QUASI - NEWTON METHODS AND THE SOLUTION OF SOME FLUID MECHANICS PROBLEMS

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ABSTRACT – In this paper we consider the application of Quasi-Newton methods to the resolution of the Cavity Problem. This is a fourth order boundary value problem governed by the Navier-Stokes equations. Its finite difference discretization represents an interesting case study for algorithms that solve sparse nonlinear systems. We conclude that the Quasi-Newton algorithms that save on linear algebra at each iteration are more efficient than the classical Newton method.

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QUASI-NEWTON METHODS AND THE SOLUTION OF SOME FLUID MECHANICS PROBLEMS [(*)]

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Abstract In this paper we consider the application of Quasi-Newton methods to the resolution of the Cavity Problem. This is a fourth order boundary value problem governed by the Navier-Stokes equations. Its finite difference discretization represents an interesting case study for algorithms that solve sparse nonlinear systems. We conclude that the Quasi-Newton algorithms that save on linear algebra at each iteration are more efficient than the classical Newton method.

Key words: Nonlinear systems of equations, Newton's method, Quasi-Newton methods, stream function, Navier Stokes equations, cavity problems.

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1.- Introduction

We consider nonlinear systems of equations

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

where $F : R^n \to R^n$ is differentiable, n is large and the Jacobian matrix $J(x)$ is sparse.

The best known algorithm for solving (1.1) is Newton's method. This is an iterative method which, at each iteration, proceeds by solving the linear system

$$J(x_k)s_k = -F(x_k) \tag{1.2}$$

and defining

$$x_{k+1} = x_k + s_k. \tag{1.3}$$

See Ortega and Rheinboldt [1970], Schwetlick [1974], Dennis and Schnabel [1983], Ostrowski [1973].

At each iteration of Newton's method, we compute the first derivatives of F and we solve the linear system (1.2). We take the point of view that computing derivatives is not very hard, at least when automatic differentation routines (Griewank [1992], Iri [1984], Rall [1984], [1987]) are available. If this is not the case, we may use the numerical differentation algorithms of Curtis, Powell and Reid [1974] and Coleman and Moré [1983]. See also Coleman, Garbow and Moré [1984]. In general, the resolution of the linear system (1.2) is a very costly computational problem, even if modern sparse techniques are used (Duff, Erisman and Reid [1989], Duff [1977], George and Ng [1987], Zlatev, Wasnieswski and Schaumburg [1981]).

Quasi-Newton methods were introduced with the aim of alleviate the computational work of the Newton iteration, but keeping some of the excellent local convergence properties of this method. See Broyden [1965], Broyden, Dennis and Moré [1973], Dennis and Moré [1977], Dennis and Schnabel [1983], Dennis and Walker [1981], Martínez [1990b].

In a typical Quasi-Newton iteration, (1.2) is replaced by

$$B_k s_k = -F(x_k) \tag{1.4}$$

and the resolution of (1.4) is inexpensive when compared with the resolution of (1.2). A systematic comparison of Quasi Newton methods for large sparse nonlinear systems has been developed in the Applied Mathematics Laboratory of the University of Campinas during the last five years. As a result, we developed the package NIGHTINGALE, where some of the most successful Quasi-Newton methods with "cheap linear algebra" have been implemented. See Broyden [1965], Dennis and Marwil [1982], Martínez [1983, 1984, 1987, 1990a], Gomes-Ruggiero, Martínez and Moretti [1992], Gomes-Ruggiero and Martínez [1992]. In Tewarson and Zhang [1987], Tewarson [1988] and Martínez and Zambaldi [1992] potentially useful methods that are not yet incorporated to NIGHTINGALE are analyzed.

The validation of nonlinear equations solvers requires a very careful selection of meaningful test problems (Moré [1989]). Some of the more interesting tests for algorithms which solve nonlinear systems come from the discretization of boundary value problems (Ortega and Rheinboldt [1970], Schwandt [1984], Watson [1979, 1980, 1983], Watson and Scott [1987], Watson and Wang [1981].) In this paper we apply several Quasi-Newton methods to the Cavity Problem (Peyret and Taylor [1985]), which is a boundary value problem governed by a fourth order partial differential equation in terms of the stream function. For low Reynolds numbers, the problem is almost linear, while, when the Reynolds number is large, the problem is highly nonlinear. We test Quasi-Newton methods for problems with increasing Reynolds numbers, up to the vicinity of a "turning point" (Rheinboldt [1986]). Going through this turning point requires the use of Homotopy or Continuation techniques (Rheinboldt [1986], Watson, Billups and Morgan [1987]) that are beyond the scope of our study.

This paper is organized as follows. In Section 2, we describe the methods implemented. In Section 3, we survey the theoretical convergence results relative to these methods. In Section 4, we describe the Cavity Problem and its discretization. In Section 5, we report our numerical experiments. The conclusions of the study are given in Section 6.

2.- The algorithms

In this section we describe briefly the methods that are compared in the present study. More detailed descriptions of these methods can be found in Gomes-Ruggiero, Martínez and Moretti [1992] and Gomes-Ruggiero and Martínez [1992]. The methods are:

(1) Newton's method.

(2) Modified Newton method.

(3) Broyden's method.

(4) Column-Updating method.

The following features are common to the implementation of the four methods:

(a) The iterations are of type (1.4) (1.3) except if $\|s_k\|_\infty \geq \Delta$ where Δ is a parameter given by the user. In this case, we replace s_k by $s_k\Delta/\|s_k\|_\infty$.

(b) At the first iteration, (1.2) is solved using the algorithm for sparse LU factorization with partial pivoting introduced by George and Ng [1987]. This factorization has proved to be more efficient than more classical sparsity schemes due stability reasons (Zambaldi [1990]). The subsequent iterations of Newton also use the George-Ng method for solving (1.2).

(c) If, in the course of a factorization, singularity or severe ill-conditioning of B_k is detected, B_k is modified in order to transform it in a "less ill-conditioned matrix" . The same decision is adopted if "near-singularity" is detected when a rank-one correction is added to B_{k-1} (methods (5) and (6)). The details of these modifications are given in Gomes-Ruggiero, Martínez and Moretti [1992].

In Newton's method, $B_k = J(x_k)$ for all $k = 0, 1, 2, \ldots$. We also choose $B_0 = J(x_0)$ in the Quasi - Newton methods of the NIGHTINGALE package. The definition of B_{k+1} in the Quasi - Newton methods for $k = 0, 1, 2, \ldots$ is as follows:

Modified Newton method:

$$B_{k+1} = B_k. \tag{2.1}$$

Broyden's method:

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)s_k^T}{s_k^T s_k} \tag{2.2}$$

where

$$s_k = x_{k+1} - x_k, \tag{2.3}$$

$$y_k = F(x_{k+1}) - F(x_k). \tag{2.4}$$

Column-Updating Method:

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)e_{j_k}^T}{e_{j_k}^T s_k} \tag{2.5}$$

where $\{e_1, \ldots, e_n\}$ is the canonical basis of $\mathbb{R}^n$, s_k and y_k are given by (2.3) and (2.4) respectively and

$$|e_{j_k}^T s_k| = \|s_k\|_\infty. \tag{2.6}$$

In Broyden's method, we have that

$$B_{k+1}^{-1} = B_k^{-1} + \frac{(s_k - B_k^{-1} y_k)s_k^T B_k^{-1}}{s_k^T B_k^{-1} y_k}. \tag{2.7}$$

Therefore,

$$B_{k+1}^{-1} = (I + u_k s_k^T) \ldots (I + u_0 s_0^T) B_0^{-1}, \tag{2.8}$$

where, for $\ell = 0, 1, \ldots, k$, we have:

$$u_\ell = s_\ell - B_\ell^{-1} y_\ell / s_\ell^T B_\ell^{-1} y_\ell. \tag{2.9}$$

By (2.8) and (2.9), Broyden's method can be implemented storing $u_0, \ldots, u_k, s_0, \ldots, s_k$ plus the LU factorization of B_0 (Matthies and Strang [1979], Griewank [1986], Gomes-Ruggiero, Martínez and Moretti [1992]).

Similarly, in the Column-Updating Method, we have that

$$B_{k+1}^{-1} = \left[I + \frac{(s_k - B_k^{-1} y_k)e_{j_k}^T}{e_{j_k}^T B_k^{-1} y_k}\right] \cdots \left[I + \frac{(s_0 - B_0^{-1} y_0)e_{j_0}^T}{e_{j_0}^T B_0^{-1} y_0}\right] B_0^{-1}. \tag{2.10}$$

So,

$$B_{k+1}^{-1} = (I + u_k e_{j_k}^T) \cdots (I + u_0 e_{j_0}^T) B_0^{-1}, \tag{2.11}$$

where

$$u_\ell = \frac{s_\ell - B_\ell^{-1} y_\ell}{e_{j_\ell}^T B_\ell^{-1} y_\ell}, \tag{2.12}$$

$\ell = 0, \ ,1, \ ,2, \ldots$. Formula (2.11) allows us to implement the Column-Updating Method for large - scale problems, storing the vectors, $u_0, \ldots, u_k$, the indices $j_0, \ldots, j_k$, and the factorization of B_0. For details of this implementation see Gomes Ruggiero and Martínez [1992]. Comparing (2.7)–(2.9) with (2.10)–(2.12), we observe that a typical iteration of the Column - Updating Method uses less computer time and less storage than Broyden for large - scale problems.

3.- Survey of Convergence Results

We assume that $F : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$, Ω an open and convex set, $F \in C^1(\Omega)$, $F(x_*) = 0$, $J(x_*)$ nonsingular, and that there exist $L, p > 0$ such that for all $x \in \Omega$,

$$||J(x) - J(x_*)|| \leq L||x - x_*||^p. \tag{3.1}$$

We consider the algorithms described in Section 2, without correction of near-singularity, and without control of the stepsize. Let us survey the convergence results related to these algorithms. Theorems 3.1 and 3.2 are related to Newton's method, the Modified Newton method and Broyden's method. These theorems say that the sequences generated by these methods are well defined and linearly convergent to x_*, if the initial point and the initial B_0 are close enough to x_* and $J(x_*)$ respectively.

Theorem 3.1 *Given $r \in (0,1)$, there exists $\varepsilon = \varepsilon(r) > 0$ such that if $||x_0 - x_*|| \leq \varepsilon$, the sequences $\{x_k\}$ generated by Newton and Modified Newton are well defined, converge to x_*, and satisfy*

$$||x_{k+1} - x_*|| \leq r \ ||x_k - x_*|| \tag{3.2}$$

for all $k = 0, 1, 2, \ldots$.

Proof. See Dennis and Schnabel [1983]. □

Theorem 3.2 *Given $r \in (0,1)$, there exist $\varepsilon = \varepsilon(r) > 0$, $\delta = \delta(r) > 0$ such that if $||x_0 - x_*|| \leq \varepsilon$ and $||B_0 - J(x_*)|| \leq \delta$, the sequence $\{x_k\}$ generated by Broyden is well defined, converges to x_*, and satisfies*

$$||x_{k+1} - x_*|| \leq r\, ||x_k - x_*|| \tag{3.3}$$

for all $k = 0, 1, 2, \ldots$.

Proof. See Dennis and Schnabel [1983]. □

Theorem 3.3 is the classical theorem on the order of convergence of Newton (quadratic when $p = 1$), and Theorem 3.4 says that the convergence of Broyden is Q-superlinear.

Theorem 3.3 *Under the hypotheses of Theorem 3.1, if $\{x_k\}$ is generated by Newton's method, there exists $c > 0$ such that*

$$||x_{k+1} - x_*|| \leq c\, ||x_k - x_*||^{p+1} \tag{3.4}$$

for all $k = 0, 1, 2, \ldots$.

Proof. See, for instance, Ortega and Rheinboldt [1970], Dennis and Schnabel [1983]. □

Theorem 3.4 *Under the hypotheses of Theorem 3.2, if $\{x_k\}$ is generated by Broyden's method, we have that*

$$\lim_{k\to\infty} ||x_{k+1} - x_*|| / ||x_k - x_*|| = 0 \tag{3.5}$$

Proof. See Dennis and Schnabel [1983]. □

Let us consider now the Column - Updating method. In 1984, Martínez proved that, under the usual hypotheses on F, this method has local and superlinear convergence *with Jacobian restarts every m iterations*. This means that we use the formula (2.5) if $k + 1$ is not a multiple of a fixed integer $m > 0$, and we set $B_{k+1} = J(x_{k+1})$ otherwise. This theoretical result is not completely satisfactory, since we know that it is satisfied by methods whose performance is poorer than the performance of the Column-Updating method. In fact, numerical experiments performed in the last ten years showed that, in most practical cases, the behavior of the Column-Updating method is very similar to the behavior of Broyden. The following results were proved recently and tend to reduce the gap between theory and practice with respect to this method.

Theorem 3.5 *Suppose that the sequence $\{x_k\}$ generated by the Column - Updating method, is well defined, converges to x_*, and satisfies (3.3). Then,*

$$\lim_{k\to\infty} ||x_{k+2n} - x_*|| / ||x_k - x_*|| = 0 \tag{3.6}$$

and

$$\lim_{k\to\infty} ||x_k - x_*||^{1/k} = 0 \tag{3.7}$$

Proof. See Martínez [1992c]. □

Theorem 3.6 *Assume that $n = 2$. Given $r \in (0,1)$, there exists $\varepsilon = \varepsilon(r) > 0$, $\delta = \delta(r) > 0$, such that if $||x_0 - x_*|| \le \varepsilon$, and $||B_0 - J(x_*)|| \le \delta$ the sequence $\{x_k\}$ generated by Column - Updating method, is well defined, converges to x_*, and satisfies (3.3), (3.6) and (3.7).*

Proof. See Martínez [1992c]. □

Theorem 3.7 *Given $r \in (0,1)$, m a positive integer, there exists $\varepsilon = \varepsilon(r) > 0$, $\delta = \delta(r) > 0$, such that if $||x_0 - x_*|| \le \varepsilon$, and $||B_k - J(x_*)|| \le \delta$ if k is a multiple of m, the sequence $\{x_k\}$ generated by Column - Updating method, except perhaps when k is multiple of m, is well defined, converges to x_*, and satisfies (3.3), (3.6) and (3.7).*

Proof. See Martínez [1992c]. □

Up to now, Theorems 3.5, 3.6 and 3.7 are the best results we have for explaining the numerical behavior of the Column-Updating method. There is still a large gap between theory and practice. In particular, we do not know yet if a local convergence result like Theorem 3.2 holds for this method if $n \neq 2$. Theorem 3.5 says that, assuming linear convergence, R- superlinear convergence (Ortega and Rheinboldt [1970]) takes place. However, this is a weak result compared with the Q-superlinear convergence of Broyden. The main problem is that it has not been found a Bounded Deterioration result (Broyden, Dennis and Moré [1973]) allowing the accumulation of infinite many small deteriorations in the updating of B_k. Such results are easy to obtain in the case of Broyden and other Least Change Secant Update (LCSU) methods (Dennis and Schnabel [1983], Dennis and Walker [1981], Martínez [1990b]) because LCSU algorithms involve orthogonal projections, which is not the case of the Column- Updating method.

4.- The Cavity Problem and its Discretization

The stream function-vorticity equations can be written in the case of a steady plane flow in the following form (Peyret and Taylor [1985]):

$$\vec{u} \cdot \overline{\nabla}\, \omega - \frac{1}{Re} \Delta\omega = 0 \tag{4.1}$$

$$\omega + \Delta\psi = 0, \tag{4.2}$$

where ψ is the stream function, ω is the vorticity, Re is the Reynolds Number and $\vec{u} = (u, v)$ is the velocity with components expressed in terms of the stream function. That is, $u = \psi_y$, $v = -\psi_x$.

Suitable boundary conditions must be added to equations (4.1) and (4.2) in order to complete the formulation of the boundary value problem.

Setting $\omega = -\nabla\psi$ in (4.1), we obtain a nonlinear fourth-order equation for the stream function:

$$P(\psi) \equiv \Delta^2\psi + Re\,[\psi_x(\Delta\psi)_y - \psi_y(\Delta\psi)_x] = 0 \tag{4.3}$$

For $Re = 0$ this equation reduces to the biharmonic linear equation

$$\Delta^2\psi = 0. \tag{4.4}$$

We assume that the cavity is the unit square $R = \{(x,y) \in I\!R^2 \mid 0 \leq x, y \leq 1\}$ and we use the boundary conditions proposed by Bourcier and François (see Peyret and Taylor [1985, p. 199]: $\psi(x,y) = 0$ on the boundary, $\frac{\partial\psi}{\partial y} = -16x^2(1-x)^2$ if $y = 1$, and $\frac{\partial\psi}{\partial n} = 0$ if $y \neq 1$.

The equation (4.3) defines, with the boundary conditions above, an elliptic fourth - order two dimensional boundary problem in a single unknown, which we attempt to solve using its finite difference aproximation.

For the aproximation of the nonlinear operator $P[\psi]$, we set (Collatz, [1973]):
$P\,[\psi_{j,k}] \approx \{20\psi_{j,k} - 8(\psi_{j+1,k} + \psi_{j,k+1} + \psi_{j-1,k} + \psi_{j,k-1}) + 2(\psi_{j+1,k+1} + \psi_{j-2,k} + \psi_{j,k+2} + \psi_{j,k-1}) + \psi_{j+2,k} + \psi_{j-2,k} + \psi_{j,k+2} + \psi_{j,k-2} + Re\,[(\psi_{j+1,k} - \psi_{j-1,k})(\psi_{j-1,k+1} - 4\psi_{j,k+1} + \psi_{j+1,k+1} + \psi_{j,k+2} - \psi_{j+1,k-1} + 4\psi_{j,k-1} - \psi_{j-1,k-1} - \psi_{j,k-2}) + \psi_{j,k+1} - \psi_{j,k-1})(\psi_{j+2,k} - 4\psi_{j+1,k} - \psi_{j-1,k} + \psi_{j+1,k+1} + 4\psi_{j-1,k} - \psi_{j-2,k} + \psi_{j+1,k+1} - \psi_{j-1,k+1})]\}$.

Using this discretization , and varying the Reynolds number Re, we obtain different nonlinear systems

$$f(x, Re) = 0 \tag{4.5}$$

where the nonlinearity increases with Re.

5.- Numerical Experiments

Our tests consist of solving the system (4.5) for $Re = 250, 500, \ldots, 2000$, using the solution of $f(x, Re) = 0$ as initial approximation for the resolution of $f(x, Re + 250) = 0$. Observe that if $Re = 0$, the system is linear, so, in absence of rounding errors, the methods described in Section 2 solve it in exactly one iteration.

A similar computational behavior was observed for different grid sizes. Here we report the results obtained dividing the interval $[0, 1]$ into 32 subintervals. Thus, the nonlinear system has $29 \times 29 = 841$ equations and unknowns.

To ensure a fair comparison, we ran the different methods in the following way: We ran the complete set of experiments using Newton's method, with the stopping criterion $\|x_{k+1} - x_k\|_\infty \leq 10^{-4}\|x_k\|_\infty$. For each experiment (identified by the Reynolds number Re), we call $\varepsilon(Re) = \|f(x(Re), Re)\|_\infty$, where $x(Re)$ is the "solution" obtained by Newton, according to the stopping criterion mentioned above. The stopping criterion used for the experiments with Quasi-Newton methods was $\|f(x_k, Re)\|_\infty \leq \varepsilon(Re)$. In this way, we ensure that Quasi-Newton methods obtain an approximate solution at least as good as the one obtained by Newton.

The results are presented in Table 1. The result of a particular experiment is represented by two numbers (NI, TIME), where NI is the number of iterations performed, and TIME is the computer CPU time used, in a SUN Workstation. Adding the CPU times for all the experiments, we observe that the Column-Updating method ranked first, with 99.92 seconds, the Modified Newton Method used 106.6 seconds, while Broyden and Newton wasted 122.4 seconds and 207.92 seconds respectively. The fact that, on average, the Modified Newton method behaved better than Broyden was quite surprising for us. We also tried to solve this set of problems using the Diagonal-Scaling method and the Row-Scaling method (Gomes-Ruggiero, Martínez and Moretti [1992]) but the results turned to be completely disappointing. In fact, these methods did not converge even for $Re = 250$.

Reynolds	Newton	Mod. Newton	Broyden	Column-Updating
250	4; 30.11	56; 25.21	70; 34.28	20; 13.88
500	4; 30.10	30; 16.71	28; 17.03	29; 17.00
750	3; 23.52	10; 10.84	17; 13.36	13; 11.84
1000	3; 24.21	19; 13.94	10; 11.13	8; 10.48
1250	3; 24.55	9; 10.88	13; 12.28	4; 9.31
1500	3; 24.88	5; 9.68	5; 9.71	6; 9.98
1750	3; 25.20	5; 9.82	5; 9.78	6; 10.12
2000	3; 25.35	4; 9.52	19; 14.83	26; 16.81

Table 1 – Numerical Experiments.

6.- Conclusions

Boundary value problems coming from the Navier-Stokes equations are very important, not only because their intrinsic relevance but also because they are representative of other problems that model physical and engineering problems.

In this paper we showed that some Quasi-Newton methods are reliable alternatives to Newton for these problems.

The NIGHTINGALE package was used for solving the Fluids Dynamics problems considered in this paper. One of the strenghts of this code is the careful treatment of the solution of the linear systems. For this purpose, we use the partial pivoting rule, which ensures numerical stability, and the static data structure introduced by George and Ng [1987]. In Newton we solve many nonlinear systems with the same Jacobian structure, so the symbolic phase of the George - Ng method, which defines the data structure, is executed only once.

In our tests we used true Jacobians at the first iteration. So, we were forced to perform a complete *LU* factorization of a sparse matrix at this iteration. We tried to alleviate this work by replacing the true Jacobian by a "False Jacobian". With that purpose, we eliminated some sub diagonals of the true Jacobian, so that the factorization became less expensive. We expected that the Quasi-Newton methods could correct this simplification, incorporating the missing information as the process progreeded. This phenomenon had ocurred in other tests concerning boundary value problems (Martínez and Zambaldi [1992]). Unhappily, in the problems studied in this paper, the behavior of Quasi - Newton methods was very sensitive to "errors" on the initial Jacobian, and their behavior turned to be very poor, even for modest simplifications (say, dropping only one sub-diagonal). According to these results, our present feeling is that Quasi-Newton methods are in fact very useful for large problems, when the structure of the Jacobian is such that the sparse *LU* factorization is possible. For *very large* problems, say, 3D boundary value problems, or nonlinear systems coming from very fine discretizations, Inexact Newton methods (Dembo, Eisenstat and Steihaug [1983]), perhaps using Quasi-Newton schemes as preconditioners (Martínez [1990b, 1992b]), seem to be the best choice. Further research is necessary to characterize problems where the performance of Quasi-Newton methods is not seriously affected by "proposital" errors on the initial Jacobian.

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