$X_{k+1} = Y_k - [F(2Y_k - X_k;\, X_k)]^{-1}\, F(X_k) \quad (10)$$

$$Y_k = X_k - [F(2Y_{k-1} - X_{k-1};\, X_{k-1})]^{-1}\, F(X_k) \quad (11)$$

which has the asymptotic convergence rate equal to 3, provided the second order derivative F" is Lipschitz continuous and corresponding divided differences $F(\cdot\,;\,\cdot)$ are Lipschitz continuous . The procedure (10) - (11) requires a little information per an iteration: two values of F and one value of the divided difference (except for the first iteration) [4].

If the computational cost for the function value evolution and / or the dimensionality of the problem is not too large, then one may use the following modification of (7)

$$X_{k+1} = X_k - [F(2u_k - X_k;\, X_k)]^{-1}\, F(X_k) \tag{12}$$

where $u_k = X_k - \frac{1}{2} B_k F(X_k)$ and $B_k = [F(2X_k - X_{k-1};\, X_k)]^{-1}$ or $B_k = [F(2X_k - u_{k-1};\, X_k)]^{-1}$ and $\beta = 1$.

SOME COMPUTATIONAL ASPECTS

The efficiency of the methods containing high order derivatives in their computational schemes relative to the Newton method for solving nonlinear integral and ordinary differential equations is discussed and indicated in [5]. But the application of them to systems of nonlinear algebraic and transcendental equations is problematic.

One substantial reason for using methods with the convergence order higher than that of the Newton method and its variants which could fail if F´is singular or badly ill-conditioned at the solution point is the fact that methods of the order $p \geq 3$ are taking advantage, at least, of a quadratic model. Therefore, they can perform succesfully for the singular Jacobian as well. It is known that even very rough approximations for the second derivatives in the method with $p \geq 3$ may ensure their numerical stability [6,7].

Although the solution of a system of linear equations is, as a rule, more economical and reliable than the inversion of the corresponding matrix, it is sometimes preferable to employ versions of iterative methods based on matrix inversion. Knowledge of the inverse operator or its approximation is desirable in many cases. It facilitates to compute a condition number and error bounds and to pass easily to interval versions of the method, at least to ones, based on the Krawczyk transformations. Interval analysis is a special kind of error analysis and an interval method together with a standard point approximation methods permits to find the roots of the equations safely and efficiently.

However, the advantages of the approach, based on solving the linear equations instead of computing inverses by (3), are not so clear for abstract spaces, e.g. the fast Fourier transformations permit to calculate the needed multiplications of linear operators with the smaller cost of computation than the solution of corresponding linear operator equations [8,9].

One of the potential ways to reduce the total time needed for computing a solution with a prescribed accuracy is the use of parallel computation. The methods with successive approximation of inverse operator based on the formula (3) offer various facilities for organizing parallel computation. Different types of matrix multiplication (inner-product, middle-product, outer-product, n^3 - parallelism) that are suitable for parallel execution on computers with certain given structure can be found in the literature, e.g. in [9] . Parallel matrix computation is a vast topic and it requires a comprehensive analysis and information on certain characteristics of the computational environment and therefore a thorough discussion of aspects of parallel computation is dropped here.

A strategy of problem solving that instead of finding the exact solution of a linear equation at each iteration solves it intentionally in an inexact way permits to save the computational work and is a daptive in the sense that low accuracy numerical solutions of linear equations are used when the solution is not reached yet and improves the accuracy as the solution is approached. In many cases, especially, for large sparse problems iterative methods are more adequate and economical

compared to direct ones. Besides, iterative methods are usually self-correcting, hence they are insensitive to small computational errors but their convergence can be quite slow in the peresence of ill-conditioning. Preconditioning techniques must be introduced to alleviate this difficulty [2], [11]. Continuous methods converge globally but slowly, whereas the iterative methods with high order convergence locally. These features can be combined in such a way that a continuous method is used first to help get into the domain of convergence of rapidly convergent method, which, then, will be turned on to improve the accuracy.

GLOBALIZATION AND IMPLEMENTATION

Usually it is not known ahead what are the complications of a problem to be solved. Construction of an appropriate model from experiments and observations involves frequently the solution of ill-posed problems. For instance, inverse problems are often nonlinear and involve very complicated subproblems. There are also many industrial problems in which the model code requires much computation time and thus must not be called too many times. The realization of shooting methods for solving two-point boundary value problems (TPBVPs) in ordinary differential equations (ODEs) leads to the solution of systems of nonlinear equations where only the function values are available. Numerical solution of certain decomposition-coordination problems in convex programming often involves the solution of systems of nonlinear equations or minimizing a function to obtain proper values for coordination parameters. In this case the user has his disposal only the values of the functions, evaluation of which, includes, basically, the solution of certain subproblems, the functions involved are not necessarily differentiable, they may belong to the almost differentiable equations. Problems of minimizing nonsmooth and discontinuous function cause serious computational problems for numerical methods. Methods based on the approximational gradient allow to handle many nonsmooth functions. Analogs of steepest descent and the conjugate gradient methods based the approximational gradient are studied in [12]. In such cases sophisticated algorithms are needed which try to find a compromise between robustness, stability and convergence speed, in particular, hybrid ones based on the polyalgorithmic approach to improve the efficiency of the resulting procedure.

The property of global convergence is a criterion of robustness of an algorithm. One of the most popular ways to quarantee the global convergence is the “continuation strategy”. But all the homotic methods suffer from the disadvantage that the Jacobian at some points may become singular. Therefore the implementation of methods with the convergence order $p \geq 3$ in conjunction with the continuation strategy may be justified. A reasonable polyalgorithmic strategy is to use a high order method if it works otherwise to switch on slower but more sure global method. Some polyalgorithmic computational schemes will be published elsewhere.

Numerical solution of TPBVPs and decomposition-coordination problems are discussed more thoroughly in [3].

The performance of methods under consideration was tested on small set of test problems containing 14 problems for the systems of nonlinear equations of Argonne National Laboratory plus Freudenstein and Roth function and Box three dimensional function for nonlinear least squares problems taken from literature [13]. Numerical experience with the methods under discussion has confirmed our theoretical considerations [3]. These promising results encourage us to carry on the investigation of properties of hybrid methods.

In conclusion, we discussed the methods under consideration mainly on the theoretical basis. One reason for doing so is that mathematical properties exhibit indisputable features of the algorithms, in contrast to the computer experiments numerical results of which presented in pa-

pers and books often show contradictory aspects. Secondly, mathematical aspects fix limits of what can be expected from the use of an algorithm.

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