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Least-Change Secant Updates of Non-Square Matrices

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LEAST-CHANGE SECANT UPDATES OF
NON-SQUARE MATRICES

by

Samih Kassem Bourji

A dissertation submitted in partial fulfillment
of the requirements for the degree
of
DOCTOR OF PHILOSOPHY
in
Mathematics

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I wish to express my appreciation to Professor Homer Walker for his continual support and encouragement. I have to admit that if it were not for his confidence in my ability and the many hours he spent advising me, this work would have never been finished.

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Samih K. Bourji
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In many problems involving the solution of a system of nonlinear equations, it is necessary to keep an approximation to the Jacobian matrix which is updated at each iteration. Computational experience indicates that the best updates are those that minimize some reasonable measure of the change to the current Jacobian approximation subject to the new approximation obeying a secant condition and perhaps some other approximation properties such as symmetry.

All of the updates obtained thus far deal with updating an approximation to an nxn Jacobian matrix. In this thesis we
consider extending most of the popular updates to the non-square case. Two applications are immediate: between-step updating of the approximate Jacobian of $f(X,t)$ in a non-autonomous ODE system, and solving nonlinear systems of equations which depend on a parameter, such as occur in continuation methods. Both of these cases require extending the present updates to include the $nx(n+1)$ Jacobian matrix, which is the issue we address here. Our approach is to stay with the least change secant formulation. Computational results for these new updates are also presented to illustrate their convergence behavior.

(74 pages)
CHAPTER I

INTRODUCTION

Many problems require the numerical solution of a system of nonlinear equations in $n$ unknowns:

(1.1) Given $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, find $X_*$ such that $F(X_*) = 0$.

For example, (1.1) arises in optimization problems, in which $F$ is the gradient of some function $f$ to be optimized, and in finding equilibrium points of nonlinear systems. Newton's method is an iterative method which proceeds at each iteration from an estimate $X$ of $X_*$ to a perhaps better estimate $X_+$. At each step one is required to evaluate the Jacobian $J(X)$ of $F(X)$. In many cases, calculation of $J(X)$ or its approximation by finite differences is either impossible, prohibitively expensive or very prone to human error. Then one tries to obtain an approximation to $J$ and updates the approximation as the iterations proceed. The resulting method is called a quasi-Newton method.

The last two decades have seen great progress in this area. Excellent surveys can be found in Dennis - Schnabel [5], Fletcher [8] and Gill - Murray - Wright [10]. All of the existing methods deal with the problem of updating a square matrix $A$ to a new update $A_+$ where $A_+$ is the "closest" matrix to $A$ subject to a secant condition and perhaps some other approximation properties.
Newton's method and quasi-Newton methods may fail to converge from bad starting points. Global strategies were developed [5],[10], [16] to improve the convergence behavior of these algorithms. Of these strategies, the Powell dogleg method was implemented in MINPACK. But even with this global method MINPACK fails on some problems, see [18].

Globally convergent homotopy algorithms were developed in 1976, see [18] and [19]. These are algorithms for solving nonlinear systems of (algebraic) equations which are convergent for almost all choices of the starting point. Thus they are globally convergent with probability one. In homotopy algorithms F is usually embedded in a map \( \rho \). For example,
\[
(1.2) \quad \rho(X,\lambda) = \lambda F(X) + (1 - \lambda)(X - a)
\]
where \( \lambda \in \mathbb{R}, X, a \in \mathbb{R}^n \). Obviously, \( \rho(X,0) = 0 \) is trivial to solve and the solution to \( \rho(X,1) = 0 \) is that of \( F(X) = 0 \).

The Jacobian of \( \rho \), \( D\rho = \left[ \frac{\partial \rho}{\partial X}, \frac{\partial \rho}{\partial \lambda} \right] = \left[ J, b \right] \), is clearly not a square matrix but rather an \( nx(n+1) \) matrix which we would like to update at each step of the iteration process.

Another interesting application involving non-square matrices is in the numerical solution of ordinary differential equations (ODE). Consider an initial value problem for an ODE system
\[
(1.3) \quad Y' = f(t,Y), \quad Y(t_0) = Y_0
\]
where \( Y \) and \( f(t,Y) \) are in \( \mathbb{R}^n \). Suppose we employ the backward
differentiation formula (BDF) methods to solve (1.3). In these methods one is asked to solve

\[
Y_n = \sum_{j=1}^{q} \alpha_j Y_{n-j} + h \beta_0 f(t_n, Y_n)
\]

where \( Y_k \) denotes the approximation to \( Y(t_k) \), \( h = t_k - t_{k-1} \) and \( q \) is the method order. The \( \alpha_j \)'s and \( \beta_0 \) are parameters. The BDF methods given by (1.4) have \( \beta_0 > 0 \). Thus they are implicit, and at each time step, one must solve a generally nonlinear algebraic system

\[
0 = F_n(Y_n) = Y_n - h \beta_0 f(t_n, Y_n) - \gamma_n
\]

\[
\gamma_n = \sum_{j=1}^{q} \alpha_j Y_{n-j}
\]

One way to solve (1.5) is to find a prediction \( Y_n(0) \) using an explicit formula and then correct using Newton's method, namely,

\[
P_n(Y_{n+1} - Y_n) = -F_n(Y_n)
\]

where \( P_n \) is an approximation of the Jacobian \( \frac{\partial F_n}{\partial Y_n} \), i.e.,

\[
P_n \approx \frac{\partial F_n}{\partial Y_n} = I - h \beta_0 J(t_n, Y_n)
\]

The solution of (1.6) over a number of time steps can be quite costly in practice, so quasi-Newton methods can be implemented to
maintain the approximate Jacobian \( P_n^m \) \( \approx \frac{\partial F_n}{\partial Y_n} \). If the ODE system is autonomous, then such updating is straightforward. If the ODE system is not autonomous, however, then the updating will be based on function values at two different values of \( t \) and the Jacobian would be \( \left[ \frac{\partial F}{\partial Y}, \frac{\partial F}{\partial t} \right] \), which is not a square matrix. Thus again we will need a non-square matrix updating method.

In quasi-Newton methods, in the square case, one updates the Jacobian \( J \), as the iterations proceed from \( X \) to \( X_+ \), subject to a secant condition

\[
J_+ S = Y
\]

where \( S = X_+ - X \) and \( Y = F(X_+) - F(X) \) and \( J_+ \) is taken as an approximation to \( J(X_+) \).

As mentioned before, all the existing methods deal with updating a square Jacobian. In this thesis, we extend the least-change secant principle (see [4] and [6]) to the \( n \times (n+1) \) Jacobian. At each step we have \( S \in \mathbb{R}^{n+1} \) and \( Y \in \mathbb{R}^n \), and for \( n \times n \) \( J \) and \( b \in \mathbb{R}^n \), we require an update \( [J_+, b_+] \) of \( [J, b] \) to satisfy a secant-like condition

\[
[ J_+, b_+ ] S = Y
\]

subject to an extended least-change principle.

We extend the first Broyden and the second Broyden updates in
which the Jacobian only has to satisfy the secant condition (1.4). We will also extend the Powell - symmetric - Broyden update in which we add the requirement that the J part of the Jacobian is to be symmetric. A formula for an extension of the sparse secant update will be presented. Also, the Davidon - Fletcher - Powell and the Broyden - Fletcher - Goldfarb - Shanno updates will be extended to the non-square case.

The updates are presented and derived independently of the algorithms that might employ them. So, they can be used in an algorithm using continuation methods such as HOMPACK or one that tries to obtain a between-step update of the Jacobian of \( f(t, X) \) in an ODE system or any other application that may come up. In Chapter 2, we review some background material on least-change secant updates. In Chapter 3 we formulate the extensions mentioned above. In Chapter 4 we test the updates in HOMPACK, a mathematical software package which deals directly with homotopy methods.
Consider the problem of finding \( x^* \in \mathbb{R}^n \) that solves
\[
(2.1) \quad F(x) = 0 ; \quad F : \mathbb{R}^n \rightarrow \mathbb{R}^n
\]
Problem (2.1) is usually solved using some iterative scheme, which starts with initial guess \( x_0 \) and produces better approximants \( \{ x_k \} \) to \( x^* \). In this chapter we will investigate the best-known such methods, namely Newton's method and some of its variants known as quasi-Newton methods.

**Notation**: Let \( \mathbb{R}^n \) denote the space of column vectors of \( n \) components and \( L(\mathbb{R}^m, \mathbb{R}^n) \) the space of matrices with \( n \) rows and \( m \) columns. In the case when \( n=m \) we will use \( L(\mathbb{R}^n) \) instead of \( L(\mathbb{R}^n, \mathbb{R}^n) \). We let \( M_{ij} \) denote the \( ij \)th entry of the matrix \( M \) and \( V_i \) the \( i \)th component of the vector \( V \). We denote general, unspecified norms by \( |.| \). The norms most useful here are the Frobenius norm, denoted by \( |.|_F \) and defined as
\[
|M|_F = \left( \sum_{i=1}^{n} \sum_{j=1}^{m} (M_{ij})^2 \right)^{1/2}
\]
for any \( M \in L(\mathbb{R}^m, \mathbb{R}^n) \); the weighted Frobenius norm \( |.|_{Q,P} = |QMP|_F \), where \( Q \in L(\mathbb{R}^n), P \in L(\mathbb{R}^m) \), \( Q \) and \( P \) are non-singular; and the \( l_2 \) norm denoted by \( |.|_2 \).
In Newton's method one is given an \( X_0 \in \mathbb{R}^n \) and generates the sequence \( \{ X_k \} \) by

For \( k = 0,1,2, \ldots \)

Solve \( J(X_k) S_k = -F(X_k) \)

Set \( X_{k+1} = X_k + S_k \)

where \( J(X_k) \) denotes the Jacobian of \( F \) at \( X_k \). For the purpose of analyzing the algorithms for solving \( F(X) = 0 \), the mapping \( F \) is assumed to have the following properties:

a) The mapping \( F \) is continuously differentiable in an open convex set \( D \).

b) There is an \( X_\ast \in D \) such that \( F(X_\ast) = 0 \) and \( J(X_\ast) \) is non-singular.

In addition to (2.2) sometimes we will need the stronger requirement that \( J \) satisfies a Lipschitz condition at \( X_\ast \): There is a constant \( L \) such that

\[
(2.3) \quad |J(X) - J(X_\ast)| \leq L |X - X_\ast|
\]

The proof of the following well-known result can be found in most books on numerical analysis, e.g., Ortega and Rheinboldt [13]

**Theorem 2.1** Let \( F : \mathbb{R}^n \longrightarrow \mathbb{R}^n \) satisfy assumptions (2.2). Then there is an open set \( O \) which contains \( X_\ast \) such that for any \( X_0 \in O \) the Newton iterates are well-defined, remain in \( O \) and converge to \( X_\ast \). Moreover, there is a sequence \( \{ \alpha_k \} \) which converges to zero
such that

\[(2.4) \quad \left| x_{k+1} - x^*_k \right| \leq \alpha_k \left| x_k - x^*_k \right| \quad k = 0,1,2,\ldots \]

If, in addition, \( F \) satisfies \((2.3)\) then there is a constant \( \beta \) such that

\[(2.5) \quad \left| x_{k+1} - x^*_k \right| \leq \beta \left| x_k - x^*_k \right|^2 \quad k = 0,1,2,\ldots \]

Although very attractive to work with, Newton's method is often not convenient, as evaluating \( J(X_k) \) at each step requires the evaluation of up to \( n^2 \) scalar functions, which could be very costly. Also solving \( J(X_k) S_k = -F(X_k) \) requires up to \( O(n^3) \) arithmetic operations. An alternative is to replace \( J(X_k) \) by some approximation \( B_k \) such that \( B_k \) is easy to evaluate and \( B_k S_k = -F(X_k) \) can be solved cheaply. A method employing such a technique is called a quasi-Newton method.

Suppose at the current step we have \( X_c \) and \( B_c \), an approximation to \( J(X_c) \); then we can solve for \( S_c \) by \( B_c S_c = -F(X_c) \) and set \( X_+ = X_c + S_c \). Now to solve for the next iterate \( X_{++} \) we need \( B_+ \), an approximation to \( J(X_+) \). If we set \( Y_c = F(X_+) - F(x_c) \), a generalization of the secant method would require \( B_+ \) to satisfy

\[(2.6) \quad B_+ S_c = Y_c. \]

Equation \((2.6)\) will be referred to as the secant condition. Since the secant condition does not uniquely determine \( B_+ \), Broyden
[1] suggested a method of choosing $B_+$ as a rank-1 update of $B$ which later was shown to be the unique matrix that solves

$$\min \ | \ \overline{B} - B_c \ |_F \ \text{subject to} \ \overline{B} S_c = Y_c$$

$\overline{B} \in L(\mathbb{R}^n)$

**Theorem 2.2** Let $B_c \in L(\mathbb{R}^n)$, $S, Y \in \mathbb{R}^n$ with $S \neq 0$. Then the unique solution to

$$\min \ | \ \overline{B} - B_c \ |_F \ \text{subject to} \ \overline{B} S = Y$$

$\overline{B} \in L(\mathbb{R}^n)$

\begin{equation}
B_+ = B_c + \frac{(Y - B_c S) S^T}{S S^T}
\end{equation}

**Proof:** See [4].

Equation (2.8) is referred to as the least-change secant update. The word update indicates that the we are not approximating $J(X_+)$ from scratch, rather we are updating the approximation $B_c$ to $J(X_c)$ into an approximation $B_+$ to $J(X_+)$. Since one is trying to solve $S_c = -B_c^{-1} F(x_c)$, it would be reasonable to update $B_c^{-1}$, rather than $B_c$, by choosing $B_+^{-1}$ to be the unique matrix that solves

$$\min \ | \ \overline{B}^{-1} - B_c^{-1} \ |_F \ \text{subject to} \ \overline{B} S_c = Y_c$$

$\overline{B}^{-1} \in L(\mathbb{R}^n)$

which would yield
(2.10,a) \[ \mathbf{B}_+^{-1} = \mathbf{B}_c^{-1} + \frac{(\mathbf{S} - \mathbf{B}_c^{-1} \mathbf{Y}_c) \mathbf{Y}_c^T}{\mathbf{Y}_c^T \mathbf{Y}} \]

or

(2.10,b) \[ \mathbf{B}_+ = \mathbf{B}_c + \frac{(\mathbf{Y} - \mathbf{B}_c \mathbf{S}) \mathbf{Y}_c^T \mathbf{B}_c}{\mathbf{Y}_c^T \mathbf{B}_c \mathbf{S}} \]

Update (2.10,b) can be obtained from update (2.10,a) by the Sherman–Morrison–Woodbury formula, clearly a different update from the one given by (2.8). This update was also suggested by Broyden [1]. As it happens, (2.8) usually perform better in practice than (2.10). Consequently, (2.8) and (2.10) are known colloquially as the good and the bad Broyden updates, respectively, and more politely as the first and second Broyden updates.

Suppose that the Jacobian matrix has some special property such as symmetry or a known pattern of sparsity. It would seem reasonable to require the updates to have that special property. Assume such matrices form an affine set \( \mathcal{A} \subseteq \mathbb{L}(\mathbb{R}^n) \); also let

\[ \mathbb{Q}(\mathbf{Y}, \mathbf{S}) = \{ \mathbf{M} \in \mathbb{L}(\mathbb{R}^n) : \mathbf{M} \mathbf{S} = \mathbf{Y} \} \]

If \( \mathcal{A} \cap \mathbb{Q}(\mathbf{Y}, \mathbf{S}) \neq \emptyset \), then a least-change secant update \( \mathbf{B}_+ \) is the element of \( \mathcal{A} \cap \mathbb{Q}(\mathbf{Y}, \mathbf{S}) \) which is the closest to \( \mathbf{B}_c \) in an inner-product norm \( \| \cdot \| \). In the event the two spaces \( \mathcal{A} \) and \( \mathbb{Q}(\mathbf{Y}, \mathbf{S}) \) are disjoint we require the least-change secant update to be as close to \( \mathbb{Q}(\mathbf{Y}, \mathbf{S}) \) as possible while remaining in \( \mathcal{A} \). For that let us
define for two affine spaces \( A_1 \) and \( A_2 \)

\[
M(A_1, A_2) = \{ M \in A_1 : |M - A_2| = |A_1 - A_2| \}
\]

for some inner-product norm \( |.| \), where \( |M - A_1| \) is the distance from \( M \) to \( A_1 \) defined by

\[
|M - A_1| = \inf \{ |M - N| : N \in A_1 \}
\]

and \( |A_1 - A_2| \) is the distance between \( A_1 \) and \( A_2 \) defined by

\[
|A_1 - A_2| = \inf \{ |M - A_2| : M \in A_2 \}.
\]

So, we are interested in solving

\[
(2.11) \quad \min_{B \in M(A, Q(Y, S))} |\overline{B} - B|_F
\]

Note that if \( A \cap Q(Y, S) \neq \emptyset \) then \( M(A, Q(Y, S)) = A \cap Q(Y, S) \)

Unless otherwise specified, \( P \) with a subscript will denote the orthogonal projection with respect to an inner-product norm onto the affine space specified by the subscript, while a superscript \( \perp \) will denote the projection orthogonal to it.

**Theorem 2.3**: Let \( A \) be an affine subset of \( L(\mathbb{R}^n) \) and \( B \in A \). The unique solution to

\[
\min_{\overline{B} \in M(A, Q(Y, S))} |\overline{B} - B|
\]

is given by

\[
(2.12) \quad \overline{B} = \lim_{k \to \infty} (P A Q(Y, S))^K B
\]

**Proof**: See [4].
Powell [14] showed if $A = S$ is the space of symmetric matrices, $B \in S$, and the norm is the Frobenius norm, then

\[(2.13) \quad B_+ = \lim_{k \to \infty} \left( P_S P_Q(Y, S) \right)^k B \]

\[= B + \frac{(Y - BS)S^T + S(Y - BS)^T}{S^T S} - \frac{S^T(Y - BS)S S^T}{(S^T S)^2} \]

Equation (2.13) is referred to as the Powell symmetric Broyden (PSB) update. Also, Greenstadt [12] showed

\[(2.14) \quad B^{-1}_+ = \lim_{k \to \infty} \left( P_S P_Q(S, Y) \right)^k B^{-1} \]

\[= B^{-1} + \frac{(S - B^{-1} Y)Y^T + Y(S - B^{-1} Y)^T}{Y^T Y} - \frac{Y^T(S - B^{-1} Y)YY^T}{(Y^T Y)^2} \]

Theorem 2.4: Let $S, Y \in \mathbb{R}^n$ with $S \neq 0$ and let $A$ be an affine subspace of $L(\mathbb{R}^n)$ with $S$ its parallel subspace. Let $P$ be the $n \times n$ matrix whose $j$th column is $P_S(\varepsilon_j S^T / S^T S) S$, where $\varepsilon_j$ is the $j$th unit coordinate vector in $\mathbb{R}^n$. Let $B \in A$. If $v$ is any solution to

\[(2.15) \quad \min \left| P v - (Y - BS) \right|_2 \]

or equivalently to

\[(2.16) \quad \min \left| P \left( \frac{v S^T}{S S S^T} \right) - (Y - BS) \right|_2 \]

\[(2.17) \quad B = B + P \left( \frac{v S^T}{S S S^T} \right) \]

Proof: See [4].

The above theorem provides an easy tool to evaluate most of the well-known least change secant updates. As an example, let $A$
be the space of sparse matrices with a special pattern of sparsity, say, if \( M \in \mathcal{A} \) then \( M \) has the sparsity pattern of some \( X \in L(\mathbb{R}^n) \). Since \( \mathcal{A} \) is a subspace we have \( S = \mathcal{A} \). We define:

\[ Z : L(\mathbb{R}^n) \rightarrow L(\mathbb{R}^n) \]

\[ (Z(M))_{ij} = \begin{cases} 0 & , X_{1j} = 0 \\
M_{ij} & , X_{1j} \neq 0 
\end{cases} i,j = 1,2,...,n \]

Also let \( S_{-j} \) be the vector formed from \( S \) by setting \( S_{1j} \) to zero if \( X_{1j} = 0 \).

Then we have \( P S M = Z( M ) \), for any \( M \in L(\mathbb{R}^n) \), so the \( j^{th} \) column of \( P \) is \( Z( \varepsilon_j S^T / S^T S ) S = ( S_{-j}^T S / S^T S ) \varepsilon_j \). Then,

\[ P = (1 / S^T S) \text{ diag } (S_{11}^T S, S_{22}^T S, \ldots, S_{nn}^T S) = \frac{1}{S^T S} D \text{. Thus,} \]

\[ v = S^T S \sum_{j=1}^{n} (S_{-j}^T S)^+ \varepsilon_j^T (Y - BS) \varepsilon_j \]

\[ = (S^T S) D^+ (Y - BS) \]

is a least-square solution to (2.15). Here \( a^+ = a^{-1} \) if \( a \neq 0 \) and \( 0^+ = 0 \), and for \( D = \text{ diag } (d_1, d_2, \ldots, d_n) \), \( D^+ = \text{ diag } (d_1^+, d_2^+, \ldots, d_n^+) \). Therefore, \( B_+ = B + Z( v S^T / S^T S ) \)

\[ = B + Z \left( \sum_{j=1}^{n} (S_{-j}^T S)^+ \varepsilon_j^T (Y - BS) \varepsilon_j S^T \right) \]
Thus,

\[
B_+ = B + \sum_{j=1}^{P} (S_j^T S_j)^+ \varepsilon_j^T (Y - BS) \varepsilon_j S_j^T
\]

Equation (2.18) is referred to as the sparse Broyden update. It was first introduced by Broyden [2] and also by Schubert [15].

Another example is the sparse symmetric update. If \( \mathcal{A} \) is as in the previous example and \( \mathcal{S} \) is the space of symmetric matrices, then

\[
(2.19) \quad \mathcal{P}\mathcal{S}\mathcal{A}(M) = \frac{1}{2} Z(M + M^T)
\]

So,

\[
\mathcal{P}\mathcal{S}\mathcal{A}(\varepsilon_j S_j^T)S = \frac{1}{2} Z(\varepsilon_j S_j^T + S_j \varepsilon_j^T)S
\]

\[
= \frac{1}{2} \left( \varepsilon_j S_j^T + S_j \varepsilon_j^T \right)S
\]

\[
= \frac{1}{2} \left( S_j^T S \varepsilon_j + \varepsilon_j^T S_j S_j^T \right)
\]

and so \( P = \frac{1}{2} \frac{S^T S}{S^T S} \)

Thus if \( v \) is any least-square solution to

\[
\min \left| \frac{1}{2} \frac{S^T S}{S^T S} (D + Z(S S^T)) v - (Y - BS) \right|_2^2 \text{ then,}
\]

\[
(2.20) \quad B_+ = B + \mathcal{P}\mathcal{S}\mathcal{A}(v S^T S) S^T S
\]

is the least change sparse symmetric update. For a different approach see [17].
**Theorem 2.5:** Let there be given vectors $S, Y \in \mathbb{R}^n$ with $S \neq 0$, an affine subspace $A \subseteq L(\mathbb{R}^n)$ with $S$ its parallel subspace, and an inner-product norm $| \cdot |$ on $L(\mathbb{R}^n)$. Set $Q = Q(Y, S)$ and its parallel subspace $Q(0, S) = N$. Then $M(\mathcal{A}, Q)$ is an affine subspace with parallel subspace $\mathcal{Q}N$; in particular,

\begin{equation}
(2.21) \quad P_{M(\mathcal{A}, Q)} A = A_+ = (I - P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}})^{-1} A_N + (I - P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}})^{-1} P_{S_{\mathcal{N}}} (\frac{Y S^T}{S^T S}) + P_{\mathcal{Q}N} A
\end{equation}

for any $A \in L(\mathbb{R}^n)$, and

\begin{equation}
(2.22) \quad M(\mathcal{A}, Q) = \{ (I - P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}})^{-1} A_N + (I - P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}})^{-1} P_{S_{\mathcal{N}}} (\frac{Y S^T}{S^T S}) + H : H \in \mathcal{Q}N \}
\end{equation}

where $A_N$ is the normal to $S$.

If $G, \overline{G} \in M(\mathcal{A}, Q)$, then $P_{\mathcal{N}} G = P_{\mathcal{N}} \overline{G}$ i.e., $G S = \overline{G} S$.

Furthermore, if $G \in M(\mathcal{A}, Q)$, then

\begin{equation}
(2.23) \quad P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}} G = P_{S_{\mathcal{N}}} P_{S_{\mathcal{N}}} (\frac{Y S^T}{S^T S})
\end{equation}

and if $A \in L(\mathbb{R}^n)$, then

\begin{equation}
(2.24) \quad A_+ = P_{\mathcal{Q}N} A + P_{\mathcal{Q}N}^\perp G.
\end{equation}

If $G \in M(\mathcal{A}, Q)$ and $A, H \in L(\mathbb{R}^n)$ then

\begin{equation}
(2.25) \quad | A_+ - H | \leq | P_{\mathcal{Q}N} (A - H) | + | P_{\mathcal{Q}N}^\perp (G - H) |.
\end{equation}

**Proof** See [6].
Equation (2.21) expresses $A_+$ as the sum of two elements, one from $\mathcal{N}^\perp$ while the other is from $(\mathcal{N}^\perp)^\perp$. Equation (2.22) characterizes all the elements of $M(\mathcal{N},Q)$ and equation (2.25) shows that least-change secant updates exhibit a very general form of bounded deterioration.

We will use (2.21) to derive the PSB formula mentioned earlier.

In this case, $S = \mathcal{N} = \{ M \in L(\mathbb{R}^n) : M = M^T, A_{nM} = 0 \}$ and for $B \in L(\mathcal{R}^n)$, $P_{S}^{-1}B = \left[I - \frac{SS^T}{S^TS}\right](-\frac{B + B^T}{2})\left[I - \frac{SS^T}{S^TS}\right]$.

Since $P_{\mathcal{N}}^{-1}(M) = M \left[I - \frac{SS^T}{S^TS}\right]$, for any $M \in L(\mathbb{R}^n)$, $P_{\mathcal{N}}^{-1}(\frac{YS^T}{S^TS}) = 0$ which gives $P_{\mathcal{N}}^{-1}(\frac{YS^T}{S^TS}) = \frac{YS^T}{S^TS}$. So, $P_{S}^{-1}P_{\mathcal{N}}^{-1}(\frac{YS^T}{S^TS}) = \frac{1}{2} \left[\frac{YS^T}{S^TS} + \frac{YS^T}{S^TS}\right]$.

Using $(I - P_{\mathcal{N}}^{-1})^{-1} = I + P_{\mathcal{N}}^{-1}P_{\mathcal{N}}^{-1} + (P_{\mathcal{N}}^{-1}P_{\mathcal{N}}^{-1})^2 + \ldots$, which is true on $(\mathcal{N})^\perp$, one can show that

$$(I - P_{\mathcal{N}}^{-1})^{-1}(\frac{1}{2} (\frac{YS^T}{S^TS} + \frac{YS^T}{S^TS})) = \frac{YS^T}{S^TS} + \frac{YS^T}{S^TS} - \frac{S^TS^YS^T}{S^TS^T} - \frac{S^TS^YS^T}{S^TS^T} \left(\frac{S^TS^T}{S^TS^T}\right)^2$$

Thus,

$$B_+ = \frac{YS^T}{S^TS} + \frac{YS^T}{S^TS} - \frac{S^TS^YS^T}{S^TS^T} [I - \frac{SS^T}{S^TS}] \left(\frac{B + B^T}{2}\right)\left[I - \frac{SS^T}{S^TS}\right]$$

If $B \in S$, then $\frac{1}{2}(B + B^T) = B$ and the PSB formula follows.

Consider now rescaling the variable space by $\bar{X} = TX$ such that $T^TT = H \in Q(Y, S)$. The symmetric secant update in this variable
space is

\[(2.26) \quad \overline{B}_+ = \overline{B} + \frac{(\overline{Y} - \overline{B} \overline{S})\overline{S} + \overline{S} (\overline{Y} - \overline{B} \overline{S})^T}{\overline{S}^T \overline{S}}
- \frac{\overline{S}^T (\overline{Y} - \overline{B} \overline{S}) \overline{S} \overline{S}^T}{(\overline{S}^T \overline{S})^2}\]

where

\[\overline{S} = TS\]
\[\overline{Y} = T^{-T}Y\]
\[\overline{B}_+ = T^{-T}B_T^{-1}\]
\[\overline{B} = T^{-T}B T^{-1}\]

Re-expressing (2.26) in the original variable space one gets:

\[(2.27) \quad B_+ = B + \frac{(Y - BS)YT + Y(Y - BS)^T}{Y^T S} - \frac{S^T (Y - BS)YS}{(Y^T S)^2} (2.27) B\]

which is the DFP update named after its discoverers Davidon [3], Fletcher and Powell [9]. Another way of stating the above is that if \(B\) is symmetric, \(Y^T S > 0\), \(T \in L(\mathbb{R}^n)\) is such that \(T^T T \in Q(Y, S)\), and \(S\) is the space of symmetric matrices, then (2.27) is the unique solution to:

\[\min_{\overline{B} \in L(\mathbb{R}^n)} | T^{-T} (\overline{B} - B) T^{-1} |_F \text{ subject to } \overline{B} \in Q(Y, S) \cap S\]

If we apply the same rescaling, use Greenstadt's update (2.14) of \(B^{-1}\) to \(\overline{B}^{-1}\) and then transform back, we get:

\[(2.28) \quad B_+^{-1} = B^{-1} + \frac{(S - B^{-1} Y)S^T + S(S - B^{-1} Y)^T}{Y^T S} - \frac{Y^T (S - B^{-1} Y)SS^T}{(Y^T S)^2}\]

Update (2.28) is known as the Broyden - Fletcher - Goldfarb -
Shanno update [2], [7], [11], [15] or simply the BFGS update. Also in this case if B is symmetric, \( S^T Y > 0 \) and T as before then \( B^{-1} \) is the unique solution to:

\[
\min_{B^{-1} \in L(\mathbb{R}^n)} \left| T(\overline{B}^{-1} - B^{-1})T \right|_F \quad \text{subject to } \overline{B}^{-1} \in Q(S,Y)\mathbb{S}
\]

Both the DFP update and the BFGS update preserve positive definiteness. For that reason the latter is called the positive definite secant update while the former is called the inverse positive definite secant update.

We now present theorems which show that quasi-Newton methods based on least-change secant updates are either q-superlinearly convergent or exhibit q-linear convergence which is optimal in certain sense.

**Definition**: Given any vector norm, Ortega and Rheinboldt [13], p 281 define the linear factor of \( \{X_k\} \) as

\[
Q_1 \{ X_k \} = \begin{cases} 
0 & \text{if } X_k = X_*, k \geq \text{some } k_0 \\
\lim_{k \to \infty} \frac{|X_{k+1} - X_*|}{|X_k - X_*|} & \text{if } X_k \neq X_*, k \geq k_0 \\
+\infty & \text{otherwise.}
\end{cases}
\]

For a given norm, the statement that \( \{X_k\} \) converges q-linearly to \( X_* \) means that \( Q_1 \{ X_k \} < 1 \), and q-superlinear convergence means that \( Q_1 \{ X_k \} = 0 \). Note that q-superlinear convergence is norm independent while linear convergence is not.

**Theorem 2.6**: Let F satisfy (2.2) and (2.3) and let \( \mathcal{A} \) be an
affine subspace with parallel subspace $S$ with the property that

\begin{equation}
B_* = P_A J(X_*)
\end{equation}

is such that $B_*$ is invertible and there exists an $r_*$ for which

\begin{equation}
|B_*^{-1} P_A J(X_*)| \leq r_* < 1
\end{equation}

Also, assume that there exists an $a \geq 0$ such that for any $X, X_+ \in D$ and $Y = F(X_+) - F(X)$, one has

\begin{equation}
|X_+ - X_*| < a(X, X_+)
\end{equation}

for every $G \in M(A, Q)$, where $\sigma(X, X_+) = \max\{|X - X_*|, |X_+ - X_*|\}$ and $M = Q(0, S)$. Under these hypotheses, if $r \in (r_*, 1)$, then there are positive integers $\varepsilon_r, \delta_r$ such that for $X_0 \in \mathbb{R}^n$ and $B_0 \in L(\mathbb{R}^n)$ satisfying $|X_0 - X_*| < \varepsilon_r$ and $|B_0 - B_*| < \delta_r$, any sequence \{ $X_k$ \} defined by

\begin{equation}
X_{k+1} = X_k - B_k^{-1} F(X_k),
\end{equation}

where $B_{k+1} = (B_k)_+$ is the unique solution to

\begin{equation}
\min_{\overline{B} \in L(\mathbb{R}^n)} |\overline{B} - B_k| \quad \text{subject to} \quad \overline{B} \in M(A, Q)
\end{equation}

satisfies $|X_{k+1} - X_*| \leq r |X_k - X_*|$ for $k = 0, 1, 2, \ldots$

Furthermore, \{ $|B_k|$ \} and \{ $|B_k^{-1}|$ \} are uniformly bounded.

The above theorem is a special case of a more general theorem given by Dennis and Walker [6].

Note that from Theorem 2.5 we have if $G \in M(A, Q)$ and $H$ in
(2.25) is replaced by $B_*$, then
\[(2.33) \quad |B_+ - B_*| \leq |P \nabla \nabla (B - B_*)| + |P_{\nabla}^\perp (G - B_*)|.
\]
So condition (2.32) combined with the fact that $|P \nabla \nabla (B - B_*)| \leq |B - B_*|$ gives:
\[(2.34) \quad |B_+ - B_*| \leq |B - B_*| + \alpha \sigma(X, X_+)^p
\]
which ensures that $B_+$ has the bounded deterioration property.

**Theorem 2.7** Suppose that the hypotheses of Theorem 2.6 hold and that for some $X_0 \in \mathbb{R}^n$ and $B_0 \in L(\mathbb{R}^n)$, \{ $X_k$ \} is a sequence defined by $X_{k+1} = X_k - B_k^{-1} F(X_k)$, where $B_k^{-1} = (B_k)_+$ as before.

Set $e_k = X_k - X_*$ for $k = 0, 1, 2, \ldots$. Then
\[
\lim_{k \to \infty} |\frac{e_{k+1}}{e_k} + B_*^{-1} P_{\nabla}^\perp J(X_*) \frac{e_k}{e_k}| = 0
\]
where $B_*$ is given by (2.30). It follows that,
\[
\lim_{k \to \infty} |\frac{e_{k+1}}{e_k}| = \lim_{k \to \infty} |B_*^{-1} P_{\nabla}^\perp J(X_*) \frac{e_k}{e_k}| \leq r_*
\]
and, hence, that \{ $X_k$ \} converges q-superlinearly to $X_*$ if and only if
\[
\lim_{k \to \infty} |P_{\nabla}^\perp J(X_*) \frac{e_k}{e_k}| = 0.
\]
In particular, \{ $X_k$ \} converges q-superlinearly to $X_*$ if $F'(X_*) \in \mathcal{A}$.

For a proof of the above theorem see [6].

As a consequence of Theorem 2.7 one concludes that all of the quasi-Newton methods discussed in this chapter are locally q-superlinearly convergent, provided $F'(X_*)$ has the structural
properties imposed on the update.
CHAPTER III

LEAST-CHANGE SECANT
UPDATES OF NON-
SQUARE MATRICES

In this chapter we will deal with the problem of updating non-square matrices. In particular, we will look at updates of matrices from $L(\mathbb{R}^{n+1}, \mathbb{R}^n)$ in the least-change secant sense. This special case has broad implications in the general context of solving non-linear systems which depends on a parameter, such as occur in continuation methods. It also applies to updating the approximation to the Jacobian of a function $F$ which depends on $t \in \mathbb{R}$ and $Y \in \mathbb{R}^n$, which is the case for between-step updating in non-autonomous differential equations.

The idea behind the updates which will follow is: Given $B = [J, b]$ where $J \in L(\mathbb{R}^n)$ and $b \in \mathbb{R}^n$, we want a $B_+ = [J_+, b_+]$, $J_+ \in L(\mathbb{R}^n)$ and $b_+ \in \mathbb{R}^n$, to be "as close as possible" to $B$ subject to a secant type condition:

$$(3.1) \quad B_+ S = Y, \quad S \in \mathbb{R}^{n+1}, \quad Y \in \mathbb{R}^n, \quad S \neq 0$$

which we will also refer to as the secant condition. We may also require that $J_+$ preserve some sparsity pattern or symmetry or
positive definiteness of $J$.

General Secant Updates. To begin, we consider the case where no restrictions are placed on $J$. For $S = (\mathbf{S}^T, t)^T$, $\mathbf{S} \in \mathbb{R}^n$, $t \in \mathbb{R}$ and $Y \in \mathbb{R}^n$, define

$$(3.2) \quad Q(Y, S) = \{ M \in L(\mathbb{R}^{n+1}, \mathbb{R}^n) : M S = Y \}$$

We assume in the following that the matrix norm is the Frobenius norm, unless otherwise specified.

We note that the formulas for the least-change secant update obtained earlier in Theorems 2.3 and 2.5 are also valid in this case, and that since the norm is the Frobenius norm,

$$P_{\gamma}(B) = (I - \frac{SS^T}{S^TS}) B$$

and

$$(I - P_{\gamma})^{-1} P_{\gamma}^{-1} (\frac{YS^T}{S^TS}) = \frac{YS^T}{S^TS}$$

where $S$ and $M$ have the same meaning as in the above mentioned theorems.

Then the least-change secant update $B_+$ is given by

$$(3.3) \quad B_+ = Q(Y, S) B = B \left[ I - \frac{SS^T}{S^TS} \right] + \frac{YS^T}{S^TS}$$

$$= B - \left[ \frac{BS_+^T}{S^TS}, \frac{BS_+}{S^TS} \right] + \left[ \frac{YS^T}{S^TS} \right]$$

Expressing (3.3) in terms of $J_+, J, b_+$ and $b$ one gets
(3.4,a) \[ J_+ = J + \frac{(Y - J \hat{S} - b \, t) \hat{S}^T}{\hat{S}^T \hat{S}} \]

and

(3.4,b) \[ b_+ = b + \frac{(Y - J \hat{S} - b \, t) \, t}{\hat{S}^T \hat{S}} \]

Note that if \( t = 0 \) then \( b_+ = b \) and \( J_+ \) is just the usual first Broyden update of \( J \).

The least-change principle does not show so clearly how to extend the second Broyden update to this case. In the square matrix case, the second Broyden update is obtained by applying the least-change principle to the inverse of the matrix to be updated; in the case at hand, there is no inverse to which to apply the principle. The principle does suggest several possibilities, however. One can write (3.1) as

(3.5) \[ J_+ \hat{S} + b_+ \, t = Y \]

Pre-multiplying both sides of (3.5) by \( J_+^{-1} \) we get

(3.6) \[ J_+^{-1} Y + d_+ \, t = \hat{S}, \quad d_+ = - J_+^{-1} b_+ \]

and this suggests taking

(3.7) \[ [ J_+^{-1}, d_+ ] = P \hat{Q}(\hat{S}, \begin{bmatrix} Y \\ t \end{bmatrix}) \left( [ J_+^{-1}, d ] \right), d = - J_+^{-1} b \]

Letting \( U = \begin{bmatrix} Y \\ t \end{bmatrix} \), we obtain

(3.8) \[ [ J_+^{-1}, d_+ ] = [ J_+^{-1}, d ] \left( I - \frac{U^T \, U}{U^T \, U} \right) + \frac{\hat{S}}{U^T \, U} U^T \]

Substituting for \( U \) its value in terms of \( Y \) and \( t \) and expressing
(3.8) in terms of \( J \) and \( d \) one gets

\[
J_{+}^{-1} = J^{-1} + \left( \frac{\hat{S}^2 - J^{-1}Y - d + t}{|Y|^2 + t^2} \right) Y^T
\]

and

\[
d_{+} = d + \left( \frac{\hat{S}^2 - J^{-1}Y - d + t}{|Y|^2 + t^2} \right) t
\]

Also in this case, if \( t = 0 \) then \( J_{+}^{-1} \) is the second Broyden update and \( d_{+} = d \).

Expressing the update in its direct form we get

\[
J_{+} = J + \left( \frac{Y - JS - b + t}{Y^T (JS + b + t) + t^2} \right) Y^T J
\]

and,

\[
b_{+} = b + \left( \frac{Y - JS - b + t}{Y^T (JS + b + t) + t^2} \right) t + Y^T b
\]

The Powell Symmetric Broyden Update. Now suppose that \( J \) is a symmetric matrix and we wish the update \( J_{+} \) to preserve the symmetry.

Let \( S \) be a subspace of \( L(\mathbb{R}^n) \) and \( M \in \mathbb{R}^n \) and \( M^T = M \).

If \( B_{+} = [ J_{+}^{+} , \ b_{+}^{+} ] \) as before, then we want \( B_{+} = P_{S \cap N}(B) \) and again by appealing to Theorem 2.5 we have

\[
B_{+} = (I - P_{S \cap N}(B))^{-1} P_{S \cap N}(B)
\]

Since \( S \) is a subspace of \( L(\mathbb{R}^{n+1}, \mathbb{R}^n) \) and therefore \( A_{N} = 0 \). Here \( N \)
= Q(0,S). If we take B = [ J , b ] and S = [ $s^t$ ] the following can be easily verified:

$$P_N B = B \left[ I - \frac{SS^T}{|S|^2} \right]$$

$$= \left[ J - \frac{B^T S S^T}{|S|^2} , b - \frac{b^T S^T}{|S|^2} \right]$$

and

$$P_S B = \left[ \frac{J + JT}{2} , b \right]$$

Now, since $\frac{YS^T}{ST}$ $\in N^\perp$ we have $P_N^\perp \left( \frac{YS^T}{ST} \right) = \frac{YS^T}{ST}$ and

$$P_S^\perp \left( \frac{YS^T}{ST} \right) = \left[ \frac{YST + YS^T}{2} , \frac{tY}{|S|^2} \right]$$

So, (3.11) reduces to

(3.12) $B_+ = \left( I - P_S P_N^\perp \right)^{-1} \left[ \frac{YST + YS^T}{2} , \frac{tY}{|S|^2} \right] + P_S^\perp B$

By Theorem 2.3 we have

(3.13) $P_S^\perp B = \lim_{k \to \infty} \left( P_S P_N^\perp \right)^k B$

so we will compute the second term of (3.12) using (3.13). We have
\[ P_N B = B - \left[ \frac{B S S^T}{|S|^2}, \frac{B S t}{|S|^2} \right], \]

so,

\[ P S P_N B = B - \frac{1}{2} \left[ \frac{B S S^T}{|S|^2}, \frac{B S t}{|S|^2} \right] - \frac{1}{2} \left[ \frac{S (B S)^T}{|S|^2}, \frac{B S t}{|S|^2} \right] \]

\[ = \frac{1}{2} B + \frac{1}{2} P_N B - \frac{1}{2} \left[ \frac{S (B S)^T}{|S|^2}, \frac{B S t}{|S|^2} \right] \]

Using an inductive argument it can be shown that

\[
(3.14) \quad (P S P_N)^k B = \frac{1}{2} B + \frac{1}{2} P_N B - \frac{1}{2} \left[ I + P S P_N + \ldots + (P S P_N)^{-1} \right] \left[ \frac{S (B S)^T}{|S|^2}, \frac{B S t}{|S|^2} \right]
\]

Therefore,

\[
(3.15) \quad P S P_N B = \frac{1}{2} B + \frac{1}{2} P_N B - \sum_{k=0}^{\infty} \left( P S P_N \right)^k \left[ \frac{S (B S)^T}{|S|^2}, \frac{B S t}{|S|^2} \right]
\]

To simplify notation, let \( \frac{S}{|S|} = \sigma \) and \( \frac{B S}{|S|} = \omega \), where \( \sigma, \omega \in \mathbb{R}^n \) and \( \tau \in \mathbb{R} \). Then

\[
\left[ \frac{S (B S)^T}{|S|^2}, \frac{B S t}{|S|^2} \right] = \left[ \sigma \omega^T, \tau \omega \right]
\]
Now, $P_P^k [ \sigma \omega^T, \tau \omega ] = [ \sigma \omega^T - \tau^2 \omega \sigma^T - \omega^T \sigma \sigma^T, 
\tau ( | \sigma |^2 \omega - \omega^T \sigma \sigma)]$

and

$$P_S \left[ \sigma \omega^T, \tau \omega \right] = | \sigma |^2 \left[ \frac{\sigma \omega_1^T + \omega_1 \sigma^T}{2}, \tau \omega_1 \right]$$

where $\omega_1 = ( I - \frac{\sigma \sigma^T}{| \sigma |^2} ) \omega$

Simple arithmetic shows

(3.16) $( P_S P_P^k ) [( \sigma \omega^T, \tau \omega ] = | \sigma |^{2k} \left[ \frac{\sigma \omega_1^T + \omega_1 \sigma^T}{2}, \tau \omega_1 \right]$ for $k = 1, 2, 3, ...$

Therefore,

(3.17) $P \sum_{k=0}^{\infty} ( P_S P_P^k ) [ \frac{\hat{S} \left( B S \right)^T}{| S |^2}, \frac{t B S}{| S |^2} ]$

$= [ \sigma \omega^T, \tau \omega ] + \sum_{k=1}^{\infty} | \sigma |^{2k} \left[ \frac{\sigma \omega_1^T + \omega_1 \sigma^T}{2}, \tau \omega_1 \right]$

$= [ \frac{\hat{S} \left( B S \right)^T}{| S |^2}, \frac{t B S}{| S |^2} ] +$

$$\frac{2 | \hat{S} |^2}{| S |^2 + t^2} \left[ \frac{\left( I - \frac{\hat{S} \hat{S}^T}{| \hat{S} |^2} \right) B S}{2 | S |^2} \right] + \left( I - \frac{\hat{S} \hat{S}^T}{| \hat{S} |^2} \right) B S \hat{S}^T$$
Combining (3.17) with (3.15) one gets

\[
(3.18) \quad P_{S|W} B = \left[ J - \frac{BS^T + \hat{S} (B S)^T}{|S|^2 + t^2} + \frac{\hat{S}^T B S \hat{S}}{|S|^2 (|S|^2 + t^2)} \right]
\]

If we let now \( V = \frac{Y}{|S|} \), the first term of (3.12) can be expressed as

\[
\sum_{k=0}^{\infty} \left( P_S P_P \right)^k \left\{ \frac{1}{2} \left[ V \sigma^T, \tau V \right] + \frac{1}{2} \left[ \sigma V^T, \tau V \right] \right\}
\]

As before, for \( k = 1, 2, 3, \ldots \)

\[
( P_S P_P )^k \left[ \sigma V^T, \tau V \right] = \frac{1}{2^{k-1}} \left[ \frac{\sigma V_1^T + V_1 \sigma^T}{2} , \tau V_1 \right],
\]

\[
V_1 = \left[ I - \frac{\sigma \sigma^T}{|\sigma|^2} \right] V
\]

Also, \( P_P \left[ V \sigma^T, \tau V \right] = 0 \) and so,

\[
( P_S P_P )^k \left[ V \sigma^T, \tau V \right] = 0 \), for \( k = 1, 2, 3, \ldots \)

then,

\[
(3.19) \quad ( I - P_S P_P )^{-1} P_S P_P \left( \frac{Y S^T}{S S^T} \right) = \left[ \frac{V \sigma^T + \sigma V^T}{2} , \tau V \right]
\]
\[
+ \frac{\sigma}{2} \sum_{k=0} |\sigma|^{2k} \left[ \frac{\sigma v_{1}^{T} + v_{1}^{T} \sigma}{2}, \tau v_{1} \right]
\]

\[
= \left[ \frac{v \sigma^{T} + \sigma v^{T}}{2}, \tau v \right] + \frac{\sigma}{2(1 - \frac{2}{2})} \left[ \frac{\sigma v_{1}^{T} + v_{1}^{T} \sigma}{2}, \tau v \right]
\]

Substituting for \( \sigma, V, \tau \) and \( V_{1} \) in (3.19) one gets

(3.20) \( (I - P S_{y} P_{y})^{-1} P S_{y} P_{y} \left( \frac{Y S_{y}}{S_{y}^{T} S_{y}} \right) \)

\[
= \left[ \frac{Y \hat{S}_{y}^{T} + \hat{S} Y^{T}}{|S|^{2} + t^{2}} - \frac{\hat{S}_{y}^{T} Y \hat{S}_{y}^{T}}{|S|^{2}(|S|^{2} + t^{2})}, \frac{2 t Y}{|S|^{2} + t^{2}} - \frac{t \hat{S}_{y}^{T} Y \hat{S}_{y}}{|S|^{2}(|S|^{2} + t^{2})} \right]
\]

From (3.11), (3.18) and (3.20) we have

(3.21,a) \( J_{+} = J + \frac{(Y - BS) \hat{S}_{y}^{T} + \hat{S}(Y - BS)^{T}}{|S|^{2} + t^{2}} - \frac{\hat{S}_{y}^{T}(Y - BS) \hat{S}_{y}}{|S|^{2}(|S|^{2} + t^{2})} \)

and,

(3.21,b) \( b_{+} = b + \frac{2 t (Y - BS)}{|S|^{2} + t^{2}} - \frac{t \hat{S}_{y}^{T}(Y - BS) \hat{S}_{y}}{|S|^{2}(|S|^{2} + t^{2})} \)

The update given by (3.21) will be referred to as the Powell symmetric Broyden update. Note that if \( t = 0 \), then the update given by (3.21,a) is the PSB update, and \( b_{+} = b \).

We will now derive an analog of the Greenstadt update in a way analogous to the derivation of the extension of the second Broyden update.

We write the secant condition as \( J_{+}^{-1} Y + d_{+} t = \hat{S} \) where as before \( d_{+} = - J_{+}^{-1} b_{+} \). The same derivation as in the symmetric
update case applied to this secant condition will yield the inverse symmetric update and is given by:

\[
\begin{align*}
J^{-1}_+ &= J^{-1} + \frac{(\hat{S} - J^{-1}Y - dt)Y^T + Y(\hat{S} - J^{-1}Y - dt)^T}{|Y|^2 + 2t^2} \\
& \quad + \frac{Y^T(\hat{S} - J^{-1}Y - dt)Y^T}{(|Y|^2 + t^2)(|Y|^2 + 2t^2)}.
\end{align*}
\]

and,

\[
\begin{align*}
d_t &= d + \frac{2t(\hat{S} - J^{-1}Y - dt)}{|Y|^2 + t^2} - \frac{tY^T(\hat{S} - J^{-1}Y - dt)Y}{(|Y|^2 + t^2)(|Y|^2 + 2t^2)}.
\end{align*}
\]

Positive Definite Updates. Now we turn our attention to updates that preserve the positive definiteness as well as the symmetry of the matrix \(J\).

To make a preliminary observation, suppose we are solving

\[
F(X, \lambda) = 0, \quad F : \mathbb{R}^{n+1} \to \mathbb{R}^n, \quad X \in \mathbb{R}^n, \quad \lambda \in \mathbb{R}.
\]

If \(Y = F(X+\hat{S}, \lambda+t) - F(X,\lambda)\), then

\[
\frac{\partial F}{\partial X} \hat{S} + \frac{\partial F}{\partial \lambda} t \equiv Y;
\]

and if \(\frac{\partial F}{\partial X}\) is positive definite, one can reasonably expect

\[
( Y - \frac{\partial F}{\partial \lambda} t )^T \hat{S} > 0. \quad \text{If } [J, b] \simeq [\frac{\partial F}{\partial X}, \frac{\partial F}{\partial \lambda}], \text{ we set } Y^\# = Y - b t \text{ and require that } (Y^\#)^T \hat{S} > 0. \text{If this is the case, then there is a symmetric positive definite matrix } W \text{ such that }
\]
Let us now scale the variable space by $\bar{X} = TX$ where $TT^T=W$, $W \in \mathbb{Q}(Y^#, \hat{S})$ and $Y^# = Y - bt$. The symmetric secant update in the new variable space is

$$(3.23,a) \quad \hat{J} = J + \frac{(Y^# - \bar{J}S)S + \bar{S}(Y^# - \bar{J}S)^T}{|S|^2 + t^2} - \frac{\bar{S}S(Y^# - \bar{J}S)S}{(|S|^2 + t^2)(|S|^2 + 2t^2)}$$

$$(3.23,b) \quad \hat{b} = b + \frac{2t(Y^# - \bar{J}S)}{|S|^2 + 2t^2} - \frac{t \bar{S}S(Y^# - \bar{J}S)^T}{(|S|^2 + t^2)(|S|^2 + 2t^2)}$$

where

$$\bar{S} = TS, \quad \bar{Y} = T^TY^#, \quad \bar{J} = T^TJ + T^{-1}$$

Expressing (3.23) in the original variable space we obtain

$$(3.24,a) \quad J = J + \frac{(Y - BS)Y^#T + Y^#(Y - BS)^T}{\hat{S}T Y^# + 2t^2} - \frac{\hat{S}T(Y - BS)Y^#}{(\hat{S}TY^# + t^2)(\hat{S}TY^# + 2t^2)}$$

and,

$$(3.24,b) \quad b = b + \frac{2t(Y - BS)}{\hat{S}T Y^# + 2t^2} - \frac{t \hat{S}T(Y - BS)Y^#}{(\hat{S}TY^# + t^2)(\hat{S}TY^# + 2t^2)}$$

Update (3.24) will be referred to as the inverse positive definite secant update. It is the analogue of the DFP update in the square matrix case.
A remark concerning the scaling of the variable space in the derivation of the positive definite updates:

Suppose the problem we are interested in solving is finding a local minimizer of \( f(X) \); \( f : \mathbb{R}^n \longrightarrow \mathbb{R} \). Setting \( \overline{X} = T \cdot X \) transforms the problem in the new variable space to finding a local minimizer of \( f(\overline{X}) = f(\overline{T}^{-1}X) \), or finding a zero of

\[
\frac{\nabla}{\overline{X}} f(\overline{X}) = \overline{T}^T \frac{\nabla}{X} f(X).
\]

If we introduce a parameter \( \lambda \) such that the problem becomes finding a zero of \( F(X,\lambda) = \overline{T}^T F(X,\lambda) \), which is mostly the case in continuation methods, one can see then why we insist on \( \overline{b} = T^T b \) and \( J = T^T J_T^{-1} \).

If we now apply the same scaling idea to the inverse symmetric update we get an update analogous to the BFGS in the square matrix case.

Let \( S^\# = \hat{S} - d \cdot t \), \( d = -J^{-1} b \), then

\[
Y^T S^\# = Y^T (\hat{S} - d \cdot t)
= Y^T J^{-1}(J \hat{S} + b \cdot t)
= Y^T J^{-1} B \cdot S
\]

Since \( Y \approx F'(X,\lambda)S \) and \( B \cdot S \approx F'(X,\lambda)S \) and we assume that \( J^{-1} \) is positive definite then it becomes reasonable to expect \( Y^T S^\# > 0 \).

Thus there exists a symmetric positive definite matrix \( U \in Q(Y,S^\#) \). Let \( U = L^T L \). Let us now scale the variable space by \( \overline{X} = L \cdot X \). The inverse symmetric update in the new variable
space is:

\[
(3.25, a) \quad \bar{J}_+^{-1} = J_+^{-1} + \left( \frac{\bar{S} - \bar{J}_+^{-1} \bar{Y} - \bar{d} t}{| \bar{Y} |^2 + 2 t^2} \right) \bar{Y}^T + \frac{\bar{Y}}{| \bar{Y} |^2 + 2 t^2} \bar{Y}^T \left( \frac{\bar{S} - \bar{J}_+^{-1} \bar{Y} - \bar{d} t}{| \bar{Y} |^2 + t^2} \right) \bar{Y} \bar{Y}^T
\]

and,

\[
(3.25, b) \quad \bar{d}_+ = \bar{d} + \frac{2 t}{| \bar{Y} |^2 + 2 t^2} \left( \frac{\bar{S} - \bar{J}_+^{-1} \bar{Y} - \bar{d} t}{| \bar{Y} |^2 + t^2} \right) \bar{Y} \bar{Y}^T \left( \frac{\bar{S} - \bar{J}_+^{-1} \bar{Y} - \bar{d} t}{| \bar{Y} |^2 + 2 t^2} \right) \bar{Y}
\]

where

\[
\bar{J} = L^T J L^{-1}, \quad \bar{Y} = L^T Y, \quad \bar{S} = L \hat{S},
\]

\[
\bar{J}_+ = L^T J_+ L^{-1}, \quad \bar{b} = L^T b, \quad \bar{b}_+ = L^T b_+
\]

If we let \( \bar{d} = - \bar{J}_+^{-1} \bar{b} \), then \( \bar{d} = - L \bar{J}^{-1} L^T b = - L \bar{J}_+^{-1} b = L d \).

Also \( \bar{d}_+ = L d_+ \). Expressing (3.25) in the original variable space we obtain

\[
(3.26, a) \quad \hat{J}_+^{-1} = \hat{J}_+^{-1} + \left( \frac{\hat{S} - \hat{J}_+^{-1} \hat{Y} - \hat{d} t}{\hat{Y}^T \hat{S}^# + 2 t^2} \right) \hat{S}^# + \hat{S}^# \left( \frac{\hat{S} - \hat{J}_+^{-1} \hat{Y} - \hat{d} t}{\hat{Y}^T \hat{S}^# + 2 t^2} \right) \hat{S}^#^T \hat{Y}^T
\]

and,

\[
(3.26, b) \quad \hat{d}_+ = d + \frac{2 t}{\hat{Y}^T \hat{S}^# + 2 t^2} \left( \frac{\hat{S} - \hat{J}_+^{-1} \hat{Y} - \hat{d} t}{\hat{Y}^T \hat{S}^# + 2 t^2} \right) \hat{Y} \hat{S}^# + \hat{S}^# \hat{Y}_+ \hat{S}^#_+^T
\]
Noting that \( \hat{S}^* = \hat{S} - \hat{d} \hat{t} = \hat{J}^{-1}(\hat{J} \hat{S} + \hat{b} \hat{t}) = \hat{J}^{-1}B S \), (3.26) can be rewritten as

\[
(3.27,a) \quad J_+^{-1} = J^{-1} + \frac{J^{-1}[(B S - Y)(B S)^T + (B S)(B S - Y)^T]J^{-1}}{Y^T J^{-1} B S + 2 t^2}
\]

\[
+ \frac{J^{-1} Y^T J^{-1} (B S - Y) (B S) (B S)^T J^{-1}}{(Y^T J^{-1} B S + t^2)(Y^T J^{-1} B S + 2 t^2)}
\]

and,

\[
(3.27,b) \quad d_+ = J^{-1} b + \frac{2 t J^{-1}(B S - Y)}{Y^T J^{-1} B S + 2 t^2}
\]

\[
+ \frac{t Y^T J^{-1}(B S - Y) J^{-1} B S}{(Y^T J^{-1} B S + t^2)(Y^T J^{-1} B S + 2 t^2)}
\]

The update given by (3.27) will be referred to as the positive definite secant update. Expressing the update in its direct form we get

\[
(3.28,a) \quad J_+ = J + \frac{2 t^2}{\sigma} \left[ Y(B S)^T + (B S) Y^T \right]
\]

\[
+ \frac{(B S)^T J^{-1}(B S) Y Y^T - \sigma}{\sigma} (B S)(B S)^T
\]

and,

\[
(3.28,b) \quad b_+ = J_+^{-1} [ b + \frac{2 t J^{-1}(B S - Y)}{Y^T J^{-1} B S + 2 t^2}]
\]
\[ - \frac{t Y^T (B S - Y) B S}{(Y^T B S + t^2)(Y^T J^{-1} B S + 2t^2)} \]

where \( D = 4t^4 + (B S) J^{-1} (B S) \sigma \)

and \( \sigma = 2(Y^T J^{-1} B S + 2t^2) + \)

\[ \frac{Y^T J^{-1} (B S - Y)(Y^T J^{-1} B S + 2t^2)}{Y^T J^{-1} B S + t^2} - Y^T J^{-1} Y \]

For \( L, M \in L(\mathbb{R}^n) \) and \( l, m \in \mathbb{R}^n \), define the inner product \(<,>_{\text{w}} \) by:

\[ <[L,l],[M,m]>_{\text{w}} = \text{tr} \{ W^{-1}LW^{-1}M^T + W^{-1}lM^T \} \]

and the induced norm is then given by:

(3.29) \[ |[M,m]|_{\text{w}}^2 = |W^{-1}M W^{-1}M^T|_F^2 + |W^{-1}m M^T|_F^2. \]

Note that the update \( B_+ = [J_+, b+] \) given by (3.24) can be viewed as the solution to

(3.30) \[ \min_{\hat{B} \in L(\mathbb{R}^{n+1}, \mathbb{R}^n)} |\hat{B} - B|_w \text{ subject to } \hat{B} \in Q(Y,S) \cap S \]

and (3.25) can be viewed as the solution to

(3.31) \[ \min_{\overline{H} \in L(\mathbb{R}^{n+1}, \mathbb{R}^n)} |\overline{H} - H|_U, \quad H = [J^{-1}, d] \]

subject to \( \overline{H} \in Q(\hat{S}, [Y]_t) \cap S \), and \( |.|_w \) and \( |.|_U \) are given.
by (3.29), where $W$ and $U$ are symmetric positive definite matrices such that $W \hat{S} = Y$ and $U \hat{S} = Y$

Before we begin with the updates that preserve the sparsity we would like to state an interesting theorem concerning the non-square matrix updates which may become useful especially when some particular updates are difficult to produce or some existing ones are hard to implement.

**Theorem 3.1** Let $A$ be an affine subspace of $L(\mathbb{R}^n)$ and $A' = A \times \mathbb{R}^n$. Also, let $Q(Y, S) = \{ M \in L(\mathbb{R}^n) : MS = Y, S, Y \in \mathbb{R}^n \}$ and $Q'(Y, S) = \{ B \in L(\mathbb{R}^{n+1}, \mathbb{R}^n) : BS = Y, S \in \mathbb{R}^{n+1}, Y \in \mathbb{R}^n \}$.

If $B^+ = [ J^+, b^+ ] = \text{proj}_{A'} Q'(Y, S) [ J^+, b ]$ where $J, J^+ \in L(\mathbb{R}^n)$ and $b, b^+ \in \mathbb{R}^n$ then $J^+ = \text{proj}_{A} Q(Y-b^+t, S)$ where $[ \hat{S} \ t ] = S, \hat{S} \in \mathbb{R}^n$, and $t \in \mathbb{R}$.

**Proof:** Suppose that $J^* \neq J^+$ is a solution to

$$
(3.32) \quad \min | J - J^* |_F \text{ subject to } J \in A \text{ and } J \hat{S} = Y - b^+t.
$$

Then $| J^* - J |_F^2 + | b^+ - b |_F^2 < | J^+ - J |_F^2 + | b^+ - b |_F^2$.

But this implies that $B^* = [ J^*, b^+ ]$ is such that

$| B^* - B |_F^2 < | B^+ - B |_F^2$, which contradicts the fact that $B^+$ is the solution to
\[ \min \mid \bar{B} - B \mid_F \text{ subject to } \bar{B} \in A \text{ and } \bar{B} S = Y. \]

Therefore the solution to (3.32) is \( J_+ \).

The above theorem says that if one has \( b_+ \) a priori, then \( J_+ \) and thus \( B_+ \) can be obtained using the corresponding square matrix updates. Though we may not have \( b_+ \) unless we obtain \( B_+ \) one may have a "good" guess for \( b_+ \) which if used in a square matrix update may produce a "good" update to \( J \).

Also note that the above theorem holds if we take the projection in the weighted Frobenius norm defined by (3.29). The proof is exactly the same as in the previous theorem.

Sparse Matrix Update. Extending the sparse matrix update to the non-square case turn out to be rather easy. The secant condition

\[ J_+ \hat{S} + b_+ t = Y \]

can be written as

\[
(3.33) \begin{bmatrix}
J_+ & b_+ \\
0^T & 0
\end{bmatrix}
\begin{bmatrix}
\hat{S} \\
t
\end{bmatrix}
= \begin{bmatrix}
Y \\
0
\end{bmatrix}
\]

where \( 0^T_n \) is a row of \( n \) zeros.

Setting \( B_+ = \begin{bmatrix} J_+ & b_+ \end{bmatrix} \), \( S = \begin{bmatrix} \hat{S} \\
t \end{bmatrix} \) and \( Y = \begin{bmatrix} Y \\
0 \end{bmatrix} \) one can write

\[
(3.33) \Rightarrow (3.34) \quad \tilde{B}_+ S = \tilde{Y}
\]
If \( B = \begin{bmatrix} J & b \\ 0^T_n & 0 \end{bmatrix} \) then one can take \( \tilde{B}_+ \) as the sparse update for the square matrix case discussed in Chapter 2.

It is an easy exercise to show that if

\[ B_+ \text{ minimizes } \| \bar{B} - B \|_F \text{ subject to } \bar{B} S = Y, \text{ then } \begin{bmatrix} B_+ \\ 0^T \end{bmatrix}_{n+1} \]

\[ \text{minimizes } \| B_* - \bar{B} \|_F \text{ subject to } B_* S = \bar{Y}, \text{ where } B_* = \begin{bmatrix} \bar{B} \\ 0^T \end{bmatrix}_{n+1}. \]

As for the sparse-symmetric update we recommend taking \( b_+ \) to be the update of \( b \) obtained by the first Broyden update and update \( J \) using the sparse-symmetric update in the square matrix case as discussed in Chapter 2 where the secant condition now is:

\[ J_+ \hat{S} = Y - b_+ t. \]
In this chapter we test each of the updates obtained in Chapter 3 on a wide range of problems. The application being used here is continuation methods. The different updates were coded in a software package, HOMPACK, which tries to find a zero of $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ using continuation methods. We begin by reviewing some basic background material on continuation methods; then we will briefly discuss HOMPACK. Then finally we will report some of the numbers obtained in the numerical testings.

Continuation Methods. Consider solving $F(X) = 0$, where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a $C^2$ map. The general idea of using the aforementioned methods is to embed $F$ in a mapping $\rho$, $\rho : \mathbb{R}^n \times [0,1] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$, such that for $\rho = \rho(X,\lambda,a)$, $\lambda \in [0,1]$, $X,a \in \mathbb{R}^n$, $\rho(X,0,a) = 0$ is trivial to solve and the zero of $\rho(X,1,a)$ is $X_* \in \mathbb{R}^n$ with $F(X_*) = 0$. The mapping $\rho$ is called a homotopy map.

The homotopy map (usually but not always) is

\begin{equation}
\rho_a(X,\lambda) = \rho(X,\lambda,a) = \lambda F(X) + (1-\lambda)(X - a)
\end{equation}
In standard continuation, the embedding parameter increases monotonically from 0 to 1 as the trivial problem $X - a = 0$ is continuously deformed to the problem $F(X) = 0$.

The theoretical foundation of all globally convergent homotopy methods is given in the following differential geometry theorem:

**Definition** Let $U \subseteq \mathbb{R}^n$ and $V \subseteq \mathbb{R}^n$ be open sets, and let $\rho : U \times [0,1] \times V \rightarrow \mathbb{R}^n$ be a $C^2$ map. $\rho$ is said to be transversal to zero if the Jacobian matrix $D\rho$ has a full rank on $\rho^{-1}(0)$. Here $D\rho = \left[ \frac{\partial \rho}{\partial X}, \frac{\partial \rho}{\partial \lambda} \right]$.

**Parametrized Sard Theorem** If $\rho(X,\lambda,a)$ is transversal to zero, then for almost all $a \in U$ the map $\rho_a(X,\lambda) = \rho(X,\lambda,a)$ is also transversal to zero; that is the Jacobian matrix has full rank on $\rho_a^{-1}(0)$.

The recipe for constructing a globally convergent homotopy algorithm to solve the non-linear system of equations

\[ (4.2) \quad F(X) = 0, \]

where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a $C^2$ map, is as follows: For an open set $U \subseteq \mathbb{R}^n$ construct a $C^2$ homotopy $\rho : U \times [0,1] \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that

1) $\rho(X,\lambda,a)$ is transversal to zero,

2) $\rho_a(X,0) = \rho(X,0,a) = 0$ is trivial to solve and has a unique
solution $X_0$, 
3) $\rho_a(X,1) = F(X)$, 
4) $\rho_a^{-1}(0)$ is bounded.

In our algorithms we use $\rho$ as in 4.1. For readers interested in studying the theory deeper we recommend [19].

HOMPACK. HOMPACK is a mathematical software package that implements several strategies;
1) an ordinary differential equation based algorithm, 
2) a normal flow algorithm, 
3) an augmented Jacobian matrix algorithm.

Our implementation of HOMPACK is restricted to the augmented Jacobian matrix algorithm. The algorithm has four major phases: prediction, correction, step size estimation, and the computation of the solution at $\lambda = 1$. In the step size estimation HOMPACK uses quasi-Newton updates rather than evaluating the Jacobian.

Starting with the predicted point $Z^{(0)} = [X^{(0)}, \lambda^{(0)}]$ the correction is performed by a quasi-Newton iteration defined by

\begin{equation}
Z^{(k+1)} = Z^{(k)} - \begin{bmatrix} A^{(k)} & 0 \\ T^{(2)}T & 0 \end{bmatrix}^{-1} \begin{bmatrix} \rho_a(Z^{(k)}) \\ 0 \end{bmatrix}, \ k = 0, 1, \ldots
\end{equation}

where $A^{(k)}$ is an approximation to the Jacobian matrix $D \rho_a(Z^{(k)})$ and $T^{(2)}$ is the tangent to the zero curve at the previous point.
on the zero curve. In HOMPACK $A^{(k)}$ is updated by the first-Broyden formula, namely:

If $M^{(k)} = \begin{bmatrix} A^{(k)} \\ T(2) \end{bmatrix}$ then

$$
M^{(k+1)} = M^{(k)} + \frac{\Delta \rho_a - M^{(k)} \Delta Z^{(k)}}{\Delta Z^{(k)T} \Delta Z^{(k)}} , \quad k = -1, 0, \ldots
$$

(4.4)

where

$$
\Delta \rho_a = \begin{bmatrix} \rho_a (Z^{(k+1)}) - \rho_a (Z^{(k)}) \\ 0 \end{bmatrix}
$$

(4.5)

and $\Delta Z^{(k)} = Z^{(k+1)} - Z^{(k)}$.

For more details on this phase or any other phase of the solution we refer the reader to [18]. Figure 4.1 shows how the main routines in HOMPACK are called.

The only modification made to HOMPACK in our testings is to change (4.4) by the different updates obtained in Chapter 3. Since in HOMPACK the sparse case is not considered we did not test the sparse update. Also, we tested one case where the update was not exact, as suggested by Theorem 1 of Chapter 3. The case was for the BFGS update. Since $b_+$ can be expressed as

$$
b_+ = J_+ J^{-1} \left[ b + \frac{2t (Y - B S)}{Y^T J^{-1} B S + 2 t^2} \right]
$$

(4.6)
Figure 4.1. A flowchart for the augmented matrix algorithm in HOMPACK.
and since $J_+$ is the "closest" matrix to $J$ in some weighted norm, we expect $J_+ = J$. So using (4.7)

$$J_+ = J + \frac{2t}{Y - B S} BT J^{-1} B S$$

as the secant condition $J_+ S = Y - B S$. So we can take $J_+$ to be the BFGS update of $J$ as in the square matrix case with the secant condition $J_+ S = Y - B S$. So

We will refer to the update given by (4.7) and (4.8) as the "approximate" BFGS update, denoted ABFGS.

Numerical Testings. The problems considered here are well-known functions and widely used. They are taken from the MINPACK test set.

1) Brown function

$$f_1(X) = 10 \left( x_2 - x_1 \right)$$

$$f_2(x) = x_1 + \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

2) Rosenbrock function

$$f_1(X) = 10 \left( x_2 - x_1 \right)$$

$$f_2(x) = \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

$$f_3(x) = \left| x_1 - \frac{1}{10} \right| + \left[ 10 \left( x_2 - 1 \right) \right]$$

$$f_4(x) = \left[ 1 - \cos \left( 2\pi x_1 \right) \right] \left[ 1 - \cos \left( 2\pi x_2 \right) \right]$$

$$f_5(x) = \left( x_1^2 + x_2^2 \right)^{\frac{1}{2}}$$

$$f_6(x) = \left( x_1^2 - x_2^2 \right)^{\frac{1}{2}}$$

$$f_7(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_8(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_9(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{10}(X) = 10 \left( x_2 - x_1 \right)$$

$$f_{11}(x) = \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

$$f_{12}(x) = \left| x_1 - \frac{1}{10} \right| + \left[ 10 \left( x_2 - 1 \right) \right]$$

$$f_{13}(x) = \left[ 1 - \cos \left( 2\pi x_1 \right) \right] \left[ 1 - \cos \left( 2\pi x_2 \right) \right]$$

$$f_{14}(x) = \left( x_1^2 + x_2^2 \right)^{\frac{1}{2}}$$

$$f_{15}(x) = \left( x_1^2 - x_2^2 \right)^{\frac{1}{2}}$$

$$f_{16}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{17}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{18}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{19}(X) = 10 \left( x_2 - x_1 \right)$$

$$f_{20}(x) = \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

$$f_{21}(x) = \left| x_1 - \frac{1}{10} \right| + \left[ 10 \left( x_2 - 1 \right) \right]$$

$$f_{22}(x) = \left[ 1 - \cos \left( 2\pi x_1 \right) \right] \left[ 1 - \cos \left( 2\pi x_2 \right) \right]$$

$$f_{23}(x) = \left( x_1^2 + x_2^2 \right)^{\frac{1}{2}}$$

$$f_{24}(x) = \left( x_1^2 - x_2^2 \right)^{\frac{1}{2}}$$

$$f_{25}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{26}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{27}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{28}(X) = 10 \left( x_2 - x_1 \right)$$

$$f_{29}(x) = \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

$$f_{30}(x) = \left| x_1 - \frac{1}{10} \right| + \left[ 10 \left( x_2 - 1 \right) \right]$$

$$f_{31}(x) = \left[ 1 - \cos \left( 2\pi x_1 \right) \right] \left[ 1 - \cos \left( 2\pi x_2 \right) \right]$$

$$f_{32}(x) = \left( x_1^2 + x_2^2 \right)^{\frac{1}{2}}$$

$$f_{33}(x) = \left( x_1^2 - x_2^2 \right)^{\frac{1}{2}}$$

$$f_{34}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{35}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{36}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{37}(X) = 10 \left( x_2 - x_1 \right)$$

$$f_{38}(x) = \left( \sum_{i=1}^{n} x_i \right) - (n+1), \quad 2 \leq i \leq n$$

$$f_{39}(x) = \left| x_1 - \frac{1}{10} \right| + \left[ 10 \left( x_2 - 1 \right) \right]$$

$$f_{40}(x) = \left[ 1 - \cos \left( 2\pi x_1 \right) \right] \left[ 1 - \cos \left( 2\pi x_2 \right) \right]$$

$$f_{41}(x) = \left( x_1^2 + x_2^2 \right)^{\frac{1}{2}}$$

$$f_{42}(x) = \left( x_1^2 - x_2^2 \right)^{\frac{1}{2}}$$

$$f_{43}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{44}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$

$$f_{45}(x) = \left( \frac{x_1^2}{4} + \frac{x_2^2}{25} - 1 \right)^{\frac{1}{2}}$$
3) Helical valley problem

\[ f_1(X) = 10 - (x_3 - 10 \varphi) \]
\[ f_2(X) = 10 \left[ (x_1^2 + x_2^2)^{1/2} - 1 \right] \]
\[ f_3(X) = x_3 \]

\[ \varphi = \begin{cases} 
\frac{1}{2\pi} \arctan \left( \frac{x_2}{x_1} \right) & \text{if } x > 0 \\
\frac{1}{2\pi} \arctan \left( \frac{x_2}{x_1} \right) + 0.5 & \text{if } x < 0 
\end{cases} \]

4) Extended Rosenbrock function (n = 4)

\[ f_{2i-1}(X) = 10 \left( x_{2i} - x_{2i-1}^2 \right) \]
\[ f_{2i}(X) = 1 - x_{2i} \]

5) Powell-singular function

\[ f_1(X) = x_1 + 10x_2 \]
\[ f_2(X) = 5^{1/2} \left( x_3 - x_4 \right) \]
\[ f_3(X) = (x_2 - 2x_3)^2 \]
\[ f_4(X) = 10^{1/2} \left( x_1 - x_4 \right)^2 \]

Problem 1 was considered as a zero finding of a nonlinear system of equations while problems 2-5 were taken as unconstrained optimization problems where the objective function to minimize is

\[ f(X) = \sum_{i=1}^{n} f_i^2 \]

Even though the Jacobian of the Brown function is not symmetric we still tested the PSB update on it as the (n-1)x(n-1) principle submatrix of the Jacobian is symmetric.
For stopping HOMPACK uses four error tolerances, they are: ARCRE, ARCAE, ANSRE, and ANSAE. The first two are used to determine when the iterates have converged to the zero curve while the last two are used for the answer at $\lambda = 1$. Unless otherwise specified, their values are:

\[
\begin{align*}
\text{ARCRE} &= \text{ANSRE} = 0.5 \times 10^{-8} \\
\text{ARCAE} &= \text{ANSAE} = 0.5 \times 10^{-22}
\end{align*}
\]

For each test made we will report the update used, the number of Jacobian evaluations (NJE), the number of function evaluations (NFE) and the point the zero curve emanated from. We refer to each update by the name of the corresponding update it extends. The computations were done in double precision on a MicroVAX running ULTRIX.

For the Brown function with the zero curve emanating from $(0,0,0,0,0)$ the zero $(1,1,1,1,1)$ of $F(X) = (f_1, f_2, f_3, f_4, f_5)$ was obtained with results given in Table 4.1.

Table 4.1  
Test results for the Brown function with the zero curve emanating from $(0,0,0,0)$.

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>6</td>
<td>39</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>15</td>
<td>137</td>
</tr>
<tr>
<td>PSB</td>
<td>6</td>
<td>39</td>
</tr>
</tbody>
</table>
The Rosenbrock function was tested from various starting points. With the zero curve emanating from \((0,0)\), we obtained the results in Table 4.2.

Table 4.2
Test results for the Rosenbrock function with the zero curve emanating from \((0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>12</td>
<td>123</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>35</td>
<td>424</td>
</tr>
<tr>
<td>PSB</td>
<td>12</td>
<td>145</td>
</tr>
<tr>
<td>BFGS</td>
<td>66</td>
<td>838</td>
</tr>
<tr>
<td>DFP</td>
<td>13</td>
<td>182</td>
</tr>
<tr>
<td>ABFGS</td>
<td>**</td>
<td>**</td>
</tr>
</tbody>
</table>

** indicates that the algorithm did not converge.
With the zero curve emanating from (.2,.2) we obtained the results in Table 4.3.

### Table 4.3

Test results for the Rosenbrock function with the zero curve emanating from (.2,.2)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>18</td>
<td>206</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>76</td>
<td>871</td>
</tr>
<tr>
<td>PSB</td>
<td>15</td>
<td>189</td>
</tr>
<tr>
<td>BFGS</td>
<td>90</td>
<td>1145</td>
</tr>
<tr>
<td>DFP</td>
<td>24</td>
<td>338</td>
</tr>
<tr>
<td>ABFGS</td>
<td>**</td>
<td>**</td>
</tr>
</tbody>
</table>
With the zero curve emanating from \((.7,.7)\) we obtained the results in Table 4.4.

### Table 4.4

Test results for the Rosenbrock function with the zero curve emanating from \((.7,.7)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>20</td>
<td>204</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>67</td>
<td>1037</td>
</tr>
<tr>
<td>PSB</td>
<td>20</td>
<td>253</td>
</tr>
<tr>
<td>BFGS</td>
<td>68</td>
<td>890</td>
</tr>
<tr>
<td>DFP</td>
<td>29</td>
<td>419</td>
</tr>
<tr>
<td>ABFGS</td>
<td>6</td>
<td>86</td>
</tr>
</tbody>
</table>
With the zero curve emanating from (.8,.8) we obtained the results in Table 4.5.

Table 4.5

Test results for the Rosenbrock function with the zero curve emanating from (.8,.8)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>55</td>
<td>871</td>
</tr>
<tr>
<td>PSB</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>BFGS</td>
<td>239</td>
<td>3834</td>
</tr>
<tr>
<td>DFP</td>
<td>38</td>
<td>587</td>
</tr>
<tr>
<td>ABFGS</td>
<td>**</td>
<td>**</td>
</tr>
</tbody>
</table>

The error tolerances here were changed from $0.5 \times 10^{-6}$ and $0.5 \times 10^{-12}$ to $0.5 \times 10^{-12}$ and $0.5 \times 10^{-30}$ respectively.
The helical valley problem was tested with two different starting points.

With the zero curve emanating from \((3,0,0)\) we obtained the results in Table 4.6.

Table 4.6

Test results for the helical valley problem with the zero curve emanating from \((3,0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>12</td>
<td>76</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>43</td>
<td>483</td>
</tr>
<tr>
<td>PSB</td>
<td>12</td>
<td>77</td>
</tr>
<tr>
<td>BFGS</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>DFP</td>
<td>12</td>
<td>78</td>
</tr>
<tr>
<td>ABFGS</td>
<td>12</td>
<td>81</td>
</tr>
</tbody>
</table>
With the zero curve emanating from \((5,0,0)\) we obtained the results in Table 4.7.

Table 4.7

Test results for the helical valley problem with the zero curve emanating from \((5,0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>11</td>
<td>67</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>36</td>
<td>376</td>
</tr>
<tr>
<td>PSB</td>
<td>11</td>
<td>68</td>
</tr>
<tr>
<td>BFGS</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>DFP</td>
<td>12</td>
<td>102</td>
</tr>
<tr>
<td>ABFGS</td>
<td>12</td>
<td>99</td>
</tr>
</tbody>
</table>
For the extended Rosenbrock function with the zero curve emanating from \((1,0,1,0)\) we obtained the results in Table 4.8.

Table 4.8
Test results for the extended Rosenbrock function with the zero curve emanating from \((1,0,1,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>20</td>
<td>210</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>28</td>
<td>392</td>
</tr>
<tr>
<td>PSB</td>
<td>25</td>
<td>308</td>
</tr>
<tr>
<td>BFGS</td>
<td>102</td>
<td>1201</td>
</tr>
<tr>
<td>DFP</td>
<td>33</td>
<td>416</td>
</tr>
<tr>
<td>ABFGS</td>
<td>87</td>
<td>1075</td>
</tr>
</tbody>
</table>
With the zero curve emanating from \((3,0,0,0)\) we obtained the results in Table 4.9.

Table 4.9

Test results for the extended Rosenbrock function with the zero curve emanating from \((3,0,0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>21</td>
<td>214</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>49</td>
<td>566</td>
</tr>
<tr>
<td>PSB</td>
<td>38</td>
<td>450</td>
</tr>
<tr>
<td>BFGS</td>
<td>103</td>
<td>1199</td>
</tr>
<tr>
<td>DFP</td>
<td>52</td>
<td>627</td>
</tr>
<tr>
<td>ABFGS</td>
<td>75</td>
<td>928</td>
</tr>
</tbody>
</table>
With the zero curve emanating from (.2, .2, .2, .2) we obtained the results in Table 4.10.

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>17</td>
<td>194</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>37</td>
<td>468</td>
</tr>
<tr>
<td>PSB</td>
<td>28</td>
<td>318</td>
</tr>
<tr>
<td>BFGS</td>
<td>303</td>
<td>4968</td>
</tr>
<tr>
<td>DFP</td>
<td>25</td>
<td>348</td>
</tr>
<tr>
<td>ABFGS</td>
<td>65</td>
<td>845</td>
</tr>
</tbody>
</table>

The usual error tolerances were used except for the BFGS which did not converge until the error tolerances were changed from $0.5 \times 10^{-8}$ and $0.5 \times 10^{-22}$ to $0.5 \times 10^{-12}$ and $0.5 \times 10^{-30}$ respectively.
With the zero curve emanating from $(3,1,0,5)$ we obtained the results in Table 4.11.

### Table 4.11

Test results for the extended Rosenbrock function with the zero curve emanating from $(3,1,0,5)$

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>80</td>
<td>833</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>103</td>
<td>1238</td>
</tr>
<tr>
<td>PSB</td>
<td>109</td>
<td>1320</td>
</tr>
<tr>
<td>BFGS</td>
<td>199</td>
<td>2343</td>
</tr>
<tr>
<td>DFP</td>
<td>100</td>
<td>1187</td>
</tr>
<tr>
<td>ABFGS</td>
<td>102</td>
<td>1291</td>
</tr>
</tbody>
</table>

In the last results the second Broyden update could only produce the answer accurate to five decimal places while the PSB update produced it to 16 decimal places, which is why it took the second Broyden method fewer Jacobian evaluation to converge. Changing the error tolerances did not improve the performance of the second Broyden update.
With the zero curve emanating from \((.9,.9,.9,.9,\)) we obtained the results in Table 4.12.

### Table 4.12

Test results for the extended Rosenbrock function with the zero curve emanating from \((.9,.9,.9,.9,\))

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>PSB</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>BFGS</td>
<td>66</td>
<td>811</td>
</tr>
<tr>
<td>DFP</td>
<td>17</td>
<td>218</td>
</tr>
<tr>
<td>ABFGS</td>
<td>35</td>
<td>451</td>
</tr>
</tbody>
</table>
And finally with the Powell-singular function the following results were obtained.

With the zero curve emanating from $(3,-1,0,1)$ we obtained the results in Table 4.13.

Table 4.13

Test results for the Powell-singular function with the zero curve emanating from $(3,-1,0,1)$.

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>24</td>
<td>234</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>73</td>
<td>827</td>
</tr>
<tr>
<td>PSB</td>
<td>24</td>
<td>266</td>
</tr>
<tr>
<td>BFGS</td>
<td>97</td>
<td>1116</td>
</tr>
<tr>
<td>DFP</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>ABFGS</td>
<td>89</td>
<td>1053</td>
</tr>
</tbody>
</table>
With the zero curve emanating from \((3,0,0,0)\) we obtained the results in Table 4.14.

Table 4.14

Test results for the Powell-singular function with the zero curve emanating from \((3,0,0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>22</td>
<td>228</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>45</td>
<td>531</td>
</tr>
<tr>
<td>PSB</td>
<td>22</td>
<td>280</td>
</tr>
<tr>
<td>BFGS</td>
<td>92</td>
<td>1071</td>
</tr>
<tr>
<td>DFP</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>ABFGS</td>
<td>86</td>
<td>1001</td>
</tr>
</tbody>
</table>
With the zero curve emanating from \((5,0,0,0)\) we obtained the results in Table 4.15.

Table 4.15

Test results for the Powell-singular function with the zero curve emanating from \((5,0,0,0)\)

<table>
<thead>
<tr>
<th>update</th>
<th>NJE</th>
<th>NFE</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Broyden</td>
<td>25</td>
<td>245</td>
</tr>
<tr>
<td>Second Broyden</td>
<td>47</td>
<td>548</td>
</tr>
<tr>
<td>PSB</td>
<td>35</td>
<td>409</td>
</tr>
<tr>
<td>BFGS</td>
<td>98</td>
<td>1124</td>
</tr>
<tr>
<td>DFP</td>
<td>**</td>
<td>**</td>
</tr>
<tr>
<td>ABFGS</td>
<td>86</td>
<td>1027</td>
</tr>
</tbody>
</table>

Conclusion and Remarks. It is not our intention to prove or claim which update is best to use for what problem. It is usually expected that updates that preserve positive definiteness of the Jacobian will work best on minimization problems, but since our algorithm for tracking the zero curve does not take into account the fact that the problem is an optimization one, and consequently no special techniques were employed, it will be difficult to deduce which update is the best one.
The above testing is limited, and more is required to make final judgements. It appears that the first Broyden update is usually best, but some other updates may converge more reliably (especially BFGS). It is our hope that further investigations into the subject and a deeper study of the behavior of the zero curves of the homotopy maps will give a better insight into how things should work. And hopefully this may tell us why the results do not reflect the usual understanding of the relative effectiveness of the various updates in the square-matrix case, namely the fact that the updates that preserve positive definiteness of the Jacobian usually perform better on minimization problems.
REFERENCES


