

A ROBUST HYBRID ALGORITHM FOR COMPUTING
MULTIPLE EQUILIBRIUM SOLUTIONS

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CS84014-R

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ABSTRACT

This paper describes a hybrid method that seeks to combine the efficiency of a quasi-Newton method capable of locating stable and unstable equilibrium configurations with a robust homotopy method that is capable of tracking equilibrium paths with turning points while exploiting symmetry and sparsity of the Jacobian matrices. Numerical results are presented for a shallow arch problem.

INTRODUCTION

Currently a great deal of interest within the structural mechanics community centers around being able to predict response of structures susceptible to limit and bifurcation point instabilities¹⁻⁴. The present investigation seeks to evolve robust and efficient techniques for such a response prediction. One such technique is a hybrid method stemming from an appropriate combination of a quasi-Newton method and a homotopy method. Unlike the previously known techniques of references [1]-[4], the present hybrid method not only "breezes" past limit points but can also locate such points to an extremely high degree of accuracy. Previous techniques experience a great deal of difficulty in

the vicinity of limit points by virtue of the fact that the tangent stiffness matrix of the structure is singular at such points.

In a recent paper⁵ Kamat, Watson and Venkayya provide an evaluation of the globally convergent quasi-Newton method and the homotopy method⁶ with regard to their suitability for solving nonlinear problems of structural analysis posed as equivalent energy minimization problems. The globally convergent quasi-Newton method, although quite efficient, has its obvious limitations in the vicinity of limit and bifurcation points and along unloading branches, especially when used in the context of energy minimization. The homotopy method⁶, on the other hand, although quite suitable for nearly all types of nonlinear problems, suffers from relative inefficiency and inability to exploit sparsity and symmetry of the Jacobian matrix of the nonlinear equations of equilibrium. The hybrid scheme proposed here overcomes the undesirable features of both these techniques, besides being more reliable and efficient.

At the outset the energy minimization approach is abandoned, and in its place an extension of the globally convergent quasi-Newton method utilizing the double dogleg strategy⁷ for solving the system of nonlinear equilibrium equations directly is considered. The most significant pay-off from this alternate approach is its suitability for locating equilibrium configurations along unloading branches. The process experiences no difficulty in utilizing nonpositive definite Jacobian matrices - a characteristic of unloading branches.

The homotopy method of reference [6], in the interest of stability and accuracy, utilized Householder reflections to obtain the kernel of a $n \times (n+1)$ matrix, thereby failing to exploit sparsity and symmetry of the

Jacobian matrices of the nonlinear equilibrium equations. The approach taken here is to use a preconditioned conjugate gradient algorithm instead, thereby providing a smooth transition in the vicinity of limit points from the quasi-Newton method that exploits sparsity and symmetry to the modified homotopy method that also exploits the same properties.

QUASI-NEWTON METHOD FOR NONLINEAR EQUATIONS

Assume the nonlinear equilibrium equations to be

$$F_i(x_1, \dots, x_n) = 0; \quad i = 1, 2, \dots, n. \quad (1)$$

The double dogleg strategy described in detail in the appendix is applied to minimize

$$f(\underline{x}) = \frac{1}{2} \underline{F}^t(\underline{x}) \underline{F}(\underline{x}). \quad (2)$$

Essentially, the strategy seeks the minimum of a quadratic model \hat{m}_C of f subject to the constraint

$$\|\underline{x} - \underline{x}_C\| \leq \delta_C, \quad (3)$$

where δ_C is the radius of the sphere, centered at the current point \underline{x}_C , within which the quadratic model can be trusted. Unlike backtracking which uses a one dimensional quadratic or cubic model in the Newton direction, the double dogleg strategy uses an n-dimensional quadratic model to choose a new direction and the shorter steplengths consistent with Eq. (3). Note that the steepest descent direction for (2) at the point \underline{x}_C is given by $\underline{s}_{cp} = -\underline{J}^t(\underline{x}_C) \underline{F}(\underline{x}_C)$, where $\underline{J}(\underline{x}_C)$ is the Jacobian matrix of $\underline{F}(\underline{x})$ at \underline{x}_C .

Next consider the quadratic model \hat{m}_C given by

$$\hat{m}_C(\underline{x}_C + \underline{s}) = \frac{1}{2} \underline{M}_C^t(\underline{x}_C + \underline{s}) \underline{M}_C(\underline{x}_C + \underline{s}), \quad (4)$$

where

$$\underline{M}_C(\underline{x}_C + \underline{s}) = \underline{F}(\underline{x}_C) + \underline{J}(\underline{x}_C)\underline{s} . \quad (5)$$

Note that $\underline{S}_C^N = -\underline{J}^{-1}(\underline{x}_C)\underline{F}(\underline{x}_C)$ is the Newton direction for (4) and it is indeed a descent direction for this quadratic model since it goes to the minimum of (4). Since (2) and (4) have the same linear terms, a quasi-Newton method for the nonlinear equations (1) can be obtained by applying the double dogleg strategy to the positive definite quadratic model (4). It should be noted that the Hessian $\underline{J}^t(\underline{x}_C)\underline{J}(\underline{x}_C)$ of the quadratic model (4) is not the same as the Hessian of f . However, the former is guaranteed to be positive definite as long as $\underline{J}(\underline{x}_C)$ is nonsingular. It is herein that lies the effectiveness of this method for locating all equilibrium configurations except critical points, whether they be stable or not. It is of course possible that a local minimizer of f may not be a solution of (1), in which case it is necessary to restart nearer to a root of $\underline{F}(\underline{x})$.

Next the details of the homotopy method of reference [6], modified to account for symmetry and sparsity using a preconditioned conjugate gradient algorithm, are presented.

HOMOTOPY METHOD USING A PRECONDITIONED CONJUGATE GRADIENT SCHEME

In this method assume the equilibrium equations have the form

$$\underline{F}(\underline{x}, \lambda) = 0 \quad (6)$$

where $\underline{x}, \underline{F}$ are n -vectors and λ is a scalar. Assuming there are no bifurcation points, the zero set of $\underline{F}(\underline{x}, \lambda)$ is a smooth curve γ which does not intersect itself, and along which $\underline{DF}(\underline{x}, \lambda) = [\underline{D}_x \underline{F}(\underline{x}, \lambda), \underline{D}_\lambda \underline{F}(\underline{x}, \lambda)]$ has rank n . At a limit point $\underline{D}_x \underline{F}(\underline{x}, \lambda)$ is singular, but the entire Jacobian matrix $\underline{DF}(\underline{x}, \lambda)$ still has rank n . It is this fact which is exploited by homotopy methods.

Let the smooth equilibrium curve γ be parameterized by arc length s , so $\underline{x} = \underline{x}(s)$, $\lambda = \lambda(s)$ on γ and

$$\underline{F}(\underline{x}(s), \lambda(s)) = 0 \quad (7)$$

identically as a function of s . Then observe that $(\underline{x}(s), \lambda(s))$ is the trajectory of the initial value problem

$$\frac{d}{ds} \underline{F}(\underline{x}(s), \lambda(s)) = [\underline{D}_{\underline{x}} \underline{F}(\underline{x}(s), \lambda(s)), \underline{D}_{\lambda} \underline{F}(\underline{x}(s), \lambda(s))] \begin{pmatrix} d\underline{x}/ds \\ d\lambda/ds \end{pmatrix} = 0, \quad (8)a$$

$$\underline{x}(0) = \underline{x}_0, \quad \lambda(0) = \lambda_0, \quad (8)b$$

where $\underline{x}_0, \lambda_0$ is some initial point on γ . Since the Jacobian matrix has rank n , the derivative $(d\underline{x}/ds, d\lambda/ds)$ is uniquely determined, and the initial value problem can be solved for $\underline{x}(s), \lambda(s)$. No Newton-type iterations are performed, and the method is not just continuation or a standard initial value technique because now both the displacements \underline{x} and the load parameter λ are dependent variables.

Note that the derivative $(d\underline{x}/ds, d\lambda/ds)$ is specified only implicitly, and special techniques are required to solve the initial value problem. For more details on the homotopy algorithm, see references [6], [8], [9].

The algorithm requires computing the kernel of the $n \times (n+1)$ matrix \underline{DF} , which has rank n . This can be easily and efficiently done for small dense matrices, but the large sparse Jacobian matrix of structural mechanics presents special difficulties. The approach taken here is to solve $\underline{DFy} = 0$ using a preconditioned conjugate gradient algorithm. This conjugate gradient algorithm will now be described.

Let $(\bar{\underline{x}}, \bar{\lambda})$ be a point on the equilibrium curve γ , and $\bar{\underline{y}}$ the unit tangent vector to γ at $(\bar{\underline{x}}, \bar{\lambda})$ in the direction of increasing arc length

s. Let $\bar{y}_k = \max_i |\bar{y}_i|$. Then the matrix

$$\underline{A} = \begin{bmatrix} \underline{DF}(\underline{x}, \lambda) \\ \underline{e}_k^t \end{bmatrix} \quad (9)$$

where \underline{e}_k is a vector with 1 in the k th component and zeros elsewhere, is invertible at $(\bar{x}, \bar{\lambda})$ and in a neighborhood of $(\bar{x}, \bar{\lambda})$ by continuity. Thus the kernel of \underline{DF} can be found by solving the linear system of equations

$$\underline{A}\underline{y} = \bar{y}_k \underline{e}_{n+1} = \underline{b}. \quad (10)$$

Given any nonsymmetric, nonsingular matrix \underline{A} , the system of linear equations $\underline{A}\underline{y} = \underline{b}$ can be solved by considering the linear system

$$\underline{A}\underline{A}^t \underline{z} = \underline{b}.$$

Since the coefficient matrix for this system is both symmetric and positive definite, the system can be solved by a conjugate gradient algorithm. Once a solution vector \underline{z} is obtained, the vector \underline{y} from the original system can be computed as $\underline{y} = \underline{A}^t \underline{z}$. An implementation of the conjugate gradient algorithm in which \underline{y} is computed directly, without reference to \underline{z} , any approximations of \underline{z} , or $\underline{A}\underline{A}^t$, was originally proposed by Hestenes¹⁰, and is commonly known as Craig's method¹¹. Each iterate \underline{y}^i minimizes the Euclidean error norm $\|\underline{y} - \underline{y}^i\|$ over the translated Krylov space

$$\underline{y}^0 + \text{span} \{ \underline{r}^0, \underline{A}\underline{A}^t \underline{r}^0, (\underline{A}\underline{A}^t)^2 \underline{r}^0, \dots, (\underline{A}\underline{A}^t)^{i-1} \underline{r}^0 \},$$

where $\underline{r}_0 = \underline{b} - \underline{A}\underline{y}^0$. Below $\langle \underline{u}, \underline{v} \rangle$ denotes the inner product $\underline{u}^t \underline{v}$.

Craig's Method:

Choose \underline{y}^0 ;

Compute $\underline{r}^0 = \underline{b} - \underline{A}\underline{y}^0$;

Compute $\underline{p}^0 = \underline{A}^t \underline{r}^0$;

For $i = 0$ step 1 until convergence do

BEGIN

$$\alpha_i = \langle \underline{r}^i, \underline{r}^i \rangle / \langle \underline{p}^i, \underline{p}^i \rangle$$

$$\underline{y}^{i+1} = \underline{y}^i + \alpha_i \underline{p}^i$$

$$\underline{r}^{i+1} = \underline{r}^i - \alpha_i \underline{A} \underline{p}^i$$

$$\beta_i = \langle \underline{r}^{i+1}, \underline{r}^{i+1} \rangle / \langle \underline{r}^i, \underline{r}^i \rangle$$

$$\underline{p}^{i+1} = \underline{A}^t \underline{r}^{i+1} + \beta_i \underline{p}^i$$

END

Let \underline{Q} be any nonsingular matrix. The solution to the system $\underline{A}\underline{y} = \underline{b}$ can be calculated by solving the system

$$\underline{B}\underline{y} = (\underline{Q}^{-1}\underline{A})\underline{y} = \underline{Q}^{-1}\underline{b} = \underline{q}. \quad (11)$$

The use of such a matrix is known as preconditioning. Since the goal of using preconditioning is to decrease the computational effort needed to solve the original system, \underline{Q} should be some approximation to \underline{A} . Then $\underline{Q}^{-1}\underline{A}$ would be close to the identity matrix, and the iterative method described above would converge more rapidly when applied to (11) than when applied to (10). In the following algorithm \underline{B} and \underline{q} are never explicitly formed. The algorithm given above can be obtained by substituting the identity matrix for \underline{Q} .

Craig's method using a preconditioner:

Choose \underline{y}^0 , \underline{Q} .

Compute $\underline{r}^0 = \underline{b} - \underline{A}\underline{y}^0$.

Compute $\tilde{\underline{r}}^0 = \underline{Q}^{-1}\underline{r}^0$.

Compute $\underline{p}^0 = \underline{A}^t \underline{Q}^{-t} \tilde{\underline{r}}^0$.

For $i = 0$ step 1 until convergence do

BEGIN

$$\alpha_i = \langle \tilde{\underline{r}}^i, \tilde{\underline{r}}^i \rangle / \langle \underline{p}^i, \underline{p}^i \rangle$$

$$\begin{aligned}
\underline{y}^{i+1} &= \underline{y}^i + \alpha_i \underline{p}^i \\
\tilde{\underline{r}}^{i+1} &= \tilde{\underline{r}}^i - \alpha_i \underline{Q}^{-1} \underline{A} \underline{p}^i \\
\beta_i &= \langle \tilde{\underline{r}}^{i+1}, \tilde{\underline{r}}^{i+1} \rangle / \langle \tilde{\underline{r}}^i, \tilde{\underline{r}}^i \rangle \\
\underline{p}^{i+1} &= \underline{A}^t \underline{Q}^{-t} \tilde{\underline{r}}^{i+1} + \beta_i \underline{p}^i
\end{aligned}$$

END

For this algorithm, a minimum of $5(n+1)$ storage locations is required (in addition to that for \underline{A}). The vectors \underline{y} , $\tilde{\underline{r}}$, and \underline{p} all require their own locations; $\underline{Q}^{-t} \tilde{\underline{r}}$ can share with $\underline{A} \underline{p}$; $\underline{Q}^{-1} \underline{A} \underline{p}$ can share with $\underline{A}^t \underline{Q}^{-t} \tilde{\underline{r}}$. The computational cost per iteration of this algorithm is:

- 1) two preconditioning solves ($\underline{Q}^{-1} \underline{v}$ and $\underline{Q}^{-t} \underline{v}$);
- 2) two matrix-vector products ($\underline{A} \underline{v}$ and $\underline{A}^t \underline{v}$);
- 3) $5(n+1)$ multiplications (the inner products $\langle \underline{p}, \underline{p} \rangle$ and $\langle \tilde{\underline{r}}, \tilde{\underline{r}} \rangle$, $\alpha \underline{p}$, $\beta \underline{p}$, and $\alpha \underline{Q}^{-1} \underline{A} \underline{p}$).

The coefficient matrix \underline{A} in the linear system of equations (10), whose solution \underline{y} yields the kernel of $\underline{D}F(\bar{\underline{x}}, \bar{\lambda})$, has a very special structure which can be exploited if (10) is attacked indirectly as follows. Note that the leading $n \times n$ submatrix of \underline{A} is $\underline{D}_x F$, which is symmetric and sparse, but possibly indefinite. Write

$$\underline{A} = \underline{M} + \underline{L} \tag{12}$$

where

$$\underline{M} = \begin{bmatrix} \underline{D}_x F(\bar{\underline{x}}, \bar{\lambda}) & \underline{c} \\ \underline{c}^t & d \end{bmatrix},$$

$$\underline{L} = \underline{u} \underline{e}_{n+1}^t, \quad \underline{u} = \begin{pmatrix} \underline{D}_\lambda F(\bar{\underline{x}}, \bar{\lambda}) - \underline{c} \\ 0 \end{pmatrix}.$$

The choice of \underline{e}_k^t as the last row of \underline{A} to make \underline{A} invertible is somewhat arbitrary, and in fact any vector (\underline{c}^t, d) outside a set of measure zero (a hyperplane) could have been chosen. Thus for almost all vectors \underline{c} the first n columns of \underline{M} are independent, and similarly almost all $(n+1)$ -vectors are independent of the first n columns of \underline{M} . Therefore for almost all vectors (\underline{c}^t, d) both \underline{A} and \underline{M} are invertible. Assume that (\underline{c}^t, d) is so chosen.

Using the Sherman-Morrison formula (\underline{L} is rank one), the solution \underline{y} to the original system $\underline{A}\underline{y} = \underline{b}$ can be obtained from

$$\underline{y} = \left[\underline{I} - \frac{\underline{M}^{-1} \underline{u} \underline{e}_{n+1}^t}{(\underline{M}^{-1} \underline{u})^t \underline{e}_{n+1} + 1} \right] \underline{M}^{-1} \underline{b}, \quad (13)$$

which requires the solution of two linear systems with the sparse, symmetric, invertible matrix \underline{M} . It is the systems $\underline{M}\underline{z} = \underline{u}$ and $\underline{M}\underline{z} = \underline{b}$ to which Craig's preconditioned conjugate gradient algorithm is actually applied.

The only remaining detail is the choice of the preconditioning matrix \underline{Q} . \underline{Q} is taken as the modified Cholesky decomposition of \underline{M} , as described by Gill and Murray¹³. If \underline{M} is positive definite and well conditioned, $\underline{Q} = \underline{M}$. Otherwise, \underline{Q} is a well conditioned positive definite approximation to \underline{M} . The Gill-Murray factorization algorithm can exploit the symmetry and sparse skyline structure of \underline{M} , and this entire scheme, Eqs. (10-13), is built around using the symmetry and sparse skyline structure of the Jacobian matrix $\underline{D}_x \underline{F}$.

DESCRIPTION OF THE HYBRID METHOD

The hybrid algorithm begins as a quasi-Newton (QN) algorithm utilizing the double dogleg strategy⁷ with an assumed or specified size of

the load or time step. If lack of sufficient progress by the QN algorithm is detected, say if the function $f = 1/2 \underline{F}^T \underline{F}$ does not decrease by 200% in 5 iterations, the size of the load step is reduced by a factor of 5 and the QN algorithm is tried again. If it still fails to make sufficient progress, then this is taken to be an indication that the Jacobian matrices are badly conditioned because of the vicinity of critical points (bifurcation or limit points). The QN algorithm is abandoned at such a point and the modified homotopy method is initiated. The homotopy method structured to exploit the sparsity of the Jacobian matrix is initiated and continued beyond the critical point, where the quasi-Newton method can be reinitiated. Recall that the quasi-Newton method used here is one which requires only that the Jacobian matrix be nonsingular and well conditioned, not necessarily positive definite.

The criterion for switching from the homotopy algorithm back to the QN algorithm is that at least 10 steps of the ODE algorithm applied to (8) have been taken (this prevents chattering back and forth between the homotopy and QN algorithms), and

$$|d\lambda/ds| \geq .5/\sqrt{n+1}. \quad (14)$$

This latter condition effectively guarantees that the first n columns of the Jacobian matrix \underline{DF} are sufficiently independent, so the QN algorithm, when restarted, should be successful. Note that the homotopy algorithm is predicated on $\text{rank } \underline{DF} = n$, which is not true at bifurcation points, and thus the homotopy algorithm has no theoretical basis near bifurcation points. In practice, however, the ODE algorithm tends to step past bifurcation points and continue on the primary branch (with a

loss in accuracy, though). Rank $\underline{DF} = n$ at limit points, and they can be calculated very accurately by the homotopy method with no difficulty.

VALIDATION OF THE HYBRID METHOD

The method just described is validated on the rather simple problem of the snap-through response of a shallow arch, shown in Figure 1. The co-rotational formulation¹² is used for the kinematic description of the frame element modeling the arch. For response prediction the quasi-Newton method is initiated with a constant load step of 400 lb. The eighth load step indicated that the QN algorithm was not making satisfactory progress in spite of cutting down the load step by a factor of 5. This was taken to be an indication of the existence of a critical point in the vicinity. The homotopy method was therefore initiated from the end of the seventh step using the displacement vector \underline{x}_7 and the tangent vector $(\underline{v}, -1)$ at the end of the seventh step. The vector \underline{v} is obtained by the solution of the equations

$$[\underline{J}(\underline{x}_7)]\underline{v} = \{P_7\}. \quad (15)$$

The decomposition of \underline{J} required for the above solution was available from the quasi-Newton solution at the end of the seventh load step. λ was interpreted as the parameter on the loading distribution at the end of the seventh load step and was accordingly set to unity. The homotopy method was carried past the point where

$$\left| \frac{d\lambda}{ds} \right| \geq 0.5/\sqrt{n+1}. \quad (16)$$

$d\lambda/ds$ is obtained from the unit tangent vectors $(d\underline{x}/ds, d\lambda/ds)$ which the homotopy method calculates. To ensure a good conditioning of the Jacobian matrix it is necessary to integrate Eqs. (8) well past the critical point. Using the displacement vector, the Jacobian matrix and the sign of $d\lambda/ds$ at the end of such an integration point the quasi-

Newton method is reinitiated. The sign of $d\lambda/ds$ tells us whether the load parameter is to be increased or decreased on subsequent steps. The QN method is continued on the unstable branch of the response curve until it fails to make satisfactory progress in spite of a reduction of the load step. The homotopy method is then initiated until condition (16) is again satisfied at which point the QN method is reinitiated.

The success of the hybrid method on problems much more complicated than the one shown in Figure 1 remains to be demonstrated. However, no difficulties are anticipated other than the necessity of refining criteria for the detection of transition points between the quasi-Newton and homotopy methods.

REFERENCES

- [1] - Wempner, G. A., "Discrete Approximations Related to Nonlinear Theories of Solids", International Journal of Solids and Structures, 7, 1581-1599, 1971.
- [2] - Riks, E., "An Incremental Approach to the Solution of Snapping and Buckling Problems", International Journal of Solids and Structures, 15, 529-551, 1979.
- [3] - Crisfield, M. A., "Incremental/Iterative Solution Procedures for Nonlinear Structural Analysis", International Conference in Numerical Methods for Nonlinear Problems, Swansea, 261-290, 1980.
- [4] - Padovan, J., "Self-Adaptive Predictor-Corrector Algorithm for Static Nonlinear Structural Analysis", NASA CR-165410, 1981.
- [5] - Kamat, M. P., L. T. Watson, and V. B. Venkayya, "A Quasi-Newton versus a Homotopy Method for Nonlinear Structural Analysis", Journal of Computers and Structures, 17, 579-585, 1983.
- [6] - Watson, L. T. and D. Fenner, "Chow-Yorke Algorithm for Fixed Points or Zeros of C^2 Maps", Association for Computing Machinery Transactions on Mathematical Software, 6, 252-260, 1980.
- [7] - Dennis, J. E. and R. Schnabel, Numerical Methods for Unconstrained Optimization and Nonlinear Equations, Prentice-Hall, Engelwood Cliffs, NJ, 1983.
- [8] - Watson, L. T., "Fixed Points of C^2 Maps", Journal of Computational and Applied Mathematics, 5, 131-140, 1979.
- [9] - Watson, L. T., "A Globally Convergent Algorithm for Computing Fixed Points of C^2 Maps", Applied Mathematics and Computation, 5, 297-311, 1979.
- [10] - Hestenes, M. R., "The Conjugate Gradient Method for Solving Linear Systems," in Proceedings of the Symposium in Applied Mathematics, 6, Numerical Analysis, AMS, New York, 83-102, 1956.
- [11] - Fadeev, D. K. and V. N. Fadeeva, Computational Methods of Linear Algebra, Freeman, London, 1963.
- [12] - Kamat, M. P., "Nonlinear Transient Analysis by Energy Minimization - Theoretical Basis for the ACTION Computer Code", NASA CR-3287, 1980.
- [13] - Gill, P. E., and W. Murray, "Newton Type Methods for Unconstrained and Linearly Constrained Optimization," Mathematical Programming, 7, 311-350, 1974.

APPENDIX

Quadratic Model

Newton's method for unconstrained minimization essentially approximates the multivariate function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ about a point \underline{x}_c by a quadratic model of the type

$$m_c(\underline{x}_+) = m_c(\underline{x}_c + \underline{S}) = f(\underline{x}_c) + \underline{S}^t \nabla f(\underline{x}_c) + \frac{1}{2} \underline{S}^t \underline{H}_c \underline{S}, \quad (\text{A-1})$$

where $\underline{S} = (\underline{x}_+ - \underline{x}_c)$ and \underline{H}_c is an approximation to the Hessian of f which is coerced to be positive definite if not already so.

To render Newton's method globally convergent, sufficiently large decreases in f values must be achieved for the step lengths taken. This can be expected to be satisfied if the following definition of acceptability of an iterate \underline{x}_+ is adopted:

$$f(\underline{x}_+) \leq f(\underline{x}_c) + \alpha \nabla f(\underline{x}_c)^t (\underline{x}_+ - \underline{x}_c) \quad (\text{A-2})$$

with $\alpha = 10^{-4}$.

There is a certain region within which the quadratic model m_c can be trusted to adequately approximate the function f . Let δ_c denote the radius of such a trust region around the current point \underline{x}_c . If the trust region is large enough, that is if

$$\delta_c \geq \| \underline{S}_c^N \|_2, \quad (\text{A-3})$$

where $\| \underline{S}_c^N \|_2$ is the distance to the Newton point from the current point \underline{x}_c , then the Newton step is taken since the Newton point is the global minimizer of m_c . In other words

$$\underline{S}_c^N = - \underline{H}_c^{-1} \nabla f(\underline{x}_c), \quad (\text{A-5})$$

$$\underline{x}_+ = \underline{x}_c + \underline{S}_c^N. \quad (\text{A-6})$$

However, if the trust region radius δ_C is less than the magnitude of the Newton step, then the direction \underline{S} is the optimum solution of the constrained problem

$$\text{Minimize } m_C(\underline{x}_C + \underline{S}), \quad (\text{A-7})$$

$$\text{such that } \|\underline{S}\| \leq \delta_C. \quad (\text{A-8})$$

From the theory of constrained optimization, the necessary and sufficient conditions for an optimum are given by

$$\underline{S} = \underline{S}(\mu) = -(\underline{H}_C + \mu \underline{I})^{-1} \underline{\nabla} f(\underline{x}_C), \mu > 0 \quad (\text{A-9})$$

$$\text{such that } \|\underline{S}(\mu)\| = \delta_C;$$

$$\text{or } \underline{S} = \underline{S}(0) = \underline{S}_C^N, \mu = 0 \quad (\text{A-10})$$

$$\text{such that } \|\underline{S}(0)\| \leq \delta_C.$$

Thus the curve $\underline{S}(\mu)$ shown in Figure 2 is a curve that runs smoothly from the Newton step when $\mu = 0$ to

$$\underline{S}(\mu) \approx -\frac{1}{\mu} \underline{\nabla} f(\underline{x}_C) \quad (\text{A-11})$$

when μ gets large. In other words, the solution to Eqs. (A-7) and (A-8) when δ_C is very small is a step length δ_C approximately in the steepest descent direction. An exact solution of Eqs. (A-7) and (A-8) to determine a direction \underline{S} requires what is known as the model trust region approach utilizing methods requiring approximately $O(n^3)$ operations. The double dogleg strategy provides an approximate solution of Eqs. (A-7) and (A-8) which is not much inferior to the exact solution but at a substantially reduced computational effort - approximately $O(n^2)$ operations after \underline{S}_C^N has been calculated.

Double Dogleg Strategy

The double dogleg (see Fig. 2) is an approximation to the $\underline{S}(\mu)$ curve that must have two of its properties: namely that the distance

from the current point \underline{x}_C increases monotonically and the value of the quadratic model function also decreases monotonically along the double dogleg. The elbows of the double dogleg are chosen to guarantee these properties. The first elbow of the double dogleg is chosen to be the Cauchy point of the quadratic model. Thus

$$\underline{x}_{cp} = \underline{x}_C + \underline{S}_{cp}, \quad (A-12)$$

where

$$\underline{S}_{cp} = -\lambda \nabla f(\underline{x}_C), \quad (A-13)$$

$$\lambda = \frac{\|\nabla f(\underline{x}_C)\|^2}{\nabla f(\underline{x}_C)^T \underline{H}_C \nabla f(\underline{x}_C)}. \quad (A-14)$$

A point \underline{x}_N is then chosen along the Newton direction such that the two desired properties of the double dogleg are satisfied. The point \underline{x}_N is chosen as (following reference [7])

$$\underline{x}_N = \underline{x}_C + \eta \underline{S}_C^N \quad (A-15)$$

where

$$\eta = 0.8v + 0.2, \quad (A-16)$$

v being a quantity determined from the relation

$$\|\underline{S}_{cp}\| \leq v \|\underline{S}_C^N\| \leq \|\underline{S}_C^N\| \quad (A-17)$$

and given by

$$v = \frac{\|\nabla f(\underline{x}_C)\|^4}{(\nabla f(\underline{x}_C)^T \underline{H}_C \nabla f(\underline{x}_C)) (\nabla f(\underline{x}_C)^T \underline{H}_C^{-1} \nabla f(\underline{x}_C))}. \quad (A-18)$$

The point \underline{x}_N is the second elbow of the double dogleg.

The next iterate \underline{x}_+ is then given by a point between \underline{x}_{cp} and \underline{x}_N such that $\|\underline{x}_+ - \underline{x}_C\| = \delta_C$. That is,

$$\underline{x}_+ = \underline{x}_C + \underline{S}_{cp} + \theta(\underline{x}_N - \underline{x}_{cp}), \quad (A-19)$$

where θ is chosen such that

$$\|\underline{S}_{cp} + \theta(\underline{x}_N - \underline{x}_{cp})\| = \delta_C. \quad (A-20)$$

For \underline{x}_+ to be an acceptable point it has to satisfy Eq. (A-2). If (A-2) is not satisfied the trust region radius must be reduced. The new trust region radius is determined by a quadratic backtracking strategy utilizing $f(\underline{x}_C)$, $f(\underline{x}_+)$ and the directional derivative $\nabla f(\underline{x})^t(\underline{x} - \underline{x}_C)$ to fit a parabola, and then taking the new trust region radius as the minimum of this parabola. The new trust region radius is given by

$$\delta_C := - \delta_C \frac{\nabla f(\underline{x}_C)^t(\underline{x}_+ - \underline{x}_C)}{2[f(\underline{x}_+) - f(\underline{x}_C) - \nabla f(\underline{x}_C)^t(\underline{x}_+ - \underline{x}_C)]} . \quad (\text{A-21})$$

If \underline{x}_+ passes the acceptability test (A-2), then a check is made to determine how well the quadratic approximation is modeling the function f and whether a larger step from \underline{x}_C using the current quadratic model should be attempted. The trust region radius is repeatedly doubled and new points \underline{x}_+ computed until either the acceptability test (A-2) fails or m_C no longer models f well. When finally an acceptable \underline{x}_+ has been found, the quadratic model must be redefined utilizing \underline{H}_+ or an approximation to it. The new trust region radius is determined as follows:

if $|\Delta f| \geq 0.75 |\Delta f_{\text{pred}}|$, set $\delta_+ = 2\delta_C$;
 if $|\Delta f| < 0.1 |\Delta f_{\text{pred}}|$, set $\delta_+ = \delta_C/2$;
 else set $\delta_+ = \delta_C$;

where

$$\Delta f = f(\underline{x}_+) - f(\underline{x}_C) , \quad \Delta f_{\text{pred}} = m_C(\underline{x}_+) - f(\underline{x}_C).$$

This completes the discussion of the double dogleg strategy. Interested readers should consult reference [7] for additional details.

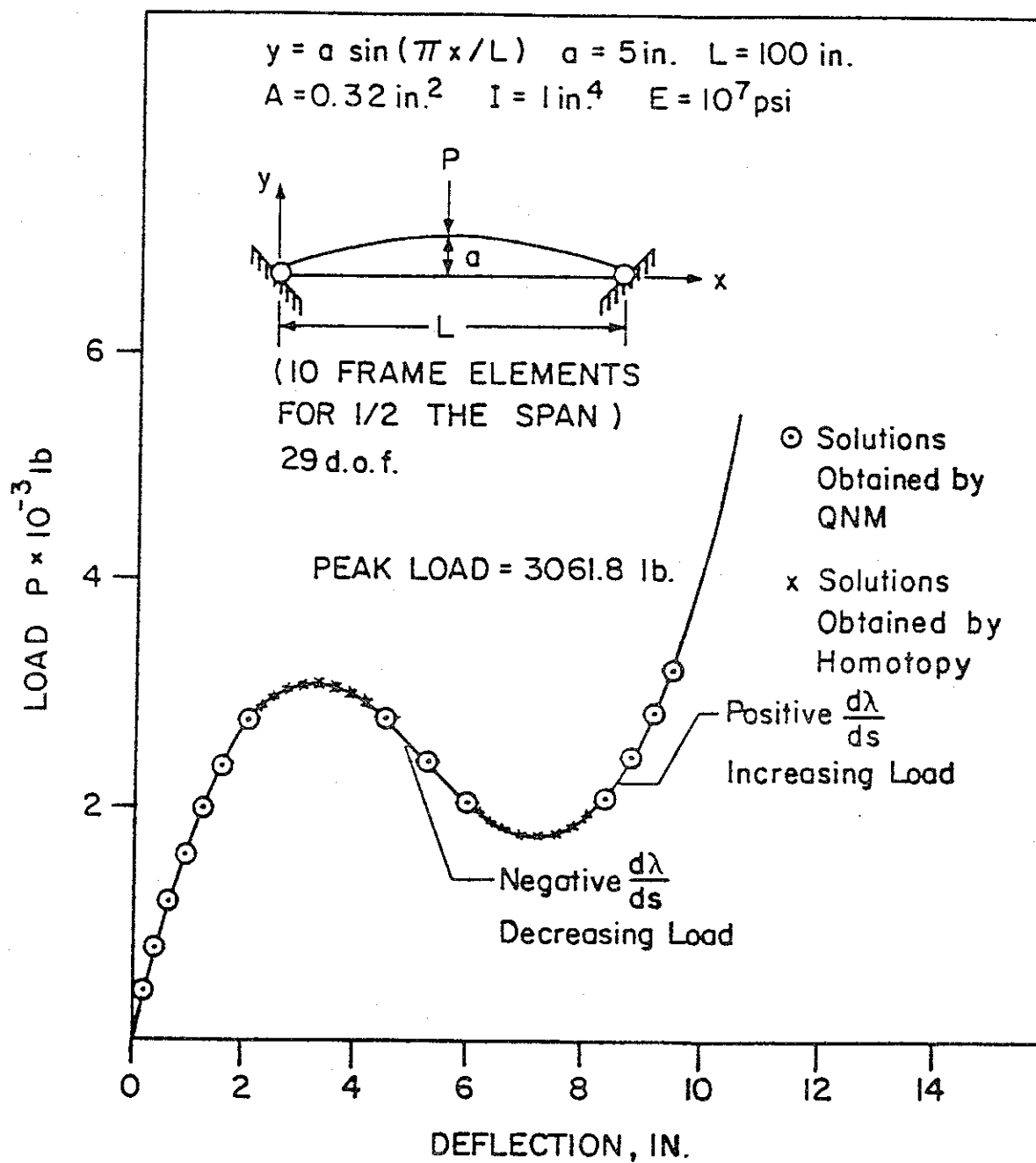


Figure 1.

FIGURE LEGEND

Figure No.

Title

1. Snap-Through Response of a Shallow Arch
2. Geometry of The Double Dogleg Step

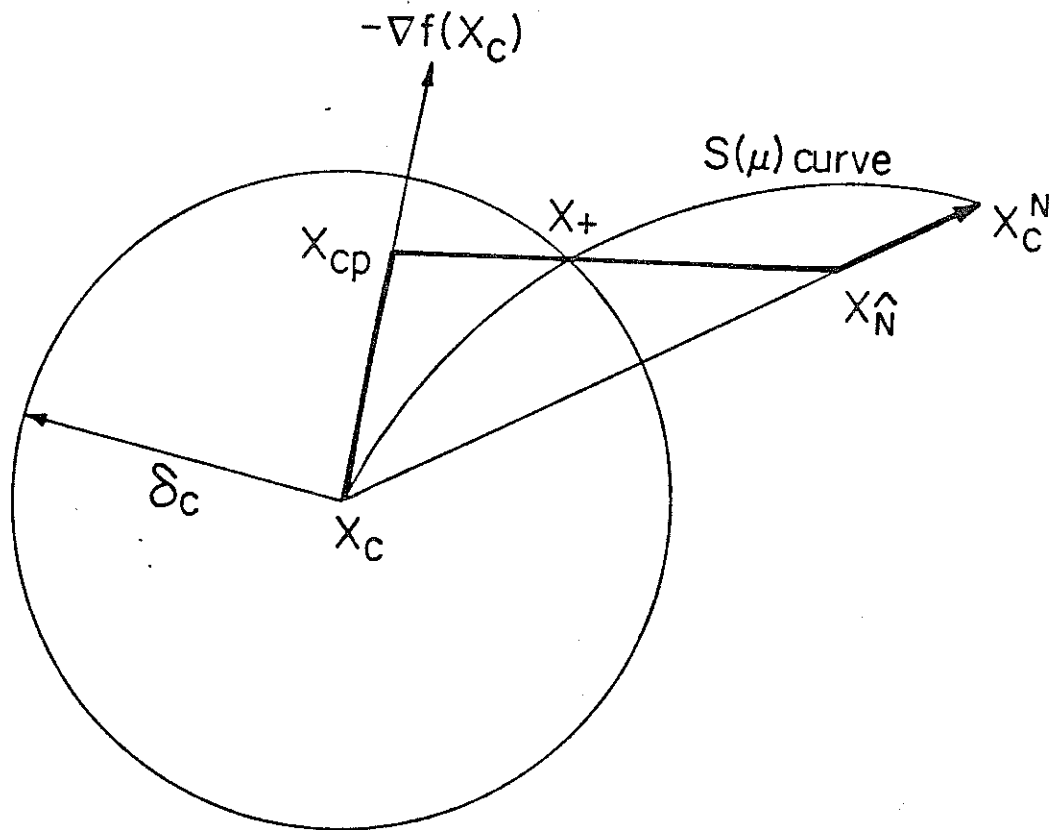


Figure 2.