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Recent Developments in Quasi-Newton Methods for Structural Analysis and Synthesis

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Introduction

ALTHOUGH the conjugate gradient method of Hestenes and Stiefel[1] as a technique for the solution of a system of linear equations has been around for a long time, the formal use of the techniques of mathematical programming, initially for structural design optimization[2] and later for linear and nonlinear structural analysis,[3-5] was first proposed by Schmit and his collaborators. More recently, in the field of structural optimization, constrained function minimization using the method of feasible directions[6,7] and the extended penalty function method[8-10] have been successfully attempted. Both of these methods of constrained function minimization involve the use of unconstrained minimization algorithms in one form or another.

The conventional method which forms the assembled stiffness matrix by an assembly of the individual element matrices and then factorizes it by a triple-factorization technique with an optimized skyline storage scheme, as outlined by Bathe and Wilson,[11] is generally believed to be more efficient than any of the unconstrained minimization algorithms for linear analysis. However, in view of the recently proposed inexpensive direct Hessian evaluation strategies, the conventional techniques may not be that cost effective, especially for large-scale problems with very small mean bandwidth.[12] The question, however, is very much open with respect to nonlinear structural analysis. Attempts to extend the technique to solve dynamic problems of structural analysis involving geometric and material nonlinearities are very promising.[13-17]

In the past, most analysts relied heavily on the conjugate directions algorithm of Powell,[18] requiring only function evaluations; the conjugate gradient algorithm of Fletcher-Reeves,[19] requiring gradient evaluations in addition; and the more powerful Davidon-Fletcher-Powell (DFP) variable metric or quasi-Newton algorithm,[20] which generates an inverse Hessian approximation on the basis of the previously known gradient information. The latter two algorithms, however, require exact line searches to insure a quadratic termination property. It was soon discovered that the performance of both these algorithms is critically sensitive to the accuracy of the line searches. In fact, not only does the performance of the DFP algorithm deteriorate rapidly as the accuracy of the line search decreases[21] but also in certain cases, in the absence of a restart, the inverse Hessian approximation becomes singular and the algorithm becomes inferior to even the steepest descent algorithm and fails to converge.[22] As is well known, even for convex problems Newton's method is not globally convergent, that is to say, a good starting point is required. So, it is natural to seek an efficient quasi-Newton method that is globally convergent. The way this is achieved is by a suitable Hessian or Hessian inverse update along with a carefully controlled steplength procedure.

The decade 1970-1980 has seen the emergence of some of the best known and most successful algorithms of unconstrained minimization. The purpose of this paper is to examine some of these algorithms for their potential of overcoming some of the problems currently facing the analysts of structural analysis and synthesis. Prominent among these problems are the lack of global convergence, difficulty in converging to a solution because of ill-conditioning, and lack of an acceptable speed and rate of convergence.

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New Algorithms and Strategies—Their Properties and Their Potential

The lack of stability of the DFP method along with its cause was briefly alluded to in the introduction. In attempting to bring out the robustness of the new algorithms by comparison to the DFP algorithm, it is worthwhile to examine the question of the stability of the DFP method more extensively. The present discussion is based on the excellent discourse provided by Refs. 21 and 23.

The DFP and Fletcher-Reeves Algorithms

Basically, in minimizing a scalar function F of a vector $\boldsymbol{x}$, the DFP method generates an inverse Hessian approximation $\boldsymbol{H}_i$ to predict a direction of travel $\boldsymbol{p}_i$ such that

$$\boldsymbol{p}_i = -\boldsymbol{H}_i \nabla F(\boldsymbol{x}_i) \tag{1}$$

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha \boldsymbol{p}_i \tag{2}$$

where α is the distance to the minimum of F along $\boldsymbol{p}_i$ and $\nabla F(\boldsymbol{x}_i)$ the gradient of F at $\boldsymbol{x}_i$. The next estimate $\boldsymbol{H}_{i+1}$ is then given by

$$\boldsymbol{H}_{i+1} = \boldsymbol{H}_i + \frac{\boldsymbol{S}_i \boldsymbol{S}_i^T}{(\boldsymbol{S}_i^T \boldsymbol{Y}_i)} - \frac{\boldsymbol{H}_i \boldsymbol{Y}_i \boldsymbol{Y}_i^T \boldsymbol{H}_i}{(\boldsymbol{Y}_i^T \boldsymbol{H}_i \boldsymbol{Y}_i)} \tag{3}$$

with

$$\boldsymbol{Y}_i = \nabla F(\boldsymbol{x}_{i+1}) - \nabla F(\boldsymbol{x}_i) \tag{4}$$

and

$$\boldsymbol{S}_i = \alpha \boldsymbol{p}_i$$

Equation (3) is derived from the requirement of stability of the algorithm, which is to say by obtaining the smallest correction to $\boldsymbol{H}_i$ in the sense of some norm such that $\boldsymbol{H}_{i+1}$ satisfies the secant relation

$$\boldsymbol{H}_{i+1} \boldsymbol{Y}_i = \boldsymbol{S}_i \tag{5}$$

and guarantees that if $\boldsymbol{H}_i$ is symmetric and positive definite so will $\boldsymbol{H}_{i+1}$. For a quadratic function F of the n-dimensional vector $\boldsymbol{x}$ the DFP algorithm has many interesting properties. In fact for a quadratic function F with a constant Hessian $\boldsymbol{G}$, Eq. (3) can be obtained by seeking a sequence of matrices $\boldsymbol{H}_i$ and eigenvectors $\boldsymbol{p}_i$, such that $\boldsymbol{H}_i \boldsymbol{G} \rightarrow \boldsymbol{I}$. For a quadratic function the minimum is guaranteed in n steps. Furthermore, in the case of a quadratic function F, the n G-orthogonal directions of search are identical to those of the Fletcher-Reeves conjugate gradient mehtod.[19] Fletcher-Reeves conjugate gradient method may also be regarded as a variable metric or as a quasi-Newton method since this method uses the formula for the search directions given by

$$\boldsymbol{p}_{i+1} = -\nabla F(\boldsymbol{x}_i) + \frac{[\nabla F(\boldsymbol{x}_i)]^T \nabla F(\boldsymbol{x}_i)}{[\nabla F(\boldsymbol{x}_{i-1})]^T \nabla F(\boldsymbol{x}_{i-1})} \boldsymbol{p}_i \tag{6a}$$

which may be rewritten as

$$\boldsymbol{p}_{i+1} = -\boldsymbol{H}_i \nabla F(\boldsymbol{x}_i) \tag{6b}$$

with

$$\boldsymbol{H}_i = -\boldsymbol{I} + \frac{\boldsymbol{p}_i [\nabla F(\boldsymbol{x}_i)]^T}{[\nabla F(\boldsymbol{x}_{i-1})]^T \nabla F(\boldsymbol{x}_{i-1})} \tag{6c}$$

Whereas the DFP algorithm does, the Fletcher-Reeves algorithm does not belong to what is known as the Huang's class of variable metric algorithm whose update formula may be written in a very compact form as[24]

$$\boldsymbol{H}_{i+1} = \boldsymbol{H}_i - \frac{\boldsymbol{H}_i \boldsymbol{Y}_i \boldsymbol{Y}_i^T \boldsymbol{H}_i}{\boldsymbol{Y}_i^T \boldsymbol{H}_i \boldsymbol{Y}_i} + \rho_i \frac{\boldsymbol{S}_i \boldsymbol{S}_i^T}{\boldsymbol{S}_i^T \boldsymbol{Y}_i} + \theta_i \boldsymbol{v}_i \boldsymbol{v}_i^T \tag{7a}$$

with

$$\boldsymbol{v}_i = (\boldsymbol{Y}_i^T \boldsymbol{H}_i \boldsymbol{Y}_i)^{1/2} \left[\frac{\boldsymbol{S}_i}{\boldsymbol{S}_i^T \boldsymbol{Y}_i} - \frac{\boldsymbol{H}_i \boldsymbol{Y}_i}{\boldsymbol{Y}_i^T \boldsymbol{H}_i \boldsymbol{Y}_i} \right] \tag{7b}$$

ρ_i and θ_i are scalar parameters that can be chosen arbitrarily. The DFP algorithm is a special case of this family with $\rho_i = 1$ and $\theta_i = 0$ for all i. Algorithms from Huang's family have the property that for the same fixed $\rho_i = \rho$, with a given $\boldsymbol{x}_0$ and $\boldsymbol{H}_0$, they generate the same sequence of points $\boldsymbol{x}_i$ even for nonquadratic functions while in addition for quadratic functions with a Hessian G, $\boldsymbol{H}_n = \rho \boldsymbol{G}^{-1}$.[25] This property of the algorithms from Huang's family have profound implications on the use of scaling to improve the performance of many of the well-known variable metric algorithms which belong to this family.

The BFGS Algorithm

Most of the earlier algorithms such as the DFP relied upon the generation of conjugate directions and exact line searches. It is only the high accuracy of the exact line search that can guarantee the generation of conjugate directions. It was wrongly believed, however, that generation of conjugate directions was necessary for guaranteeing the quadratic termination property.[26] An exact line search is the most expensive part of the algorithm. It would be highly desirable to remove this requirement, if at all possible, if in doing so the positive definiteness of the inverse Hessian approximation and the ultimate convergence of the algorithm could be guaranteed.

Positive definiteness of the matrices $\boldsymbol{H}_i$ is a highly desirable property for many reasons. First, if $\boldsymbol{H}_i$ is positive definite then a reduction in the value of the function to be minimized is guaranteed. Second, in the neighborhood of the minimum most functions can be reasonably well approximated by a quadratic function, that is to say, by a second-order Taylor expansion with a positive definite Hessian. Since $\boldsymbol{H}_i$ is an approximation to the inverse Hessian requiring it to be positive definite is a natural choice. Finally, guaranteeing $\boldsymbol{H}_i$ to be positive definite avoids the case of singular $\boldsymbol{H}_i$. With a singular $\boldsymbol{H}_i$ all subsequent search directions will not span the whole R^n and it will not be possible to attain the minimum of the function.[27] In algorithms such as the DFP which require exact line searches, numerical inaccuracies have been found to cause the matrices to be singular or indefinite.[28]

Attempts at using the DFP update while replacing the exact line search by a single function evaluation in the direction $\boldsymbol{p}_i$ so as to guarantee a reasonable function decrease, while maintaining positive definiteness of the approximating matrices $\boldsymbol{H}_i$ by updating over an interval for which $\boldsymbol{p}_i^T \boldsymbol{Y}_i > 0$, have been successful in most cases. But in a few cases failure occurs by $\boldsymbol{H}_i$ becoming singular. A new update formula which maintains positive definiteness and symmetry of the Hessian inverse while abandoning the exact line searches was proposed simultaneously by Broyden,[29,30] Fletcher,[31] Goldfarb,[32] and Shanno[33] and is known as the BFGS update formula defined by

$$\boldsymbol{H}_{i+1} = \left(\boldsymbol{I} - \frac{\boldsymbol{S}_i \boldsymbol{Y}_i^T}{\boldsymbol{Y}_i^T \boldsymbol{S}_i}\right) \boldsymbol{H}_i \left(\boldsymbol{I} - \frac{\boldsymbol{Y}_i \boldsymbol{S}_i^T}{\boldsymbol{Y}_i^T \boldsymbol{S}_i}\right) + \frac{\boldsymbol{S}_i \boldsymbol{S}_i^T}{\boldsymbol{Y}_i^T \boldsymbol{S}_i} \tag{8}$$

Equation (8) is a special case of Huang's family with $\rho_i = 1$, $\theta_i = 1$. It has the important property that successive inverse

Hessian approximations are symmetric and positive definite if H_0 has these properties. Numerical experiments with the BFGS algorithm, details of which may be found in Ref. 34, suggest that this algorithm is superior to all the known variable metric algorithms.[26]

Scaling to Eliminate Ill-Conditioning and Improve Algorithm Performance

Poor scaling of the variables or severely ill-conditioned systems, such as those encountered during the application of Fiacco-McCormick's sequential unconstrained minimization technique,[35] can easily mar the performance, or even lead to a complete failure, of even the more robust of the variable-metric algorithms such as the DFP and BFGS.

Basically, for an ill-conditioned problem the condition number (the ratio of the largest to the smallest eigenvalues of the Hessian of the function) is large. For a quadratic function $F(x)$ with a Hessian G and a minimizer x^*, if quasi-Newton updates H_i from a uniformly positive definite family are used for minimization, it can be shown that[36]

$$F(x_{i+1})-F(x^*)<\left[\frac{\kappa(R_i)-1}{\kappa(R_i)+1}\right]^2(F(x_i)-F(x^*)) \tag{9}$$

holds at every step i where

$$R_i=G^{1/2}H_iG^{1/2}$$

and $\kappa(R_i)$ denotes its condition number. To improve convergence the term

$$\frac{\kappa(R_i)-1}{\kappa(R_i)+1}$$

must be made as small as possible. If for some i, $\kappa(R_i)>\kappa(G)$ the convergence rate will be worse than that for the steepest descent, which is linear.

Several remedies have been proposed to overcome ill-conditioning. Powell[37] recommends a very carefully controlled stepping scheme in a search direction obtained by combination of the steepest descent and quasi-Newton directions. The method uses an update formula for the Hessian that satisfies the secant relation while guaranteeing that the new Hessian approximation is not singular. The result is an adaptive variable metric method that is suitable for unconstrained minimization of a function $F(x)$ which need not be convex. Oren and Luenberger[23] recommend appropriate choice of parameters in the updating formula of the Broyden family (a subset of Huang's family) of algorithms as a means of efficient scaling of the objective function. Oren and Spedicato[38] and Davidon[39] have suggested an appropriate choice of these update parameters which minimize the condition number of the matrix $H_i^{-1}H_{i+1}$. Dennis and Mei[40] use a combination of Davidon's update scheme and a modified Powell strategy.[37]

As far as the self-scaling variable metric methods are concerned, Oren and Luenberger[23] were the first to show that if $F(x)$ is of the form

$$F(x)=\tfrac{1}{2}(x-x^*)G(x-x^*)+F(x^*)$$

proper choice of γ_i in the update formula for the Broyden family of variable metric algorithms, defined by

$$H_{i+1}-[H_i-(H_iY_iY_i^TH_i/Y_i^TH_iY_i)+\theta_iv_iv_i^T]\gamma_i + (S_iS_i^T/S_i^TY_i) \tag{10}$$

with v_i defined as in Eq. (7b), insures at each iteration a reduction in the condition number of the matrix $R_i=G^{1/2}H_iG^{1/2}$. Subsequently, Oren and Spedicato[38] derived the relationship for minimizing the condition number of the matrix $H_i^{-1}H_{i+1}$ as

$$\theta_i=b(c-b\gamma_i)/\gamma_i(ac-b^2) \tag{11a}$$

where

$$a=Y_i^TH_iY_i,\quad b=S_i^TY_i,\quad c=S_i^TH_i^{-1}S_i \tag{11b}$$

Oren and Luenberger show that a proper choice of γ_i can improve the stepwise rate of convergence of the updates defined by Eq. (10) while $\gamma_i=1$ and $\theta_i=0$ (i.e., the DFP method) can in some cases lead to an increase in the condition number of R_i over R_{i+1}. They also established the existence of a continuum of values of γ_i which not only improves the rate of convergence of the algorithms but also makes the sequence of Eq. (10) self-scaling. Later, Spedicato[41] and Shanno and Phua[42] showed that the same effect can also be achieved by a single initial scaling of H_0. Spedicato[41] suggested using the reciprocals of the true diagonal elements of the Hessian, evaluated at the initial point x_0, as the elements of H_0. In some cases these may be computationally expensive to obtain and hence the suggestions by Shanno and Phua are much more appealing. The scaling

$$\gamma_i=b/a \tag{12}$$

obtained by setting $\theta_i=1$ corresponding to the BFGS update has been found by them to be suitable especially on large-scale problems. According to Shanno and Phua the more sophisticated values of γ_i proposed by Oren and Spedicato[38] are markedly superior to the initially scaled Broyden's family of updates on homogeneous functions of the type

$$F(x)=(1/r)(x-x^*)g(x)+F(x^*) \tag{13}$$

defined as such by Jacobson and Oksman.[43]

The idea of scaling can be extended to conjugate gradient methods also. An initial scaling coupled with a restart criterion that is function dependent have led to what are known as memoriless quasi-Newton methods. An extensive discussion of the basis for the scaling and the restart criterion for such methods may be found in Ref. 44.

Finally, Boggs[45] has recommended the conversion of the unconstrained minimization problem into that of integrating a stiff system of differential equations to be solved using concepts from singular perturbation theory. Basically, the steepest descent method applied to the original minimization problem as

$$x_{i+1}=x_i-\gamma_i\nabla F(x_i) \text{ with } x_0 \text{ given}$$

is regarded as being Euler's method for integrating a differential equation of the form

$$x'=-\nabla f(x);\quad x(0)=x_0 \tag{14a}$$

A linearized Taylor's expansion of the right-hand side of the above equation about the minimizer x^* yields

$$x'=-F''(x^*)[(x-x^*)]=[G(x^*)][x-x^*] \tag{14b}$$

The ill-conditioned minimization problem characterized by a high condition number of G implies that the differential equation (14b) is stiff. By an application of the steepest descent method, the system x is separated into nonsingular or slowly varying part y and the singular or rapidly varying part z. The solution of the differential equation (14a) based on an asymptotic expansion leads to expressions for the boundary-layer terms with Euler's method being used for the nonsingular parts and the quasi-Newton method being used for

the singular parts. Details of these expressions, the computer implementation of the criteria for separation of the variables into singular and nonsingular parts, and other relevant material may be found in Ref. 45. According to Boggs, the approach is better able "to smooth the geometry" than Powell's method[37] which uses a combination of the steepest descent and quasi-Newton directions.

Thus, basically, the methods for overcoming ill-conditioning may be regarded as falling into three groups, namely the adaptive techniques of Powell and Dennis and Mei; the self-scaling variable metric methods of Oren, Luenberger, Spedicato, and Davidon; and the singular perturbation technique of Boggs.

Switching of Algorithms

Somewhat similar to the adaptive algorithms, a combined conjugate-gradient quasi-Newton minimization algorithm has been suggested by Buckley.[46] Interactive switching between quasi-Newton and conjugate-gradient algorithms has also been proposed by Hazelrig et al.[47] But, whereas Buckley addresses the question of keeping the increase of storage requirements in switching from the conjugate-gradient to quasi-Newton to a minimum, Hazelrig et al. do not address this question. Hazelrig et al. simply recognize the fact that not all algorithms suit all problems and suggest measures of progress that are considered in making a switch from the quasi-Newton to the conjugate-gradient algorithms and vice versa. The objective of Buckley is to get a convergence rate somewhere between the linear convergence rate of the conjugate-gradient algorithm and the superlinear convergence rate of the quasi-Newton algorithms while reducing their usual requirement of storage locations from $n(n+1)/2$ to $m(2n+2)$ where m is the frequency at which quasi-Newton updates are attempted. This is done by rewriting the BFGS update formula in the form

$$\boldsymbol{H}_{i+1}=\boldsymbol{H}_i+\boldsymbol{\eta}_i\left[\frac{\beta-1}{b}\boldsymbol{S}_i-\frac{\beta}{a}\boldsymbol{\eta}_i\right]^T+\boldsymbol{S}_i\left[\frac{b+(1-\beta)a}{b^2}\boldsymbol{S}_i-\frac{\beta-1}{b}\boldsymbol{\eta}_i\right]^T$$

with $a=\boldsymbol{Y}_i^T\boldsymbol{H}_i\boldsymbol{Y}_i=\boldsymbol{Y}_i^T\boldsymbol{\eta}_i$, $b=\boldsymbol{S}_i^T\boldsymbol{Y}_i$, and $\boldsymbol{\eta}_i=\boldsymbol{H}_i\boldsymbol{Y}_i$. Since it is only the vectors $\boldsymbol{\eta}_i$ and $\boldsymbol{d}_{i+1}$ that are required, knowing some of the previous $\boldsymbol{\eta}_i$ and $\boldsymbol{d}_i$ explicit storage for $\boldsymbol{H}_i$ or $\boldsymbol{H}_{i+1}$ is eliminated by storing only the two vectors $\boldsymbol{\eta}_i$ and $\boldsymbol{S}_i$ and the two scalars a and b, requiring $2n+2$ locations at each update over and above those required for the conventional conjugate-gradient method. Since the vectors $\boldsymbol{\eta}_i$ are not updated at every step, Buckley suggests criteria to guarantee that the update scheme produces descent directions. Furthermore, when the allotted storage limit is eventually reached because of the accumulation of a lot of update data, some of the update data have to be discarded in favor of the other. Buckley recommends discarding all current updates and starting afresh. Unfortunately, Buckley's numerical experiments with this new hybrid algorithm indicates that its performance is at best comparable with that of Powell's conjugate-gradient algorithm with restarts.[48]

Algorithms That Exploit Sparsity

Past experiments using minimization algorithms for structural analysis reveal that at least for small-scale problems the energy minimization technique is better suited than most other incremental techniques for solving highly nonlinear problems.[13] Extension of the minimization algorithms to large-scale problems centers on reducing the storage requirements of the second-order quasi-Newton methods (BFGS, DFP,[26] etc.) or improving the efficiency of the first-order conjugate-gradient techniques. In the past few years the mathematicians and computer scientists have been attacking the problem areas that inhibit the extension of the minimization algorithms to large-scale problems. Two alternatives are presently available: 1) the preconditioned or scaled conjugate-gradient technique or 2) the variable metric methods that exploit sparsity and utilize singular perturbation theory or scaling to eliminate ill-conditioning.[42,44,45] Some of the variable metric methods that exploit sparsity are discussed next.

Schubert's Algorithm

The first attempts at exploiting sparsity in the matrix updating process appear to have been those of Schubert[49] who proposed a modification of Broyden's method[50] for solving sparse nonlinear systems of equations

$$\boldsymbol{F}(\boldsymbol{x})=\boldsymbol{0} \tag{15}$$

The iterates are computed by

$$\boldsymbol{B}_i\boldsymbol{p}_i=-\boldsymbol{F}(\boldsymbol{x}_i) \tag{16}$$

$$\boldsymbol{x}_{i+1}=\boldsymbol{x}_i+t_i\boldsymbol{p}_i \tag{17}$$

where $\boldsymbol{B}_i$ is the current approximation of the Jacobian matrix of $\boldsymbol{F}(\boldsymbol{x})$. $\boldsymbol{B}_i$ is updated row by row according to

$$\boldsymbol{B}_{i+1}^{(k)}=\boldsymbol{B}_i^{(k)}+\frac{[F_k(\boldsymbol{x}_{i+1})-(1-t_i)F_k(\boldsymbol{x}_i)]\hat{\boldsymbol{p}}_i}{t_i\hat{\boldsymbol{p}}_i^T\hat{\boldsymbol{p}}_i} \tag{18}$$

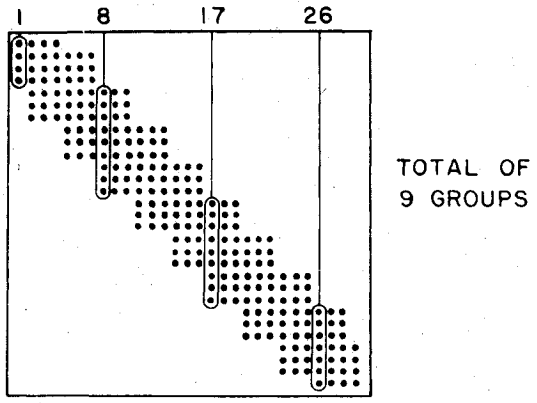
where $\boldsymbol{B}_i^{(k)}$ is the kth row of $\boldsymbol{B}_i$ and $\hat{\boldsymbol{p}}_i$ is obtained from $\boldsymbol{p}_i$ by setting to zero those coordinates corresponding to known zeros in $\boldsymbol{B}_i^{(k)}$. Note that $\hat{\boldsymbol{p}}_i$ is also dependent on k.

However, the method has the drawback that it cannot retain the symmetry of the resulting matrix even when starting with a symmetric, positive definite one. Not only does this place slightly increased demands on storage, but it also requires special sparse linear equation solvers that can accommodate matrices that are not symmetric and positive definite. Our experiments with Schubert's sparse update algorithm indicate that the technique is not suitable for nonlinear problems of structural analysis, wherein the Hessians are symmetric, banded, and mostly positive definite.

Curtis-Powell-Reid Strategy (CPR) and Powell-Toint Strategy (PT)

Because of sparisty the full Newton method, wherein the Hessian matrix is evaluated at each iteration, does appear to be a viable alternative, especially if sparsity and/or symmetry can be exploited, not only in the solution of the resulting linear systems of equations but in the estimation of the relatively few nonzero entries in the Hessian matrix. Such a technique was proposed by Curtis, Powell, and Reid[51] and will be referred to as the CPR strategy. The method divides the columns of the Hessian into groups, so that in each group the row numbers of the unknown elements of the column vectors are all different. After the formation of the first group, other groups are formed successively by applying the same strategy to columns not included in the previous groups. As seen from Fig. 1, which shows the stiffness matrix for a 29 degree-of-freedom model of half the arch of Fig. 5, the number of such groups for banded matrices of typical finite-element models is usually a very small number by comparison with the number of degrees of freedom of the model. After an initial calculation of the gradient vector, the additional gradient evaluations needed to evaluate all the nonzero elements of the Hessian using one-sided finite-difference approximations equal the number of column groups. Thus, using forward differences

$$B_{k\ell}=\frac{\partial g_k}{\partial x_\ell}\approx\frac{g_k(\boldsymbol{x}+h_\ell\boldsymbol{e}_\ell)-g_k(\boldsymbol{x})}{h_\ell} \tag{19}$$



$$\nabla_i \pi(q_1+h_1, \ldots, q_8+h_8, \ldots, q_{17}+h_{17}, \ldots, q_{26}+h_{26}, \ldots) - \nabla_i \pi(q_1, q_2, \ldots, q_{29}) = B_{ij} h_j$$

Fig. 1 Curtis-Powell-Reid (CPR) strategy.

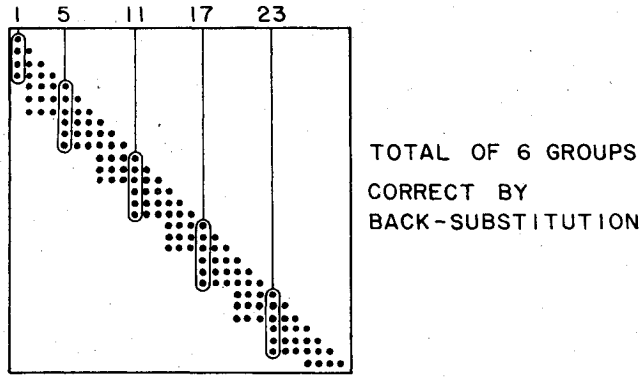


Fig. 2 Powell-Toint (PT) strategy.

where e_ℓ is the ℓth coordinate vector and h_ℓ is a suitable step size. Each step size may be adjusted such that the greatest ratio of roundoff to truncation error for any column of the Hessian falls within a specified range. However, such an adjustment of the step sizes would necessitate a significantly large number of gradient evaluations, thereby rendering the CPR strategy perhaps altogether ineffective. Hence, to economize on the number of gradient evaluations, the step sizes are not allowed to leave the range

$$[\max(\epsilon \mid x_\ell \mid, \eta h_{u\ell}), h_{u\ell}] \tag{20}$$

where ϵ is the greatest relative roundoff in a single operation, η the relative machine precision, and $h_{u\ell}$ an upper bound of h_ℓ. Unfortunately, the CPR strategy does not account for symmetry of the Hessian matrix in the formation of the groups. Powell and Toint in their recent paper[52] have proposed two new strategies which not only account for sparsity but also symmetry in the formation of the groups, thereby reducing the number of gradient evaluations for estimating the Hessian even further (see Fig. 2). One of these strategies known as the substitution method is extremely well suited for banded matrices.

The substitution method described by Powell and Toint in Ref. 52 is obtained by applying the CPR strategy to the lower triangular part, L of the symmetric Hessian, B as shown in Fig. 2. Simple back substitution is then used to correct the elements of B.[52]

Toint's Algorithm for Sparse Systems

Toint has recently proposed an algorithm[53,54] which finds updating formulas for symmetric matrices that preserve known sparsity conditions. The update is obtained by calculating the smallest correction matrix in the Frobenius norm subject to some linear constraints which include the sparsity conditions. Precisely, let A be a given symmetric matrix with sparsity conditions

$$A_{ij}=0, \quad (i,j)\in I \tag{21}$$

where I is some set of indices. The updating problem is to find a correction matrix E such that

$$A^*=A+E \tag{22}$$

$$A^{*t}=A^* \tag{23}$$

$$A^*x=y \text{ for given vectors } x,y \tag{24}$$

$$A^*_{ij}=0, \quad (i,j)\in I \tag{25}$$

Define the vectors $x(i)$ by

$$x(i)_j=\begin{cases} x_j, & (i,j)\ I \\ 0, & (i,j)\in I \end{cases} \tag{26}$$

and the matrix Q by

$$Q_{ij}=x(i)_j x(j)_i+\|x(i)\|^2\delta_{ij} \tag{27}$$

Let λ be the solution of the linear system (which has the same sparsity pattern as A)

$$Q\lambda=y-Ax \tag{28}$$

Then Toint proves that the correction matrix E is given by

$$E_{ij}=\begin{cases} 0, & (i,j)\in I \\ \lambda_i x_j+\lambda_j x_i, & (i,j)\ I \end{cases} \tag{29}$$

In our notation, $A=B_i$, the current approximation to the Hessian matrix of $F(x)$ at x_i, $A^*=B_{i+1}$, $x=t_i p_i=x_{i+1}-x_i$, $y=g_{i+1}-g_i=\nabla F(x_{i+1})-\nabla F(x_i)$. More details of this algorithm may be found in Ref. 53.

To solve the minimization problem starting with an initial guess x_0 for the vector of unknowns and an initial guess for the Hessian B_0, a direction of travel p_i is generated by a constrained minimization of a local quadratic approximation of the potential function $F(x)$. The function is then minimized along this direction by a cubic line search to obtain a new starting point x_{i+1}. Next, the Hessian is updated at this new point and the iteration is repeated. Presumably to minimize storage requirements, Toint proposes the solution of the constrained minimization of the quadratic function by a Levenberg-Marquardt procedure[54] which is similar to a conjugate-gradient scheme. The updating procedure also involves the solution of a sparse linear system of equations with the same sparsity pattern as the Hessian. Again, presumably for the same reasons as before, Toint proposes the solution of this system also by a conjugate-gradient scheme.

Results and Conclusions

As is evident from the previous discussions the advances in quasi-Newton methods have been significant and they offer several possibilities for improvement of the existing methods for solution of the problems of nonlinear structural analysis and synthesis. In light of the experiences derived from previous work[15] the authors choose to examine only a few of the most promising alternatives and because of limitations of space, concern themselves mainly with illustrations in the field of structural analysis.

By way of applications to structural synthesis, Ref. 55 reports the successful use of Bogg's singular perturbation-based algorithm in solving nonlinearly constrained problems utilizing an interior penalty function method. The modified SUMT so evolved has been found to be much more robust than the conventional SUMT proposed by Fiacco-McCormick,[35] especially in overcoming ill-conditioning of the penalty function resulting from an inappropriate choice of the penalty parameter or a poor scaling of the design variables.

With regard to nonlinear structural analysis, four methods are selected for consideration in this paper. First is the quasi-Newton method proposed by Kamat, Watson, and VandenBrink[15] and referred to as NA. This method uses a direct evaluation of the Hessian H_i by the PT strategy[52] with possibly a modification rendering it suitable for the generation of a descent direction using any one of the techniques proposed by Dennis and Schnabel,[56] Gill and Murray,[57] and Fiacco and McCormick.[58] To prevent divergence the scalar t_i along the direction

$$p_i = -H_i^{-1} \nabla g_i(x_i)$$

from the point x_i is determined such that it leads to reduction of the gradient norm. The details of the scheme for evaluating an appropriate t_i is outlined by Broyden.[50]

The second method is a quasi-Newton method identical to NA except that it uses the CPR strategy[51] instead of the PT strategy for the evaluation of the Hessian. The third is a quasi-Newton method similar to NA except that after an initial evaluation of the Hessian by the PT strategy, it is updated using Toint's sparse updates until such time as the updated Hessian approximation ceases to yield a direction of descent. At such time the Hessian is evaluated by the PT strategy. This method is referred to as the TUNA method. The last method is Shanno's variable metric algorithm that uses initial scaling to overcome ill-conditioning and accelerate convergence.

The performance of the above four algorithms will be evaluated relative to the well-known Broyden-Fletcher-Goldfarb-Shanno algorithm[33] utilizing the Hessian inverse updates. Although indications of their favorable performance relative to different methods of nonlinear analysis employed by other investigators are also available, it is deemed appropriate not to present such comparisons because of possible lack of appropriate normalization basis, coding structure, etc. Since all of the algorithms considered herein were used in conjunction with a common nonlinear structural analysis code, ACTION[13], the comparison to be presented is apt to be more meaningful and less sensitive to coding sophistications.

For evaluating the performance of the various algorithm problems of structural analysis involving only geometric nonlinearity are considered. Figure 3 illustrates the dynamic buckling of a shallow elastic arch[59] under a distributed step loading, while Fig. 4 illustrates the dynamic response of an elastic clamped beam to a step-concentrated load.[60] The snap-through buckling of a shallow elastic arch shown in Fig. 5 was obtained using displacement incrementation. This problem is used for the purposes of evaluating the performance of Shanno's algorithm.

Results of these investigations are presented in Tables 1-3. In these tables, N denotes the number of degrees of freedom of the finite-element displacement model used. In the case of

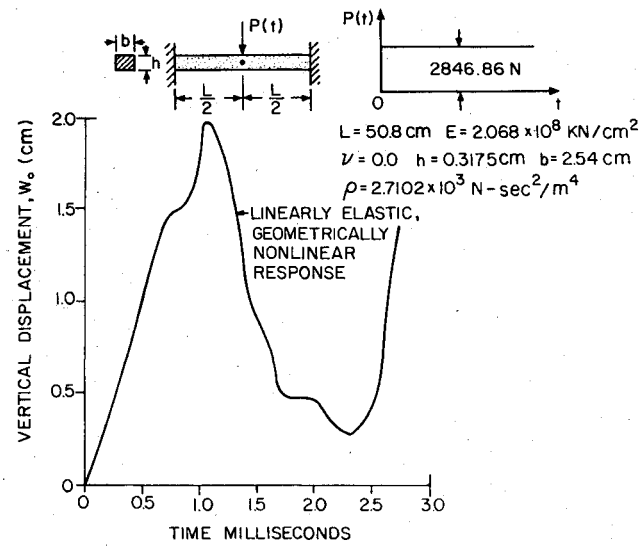


Fig. 4 Dynamic response of a clamped elastic beam.

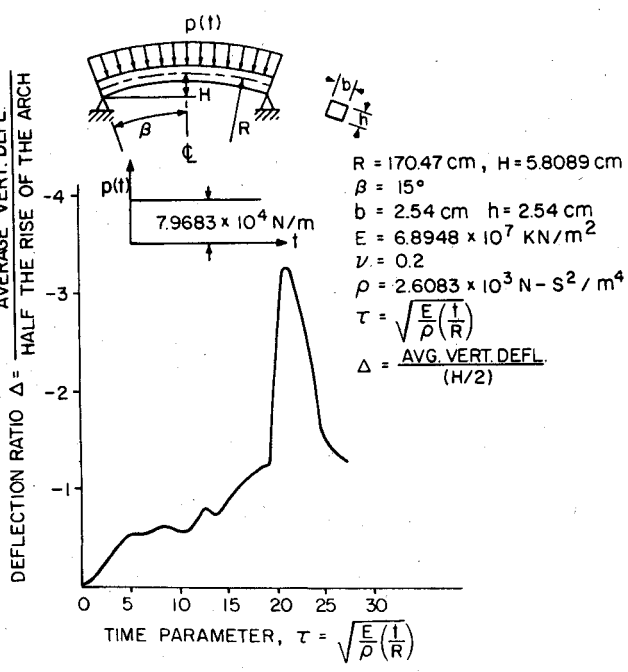


Fig. 3 Dynamic buckling of a shallow elastic arch.

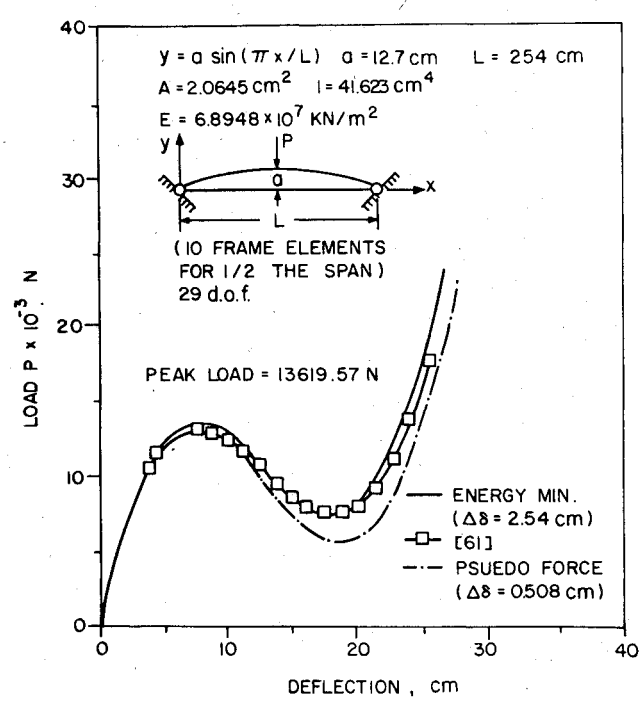


Fig. 5 Static snap-through buckling of a shallow arch.

Table 1 Results for the elastic shallow arch (Fig. 3) ($N=59$, $\Delta T=2.5\times10^{-5}$ s)

Algorithm	Normalized CPU time	Normalized function and gradient evaluations
BFGS	1.0	1.0
NA/CPR	0.835	0.938
NA/PT	0.684	0.745
TUNA	0.628	0.535

Table 2 Results for the elastic clamped beam (Fig. 4) ($N=58$, $\Delta T=1.0\times10^{-5}$ s)

Algorithm	Normalized CPU time	Normalized function and gradient evaluations
BFGS	1.0	1.0
NA/CPR	0.898	1.053
NA/PT	0.670	0.678

Table 3 Results for the shallow arch (Fig. 5) ($N=89$, $\Delta\delta=2.54$ cm)

Algorithm	Normalized CPU time	Normalized function and gradient evaluations
Shanno/without scaling	1.0	1.0
Shanno/with scaling	0.595	0.66
TUNA	0.328	0.39

dynamic response, the Newmark-Beta algorithm with $\beta=\frac{1}{4}$, $\gamma=0.5$ and a lumped mass model are implied. For consistency of comparison, constant size displacement step ($\Delta\delta$) or time step (Δt) as the case may be was used. All results are normalized with those for the BFGS algorithm.

For those small-scale time-dependent problems for which the BFGS algorithm can be used it is indeed a highly efficient algorithm in spite of its sluggishness in the first time step. For large-scale problems which inhibit its use because of excessive core requirements, the best alternatives appear to be the TUNA and the NA algorithms using the PT strategy. Shanno's algorithm utilizing initial scaling, although instrumental in accelerating the convergence significantly, appears to be no match for the NA algorithm, at least on the problem for which it is tested. The effectiveness of scaling on Hessian updates rather than on the inverse updates remains to be evaluated among the many other alternatives discussed in this paper. Limited indications of similar performances of these algorithms exist for problems involving even elastic-plastic large-deformation behavior, but because of the need for further evaluation in this rather complex case the authors defer the presentation of results for this class of problems. The conclusions in this case are a function of the size of the model, type and degree of nonlinearity, and the extent of the response prediction interval.

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