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CONVERGENCE THEOREMS FOR LEAST-CHANGE SECANT UPDATE METHODS*

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Abstract. The purpose of this paper is to present a convergence analysis of least change secant methods in which part of the derivative matrix being approximated is computed by other means. The theorems and proofs given here can be viewed as generalizations of those given by Broyden–Dennis–Moré [J. Inst. Math. Appl. 12 (1973), pp. 223–246] and by Dennis–Moré [Math. Comp., 28 (1974), pp. 549–560]. The analysis is done in the orthogonal projection setting of Dennis–Schnabel [SIAM Rev., 21 (1980), pp. 443–459] and many readers might feel that it is easier to understand. The theorems here readily imply local and q-superlinear convergence of all the standard methods in addition to proving these results for the first time for the sparse symmetric method of Marwil and Toint and the nonlinear least-squares method of Dennis–Gay–Welsch.

1. Introduction. The methods of interest in this paper are iterative methods for solving

$$F(x)=0, \qquad F:\mathbb{R}^n \to \mathbb{R}^n \tag{1.1}$$

in the case when the complete computation of F' is infeasible. In these methods it is assumed that, after k iterations, x_k, $F(x_k)$, and a nonsingular matrix $B_k \approx F'(x_k)$ or B_k^{-1} are available. The next iterate x_{k+1} is chosen with the use of s_k, the quasi-Newton step defined by $B_k s_k = -F(x_k)$. The goal is to be able, eventually, to take $x_{k+1} = x_k + s_k$, and to this end one wishes to choose B_{k+1} to look as much like $F'(x_{k+1})$ as is feasible.

Often, in practice, $F'(x_{k+1})$ is partially available either from some special purpose approximation method or from actual evaluation of partial derivatives. Thus we consider approximations of the form

$$F'(x_{k+1}) \approx B_{k+1} = C(x_{k+1}) + A_{k+1}, \tag{1.2}$$

where $C(x_{k+1})$ is a "computed part" of $F'(x_{k+1})$ determined by a function C from $\mathbb{R}^n$ to $\mathbb{R}^{n\times n}$, the space of real $n\times n$ matrices, and where A_{k+1} is an "approximated part" of $F'(x_{k+1})$ chosen to look as much like $[F'(x_{k+1}) - C(x_{k+1})]$ as is feasible.

Throughout this paper we need the following conditions on F and C.

The standard hypothesis on F and C. Let F be differentiable in an open convex neighborhood Ω of a point $x_* \in \mathbb{R}^n$ for which $F(x_*)=0$, and let $\gamma \geqq 0$, $\gamma_c \geqq 0$ and $p \in (0, 1]$, be such that, for $x \in \Omega$,

$$|F'(x) - F'(x_*)| \leqq \gamma |x - x_*|^p \quad \text{and} \quad |C(x) - C(x_*)| \leqq \gamma_c |x - x_*|^p,$$

where $|\cdot|$ denotes a vector norm and its subordinate operator norm.

In the next section, we introduce an interesting and important example, which we use for illustrative purposes in the sequel, in which (1.2) is a very natural form for B_{k+1} to take. A particular approach to choosing A_{k+1}, which we review below, is fundamental to the methods considered here.

In choosing A_{k+1}, it is reasonable to make use of currently available information about $[F'(x_{k+1}) - C(x_{k+1})]$. Information which is characteristically used in determining

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A_{k+1} is contained in vectors $s_k = x_{k+1} - x_k$ and $y_k \approx [F'(x_{k+1}) - C(x_{k+1})]s_k$. One requires that A_{k+1} be in or near the affine subspace $\mathcal{Q}(y_k, s_k) \subseteq \mathbb{R}^{n\times n}$, where for any $s, y \in \mathbb{R}^n$ with $s \neq 0$, $\mathcal{L}(y, s) = \{M \in \mathbb{R}^{n\times n}: Ms = y\}$ is the set of matrix generalizations of quotients of y by s. Also, it is often known that F' or $(F' - C)$ has some special structure such as symmetry or a particular pattern of sparsity. This information about $[F'(x_{k+1}) - C(x_{k+1})]$ can usually be exploited by requiring that A_{k+1} be in some affine subspace $\mathcal{A} \subseteq \mathbb{R}^{n\times n}$, the elements of which reflect the special structure of F' or $(F' - C)$.

Dennis and Schnabel [14] outline a criterion for choosing A_{k+1} as follows. If A_{k+1} is required to be in an affine subspace $\mathcal{A} \subseteq \mathbb{R}^{n\times n}$ then set $s_k = x_{k+1} - x_k$, choose $y_k \approx P_{\mathcal{A}}[F'(x_{k+1}) - C(x_{k+1})]s_k$, and select A_{k+1} to uniquely solve

$$\min_{\bar{A} \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y_k, s_k))} \|\bar{A} - A_k\|,$$

where $\|\cdot\|$ is a given inner-product norm on $\mathbb{R}^{n\times n}$, $P_{\mathcal{A}}$ is the corresponding projection onto $\mathcal{A}$, and for any affine subspaces $\mathcal{A}_1, \mathcal{A}_2 \subseteq \mathbb{R}^{n\times n}$, $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ is the set of elements of $\mathcal{A}_1$ for which the distance to $\mathcal{A}_2$ in the norm $\|\cdot\|$ is minimal.

This way of picking A_{k+1} is called the *least-change secant criterion*, because it calls for making the smallest possible change in A_k to get A_{k+1} consistent with making A_{k+1} look as much like a matrix generalization of the quotient of y_k by s_k as any element of $\mathcal{A}$ can. If A_{k+1} is determined according to this criterion, then we call it a *least-change secant update* of A_k. The *secant* part of the name refers to the way y_k is usually chosen. In a very important subclass of these methods, one uses $C(x) \equiv 0$ and chooses $y_k = F(x_{k+1}) - F(x_k)$, so that if $n = 1$ and $\mathcal{A} = \mathbb{R}^1$, then the secant method results.

Both the affine subspace $\mathcal{A}$ and the norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$ play critical roles when determining A_{k+1} by the least-change secant criterion. The norm $\|\cdot\|$ is often taken to be the Frobenius norm on $\mathbb{R}^{n\times n}$, denoted here by $\|\cdot\|_{\mathcal{F}}$ and defined by $\|M\|_{\mathcal{F}} = (\text{tr}\,\{MM^T\})^{1/2}$ for $M \in \mathbb{R}^{n\times n}$. With $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$, $C(x) \equiv 0$ and $y_k = F(x_{k+1}) - F(x_k)$, Broyden's method [3], [7], [12] results when $\mathcal{A} = \mathbb{R}^{n\times n}$, and the Powell symmetric Broyden (PSB) method [24], [7], [12] results when $\mathcal{A}$ is the subspace of symmetric matrices in $\mathbb{R}^{n\times n}$. If $\mathcal{A}$ is some subspace of sparse matrices, then the resulting method is the Schubert or sparse Broyden method [27], [6], [21]. If the matrices in $\mathcal{A}$ are further restricted to be symmetric as well as sparse, then one obtains the sparse symmetric update methods of Marwil [21] and Toint [32]. (See [14] for proofs.)

In addition to the Frobenius norm, other norms on $\mathbb{R}^{n\times n}$ are of interest when there is some natural scaling associated with the problem (1.1). For example when F' is positive-definite and symmetric at a solution x_* of (1.1), then a choice of a factorization $F'(x_*) = J_* J_*^T$ suggests a problem $\hat{F}(\hat{x}) \equiv J_*^{-1} F(J_*^{T^{-1}}\hat{x}) = 0$ induced by the scaling $\hat{x} = J_*^T x$, which has the desirable property that $\hat{F}'(\hat{x}_*) = I$, where $\hat{x}_* = J_*^T x_*$. To further illustrate the desirable properties of this scaling, consider the problem of minimizing a nonlinear functional $f: \mathbb{R}^n \to \mathbb{R}^1$, in which one seeks to solve $F(x) \equiv \nabla f(x) = 0$. In this case, the assumption that $F'(x_*)$ is positive definite and symmetric is reasonable, and the scaling yields a variable space for which the contour curves of the quadratic approximation of f at x_* are circular. Of course, the matrix $F'(x_*)$ which determines the ideal scaling is unknown in practice. Nevertheless, one can exploit the existence of a natural scaling in iterative procedures for solving (1.1).

Once a scaling is chosen, then A_{k+1} can be determined by first scaling A_k, s_k and y_k, to get $\hat{A}_k$, $\hat{s}_k$ and $\hat{y}_k$, respectively, then obtaining $\hat{A}_{k+1} \in \hat{\mathcal{A}}$ as a least-change secant update on the scaled problem, and finally removing the scale to get A_{k+1}. If $\hat{\mathcal{A}} \neq \mathcal{A}$ then $\hat{A}_{k+1}$ may be elusive but if a choice of a (nonsingular) scaling matrix J is made and if the norm on $\mathbb{R}^{n\times n}$ for the scaled problem is the Frobenius norm, then such a procedure is equivalent to selecting A_{k+1} to uniquely solve

$$\min_{\bar{A}\in\mathcal{M}(\mathcal{A},\,\mathcal{Q}(y_k,\,s_k))} \|\bar{A}-A_k\|_W,$$

where W is the positive-definite, symmetric "weight" matrix $W=JJ^T$ and $\|\cdot\|_W$ is the "weighted" Frobenius norm on $\mathbb{R}^{n\times n}$ defined by

$$\|M\|_W=(\mathrm{tr}\,\{W^{-1}MW^{-1}M^T\})^{1/2}$$

for $M\in\mathbb{R}^{n\times n}$.[1]

To clarify the relation between the weighted and unweighted Frobenius norms, we note that if W is any positive-definite, symmetric matrix and if $W=JJ^T$ is any factorization of W, then

$$\|M\|_W^2=\mathrm{tr}\,\{J^{T^{-1}}J^{-1}MJ^{T^{-1}}J^{-1}M^T\}=\|J^{-1}MJ^{T^{-1}}\|^2$$

for $M\in\mathbb{R}^{n\times n}$. A useful conceptual way to view this relation is as $\|M\|_W=\|\hat{M}\|$, where $\hat{M}=J^{-1}MJ^{T^{-1}}$.

By a *fixed-scale least-change secant update method*, we mean a method in which each successive A_{k+1} is a least-change secant update of its predecessor A_k and in which the *same* inner-product norm on $\mathbb{R}^{n\times n}$ is chosen at every iteration. Examples of methods of this type are those named above. There is a more general class of methods which we call *(iteratively) rescaled least-change secant update methods.* In these methods, the problem (1.1) is assumed to have an associated unknown natural scaling, and the norm on $\mathbb{R}^{n\times n}$ used to determine each least-change secant update is itself updated at each iteration to reflect current information about the natural scaling. Examples of rescaled least-change secant update methods are a single-rank update method due to Pearson [23], [7], which is obtained with $\mathcal{A}=\mathbb{R}^{n\times n}$, and the Davidon–Fletcher–Powell (DFP) method [8], [17], [7], [12], in which $\mathcal{A}$ is the subspace of symmetric matrices in $\mathbb{R}^{n\times n}$. In both of these methods, $C(x)\equiv 0$, $y_k=F(x_{k+1})-F(x_k)$, and the norm on $\mathbb{R}^{n\times n}$ used to define a least-change secant update after k iterations is a weighted Frobenius norm $\|\cdot\|_W$, where W is any positive-definite, symmetric matrix satisfying $Ws_k=y_k$ (so $\mathcal{A}=\hat{\mathcal{A}}$).

In addition to methods of the above type, in which all or part of B_{k+1} is determined from B_k by the least-change secant criterion, there are methods in which all or part of B_{k+1}^{-1} is determined from B_k^{-1} by an inverse analogue of the least-change secant criterion. In these methods, one considers approximations of the form

$$F'(x_{k+1})^{-1}\approx B_{k+1}^{-1}\equiv K_{k+1}=C(x_{k+1})+A_{k+1},$$

where $C(x_{k+1})$ is a "computed part" of $F'(x_{k+1})^{-1}$ determined by $C:\mathbb{R}^n\to\mathbb{R}^{n\times n}$ and where A_{k+1} is an "approximated part" of $F'(x_{k+1})^{-1}$ chosen to look as much like $[F'(x_{k+1})^{-1}-C(x_{k+1})]$ as is feasible. The *least-change inverse-secant criterion* for determining A_{k+1} is the following: If A_{k+1} is required to be in an affine subspace $\mathcal{A}\subseteq\mathbb{R}^{n\times n}$, then set $s_k=x_{k+1}-x_k$, choose y_k and w_k such that $\{P_{\mathcal{A}}[F'(x_{k+1})^{-1}-C(x_{k+1})]+C(x_{k+1})\}y_k\approx s_k$ and $w_k\approx P_{\mathcal{A}}[F'(x_{k+1})^{-1}-C(x_{k+1})]y_k$, and select A_{k+1} to uniquely solve

$$\min_{\bar{A}\in\mathcal{M}(\mathcal{A},\,\mathcal{Q}(w_k,\,y_k))} \|\bar{A}-A_k\|,$$

where $\|\cdot\|$ is a given inner-product norm on $\mathbb{R}^{n\times n}$ and $P_{\mathcal{A}}$ is the associated orthogonal projection onto $\mathcal{A}$.

[1] Notice that this is a different definition of the weighted Frobenius norm from that usually used in this context. It has been changed to reflect invariance with respect to factorization of W.

By a *fixed-scale least-change inverse-secant update method*, we mean a method in which each successive A_{k+1} is determined from its predecessor A_k according to this criterion with the *same* inner-product norm on $\mathbb{R}^{n\times n}$ at each iteration. With $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$, $C(x)\equiv 0$, $y_k = F(x_{k+1}) - F(x_k)$ and $w_k = s_k$, examples of fixed-scale least-change inverse-secant update methods are provided by a method of Broyden [3], in which $\mathcal{A} = \mathbb{R}^{n\times n}$, and a method of Greenstadt [19] in which $\mathcal{A}$ is the subspace of symmetric matrices in $\mathbb{R}^{n\times n}$. These methods have been found in practice to be generally less successful than their respective least-change secant update counterparts, namely, the usual Broyden's method and the PSB method.

There are also *(iteratively) rescaled least-change inverse-secant update methods*, in which the problem (1.1) is assumed to have an associated ideal scaling and the norm on $\mathbb{R}^{n\times n}$ used to determine least-change inverse-secant updates is updated at each iteration to reflect current information about the ideal scaling. Examples of such methods, in which $C(x)\equiv 0$, $y_k = F(x_{k+1}) - F(x_k)$ and $w_k = s_k$, are a single-rank update method due to G. McCormick (see Pearson [23]), obtained by taking $\mathcal{A} = \mathbb{R}^{n\times n}$, and the Broyden–Fletcher–Goldfarb–Shanno (BFGS) method [4], [5], [16], [18], [28], [12], [26], which results when $\mathcal{A}$ is the subspace of symmetric matrices in $\mathbb{R}^{n\times n}$. In both of these methods, the norm on $\mathbb{R}^{n\times n}$ after k iterations is taken to be weighted Frobenius norm $\|\cdot\|_W$, where W is a positive-definite, symmetric matrix satisfying $Wy_k = s_k$ (so again, $\mathcal{A} = \hat{\mathcal{A}}$).

We strongly suspect that the partially computed rescaled least-change inverse-secant update methods may turn out to be valuable new tools for dealing with problems in which $C(x)$ is not only feasible to compute, but for which $C(x_k)s = -F(x_k)$ is more desirable to solve than $(C(x_k) + A_k)s = -F(x_k)$, where C and A take their meaning from (1.2). We will suggest such a case in § 5.

In this paper, we exploit the projections and associated techniques used by Dennis and Schnabel [14] in deriving least-change secant updates in order to make general convergence statements for methods using such updates. The results offered here unify, simplify and extend previously known local convergence results for such methods [7]. Furthermore, the focus on the role of orthogonal projections onto approximating subspaces, in the proofs of these results, seems better in keeping with the philosophy of least-change secant updates than approaches taken in proofs of previous results.

In § 2, a new expression for the least-change secant update is offered. This expression lends itself to the formulation of a theorem to the effect that least-change secant updates exhibit a very general form of a phenomenon known as bounded deterioration. In § 3, the results of § 2 are applied in conjunction with the results of the appendix described below to obtain general local linear and superlinear convergence theorems for fixed-scale least-change secant update methods. With the aid of a lemma relating certain weighted Frobenius norms, these theorems are adapted in § 4 to yield analogous results for rescaled least-change seçant update methods. In § 5, the corresponding theorems are stated for fixed-scale and for rescaled least-change inverse-secant update methods. The results offered here are so formulated that if the functions under consideration satisfy the standard hypothesis and if $\mathcal{A}$ is chosen properly then local superlinear convergence is assured not only for the methods named above but also for a broad range of variations of those methods in which C is not zero. Examples of such variations are the nonlinear least-squares algorithms of Dennis–Gay–Welsch [13], which we draw upon in the following for illustrative purposes, and the Hessian approximation for the augmented Lagrangian exploited by Tapia [31].

Fundamental to our analysis are certain results concerning the local convergence of general quasi-Newton iterations of the form

$$x_{k+1} = x_k - B_k^{-1}F(x_k)$$

for solving (1.1). These results are generalizations of the bounded deterioration theorems of Broyden–Dennis–Moré [7] and of the characterization of superlinear convergence given by Dennis and Moré [11]. We feel that they are interesting and attractive in their own right, and we have accordingly separated them in an appendix which is essentially independent of the main body of the paper.

2. Least-change secant updates. Suppose that one is given $A \in \mathbb{R}^{n\times n}$, an affine subspace $\mathcal{A} \subseteq \mathbb{R}^{n\times n}$, and vectors $s, y \in \mathbb{R}^{n\times n}$ with $s \neq 0$. Assume that an inner-product norm $\|\cdot\|$ is specified on $\mathbb{R}^{n\times n}$, and denote $\mathcal{Q}(y, s)$ by $\mathcal{Q}$ for convenience. In accordance with the introduction, we define the least-change secant update of A in $\mathcal{A}$ (denoted by A_+) to be the unique solution of the problem

$$\min_{\bar{A}\in\mathcal{M}(\mathcal{A},\,\mathcal{Q})} \|\bar{A}-A\|.$$

This is to say that A_+ is the element of $\mathcal{A}$ nearest to A of all the nearest points of $\mathcal{A}$ to $\mathcal{Q}$.

It is shown in [14] that, if $A \in \mathcal{A}$, then A_+ is given by

$$A_+ = \lim_{k\to\infty} (P_{\mathcal{A}}P_{\mathcal{Q}})^k A. \tag{2.1}$$

Unless indicated otherwise, our convention throughout this paper is that the projection which is orthogonal with respect to a given inner-product norm and which maps onto a given affine subspace is denoted by "P", with the subspace or affine subspace indicated as a subscript. The projection orthogonal to this projection is indicated by a superscript "$\perp$". Thus $P_{\mathcal{A}}$ and $P_{\mathcal{Q}}$ are the orthogonal projections onto $\mathcal{A}$ and $\mathcal{Q}$, respectively, while $P_{\mathcal{A}}^{\perp} = I - P_{\mathcal{A}}$ and $P_{\mathcal{Q}}^{\perp} = I - P_{\mathcal{Q}}$. For questions concerning orthogonal projections in inner-product spaces see Halmos [20].

In the case $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$ and $A \in \mathcal{A}$, the following expression is given in [14] for A_+:

$$A_+ = A + P_{\mathcal{S}}\left(\frac{vs^T}{s^Ts}\right), \tag{2.2}$$

where $\mathcal{S}$ is the parallel subspace to $\mathcal{A}$ and where v is any solution of the linear least-squares problem

$$\min_{v\in\mathbb{R}^n} \left| P_{\mathcal{S}}\left(\frac{vs^T}{s^Ts}\right)s - (y - As)\right|_2^2,$$

in which $|\cdot|_2$ denotes the Euclidean norm on $\mathbb{R}^n$.

To obtain an extension of (2.1) valid for an arbitrary $A \in \mathbb{R}^{n\times n}$, we observe that $A_+ = (P_{\mathcal{A}}A)_+$ for every $A \in \mathbb{R}^{n\times n}$. Indeed, if $\bar{A} \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$, then

$$\|\bar{A}-A\|^2 = \|\bar{A} - P_{\mathcal{A}}A - P_{\mathcal{A}}^{\perp}A\|^2 = \|\bar{A} - P_{\mathcal{A}}A\|^2 + \|P_{\mathcal{A}}^{\perp}A\|^2,$$

and it follows that the solutions of

$$\min_{\bar{A}\in\mathcal{M}(\mathcal{A},\,\mathcal{Q})} \|\bar{A}-A\| \quad\text{and}\quad \min_{\bar{A}\in\mathcal{M}(\mathcal{A},\,\mathcal{Q})} \|\bar{A}-P_{\mathcal{A}}A\|,$$

are identical. From this observation and (2.1), one sees immediately that

$$A_+ = \lim_{k\to\infty} (P_{\mathcal{A}}P_{\mathcal{Q}})^k P_{\mathcal{A}}A \tag{2.3}$$

for every $A \in \mathbb{R}^{n\times n}$.

We now derive a general expression for A_+ by a straightforward evaluation of the limit of iterated projections in (2.3). This general expression is, of course, equivalent to (2.2) when $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$ and $A \in \mathcal{A}$. Although (2.2) and similar expressions in [14] are very useful for deriving many of the best known update formulas, this general expression is better suited to our purposes than (2.2) even in the case $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$ and $A \in \mathcal{A}$. In the lemma below, we offer an expression for a general limit of iterated projections and, in addition, a useful characterization of $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ for general affine subspaces $\mathcal{A}_1$ and $\mathcal{A}_2$. The expression in the lemma then yields the desired general expression for A_+.

Suppose that $\mathcal{A}_1$ and $\mathcal{A}_2$ are affine subspaces of $\mathbb{R}^m$. For a given inner product on $\mathbb{R}^m$, let P_1 and P_2 be the respective orthogonal projections onto $\mathcal{A}_1$ and $\mathcal{A}_2$. For appropriate subspaces $\mathcal{S}_1$, $\mathcal{S}_2$ and vectors $x_1 \in \mathcal{S}_1^\perp$, $x_2 \in \mathcal{S}_2^\perp$, one has

$$\begin{aligned} \mathcal{A}_i &= \{x_i + x : x \in \mathcal{S}_i\}, \qquad & i &= 1, 2, \\ P_i x &= x_i + Q_i x, & i &= 1, 2, \quad x \in \mathbb{R}^m, \end{aligned} \tag{2.4}$$

where Q_i is the orthogonal projection onto $\mathcal{S}_i$ and $\mathcal{S}_i$ is the subspace parallel to $\mathcal{A}_i$. Note that $P_i(0) = x_i$ is called the *normal* to $\mathcal{A}_i$.

LEMMA 2.1. *For* $x \in \mathbb{R}^m$,

$$\begin{aligned} x_+ &\equiv \lim_{k\to\infty} (P_1P_2)^k P_1 x \\ &= \left[\sum_{j=0}^{\infty} (Q_1Q_2)^j\right] x_1 + \left[\sum_{j=0}^{\infty} (Q_1Q_2)^j\right] Q_1 x_2 + Qx \\ &= (I - Q_1Q_2)^{-1} x_1 + (I - Q_1Q_2)^{-1} Q_1 x_2 + Qx, \end{aligned} \tag{2.5}$$

where Q is the orthogonal projection onto $\mathcal{S}_1 \cap \mathcal{S}_2$ and $(I - Q_1Q_2)^{-1}$ is the inverse of the restriction of $(I - Q_1Q_2)$ to $(\mathcal{S}_1 \cap \mathcal{S}_2)^\perp$. Furthermore, $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ is an affine subspace of $\mathbb{R}^m$ with parallel subspace $\mathcal{S}_1 \cap \mathcal{S}_2$, $P_{\mathcal{M}(\mathcal{A}_1,\mathcal{A}_2)} x = x_+$ for $x \in \mathbb{R}^m$, and

$$\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2) = \{(I - Q_1Q_2)^{-1} x_1 + (I - Q_1Q_2)^{-1} Q_1 x_2 + x : x \in \mathcal{S}_1 \cap \mathcal{S}_2\}.$$

Proof. We use induction on k to establish that for any $x \in \mathbb{R}^m$,

$$(P_1P_2)^k P_1 x = \left[\sum_{j=0}^{k-1} (Q_1Q_2)^j\right] x_1 + \left[\sum_{j=0}^{k-1} (Q_1Q_2)^j\right] Q_1 x_2 + (Q_1Q_2)^k P_1 x \tag{2.6}$$

for all $k \geqq 1$. If (2.6) holds for all $k \geqq 1$, then one sees from the technical Lemma 2.2 below, by taking limits as $k \to \infty$, that

$$\begin{aligned} x_+ &= \left[\sum_{j=0}^{\infty} (Q_1Q_2)^j\right] x_1 + \left[\sum_{j=0}^{\infty} (Q_1Q_2)^j\right] Q_1 x_2 + QP_1 x \\ &= (I - Q_1Q_2)^{-1} x_1 + (I - Q_1Q_2)^{-1} Q_1 x_2 + QP_1 x. \end{aligned}$$

Since $QP_1 = Q$, (2.5) follows. To start the induction, we have from (2.4) that for any $x \in \mathbb{R}^m$,

$$(P_1P_2)P_1 x = P_1(P_2(P_1(x))) = x_1 + Q_1(x_2 + Q_2P_1x) = x_1 + Q_1x_2 + Q_1Q_2P_1x, \tag{2.7}$$

which is (2.6) for $k = 1$. If (2.6) holds for any $k \geqq 1$, then since $(P_1P_2)^k P_1 x \in \mathcal{A}_1$, we have from (2.4) and (2.7) that

$$
\begin{aligned}
(P_1P_2)^{k+1}P_1x &= x_1+Q_1[x_2+Q_2(P_1P_2)^kP_1x] = x_1+Q_1x_2+Q_1Q_2[(P_1P_2)^kP_1x] \\
&= x_1+(Q_1Q_2)\left[\sum_{j=0}^{k-1}(Q_1Q_2)^j\right]x_1 \\
&\quad +Q_1x_2+(Q_1Q_2)\left[\sum_{j=0}^{k-1}(Q_1Q_2)^j\right]Q_1x_2+(Q_1Q_2)(Q_1Q_2)^kP_1x \\
&= \left[\sum_{j=0}^{k}(Q_1Q_2)^j\right]x_1+\left[\sum_{j=0}^{k}(Q_1Q_2)^j\right]Q_1x_2+(Q_1Q_2)^{k+1}P_1x,
\end{aligned}
$$

and the induction is complete.

It is essentially shown in [14, lemma following Thm. 3.1] that $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ is an affine subspace of $\mathbb{R}^m$ with parallel subspace $\mathcal{S}_1 \cap \mathcal{S}_2$. For completeness, we prove this result here. Note that $x \in \mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ if and only if $x \in \mathcal{A}_1$ and the distance from x to $\mathcal{A}_2$ is minimal, i.e., if and only if x solves

$$\min_{\bar{x}\in\mathcal{A}_1} \|\bar{x}-P_2\bar{x}\|.$$

Now $\|\bar{x}-P_2\bar{x}\| = \|\bar{x}-x_2-Q_2\bar{x}\| = \|Q_2^\perp\bar{x}-x_2\|$ for every $\bar{x}\in\mathbb{R}^m$, so $x \in \mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ if and only if x solves

$$\min_{\bar{x}\in\mathcal{A}_1} \|Q_2^\perp\bar{x}-x_2\|.$$

This is to say that $x \in \mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ if and only if $x \in \mathcal{A}_1$ and $Q_2^\perp x$ is the (unique) orthogonal projection of x_2 onto the affine subspace $Q_2^\perp(\mathcal{A}_1)$. Let x_0 be any element of $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$. One sees that $x \in \mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ if and only if $x \in \mathcal{A}_1$ and $Q_2^\perp x = Q_2^\perp x_0$, i.e., if and only if $(x-x_0) \in \mathcal{S}_1 \cap \mathcal{S}_2$. It follows that $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$ is an affine subspace of $\mathbb{R}^m$ with parallel subspace $\mathcal{S}_1 \cap \mathcal{S}_2$.

It follows from [14, Thm. 3.1] that $P_{\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)}\, x = x_+$ for $x \in \mathcal{A}_1$. From this, one concludes that $P_{\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)}x = x_+$ for arbitrary $x \in \mathbb{R}^m$ via the same elementary argument by which (2.3) is obtained from (2.1). An immediate consequence is that

$$\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2) = \{(I-Q_1Q_2)^{-1}x_1+(I-Q_1Q_2)^{-1}Q_1x_2+x : x\in\mathcal{S}_1\cap\mathcal{S}_2\},$$

and the proof is complete. Note that $[(I-Q_1Q_2)^{-1}x_1+(I-Q_1Q_2)^{-1}Q_1x_2]$ is in $(\mathcal{S}_1 \cap \mathcal{S}_2)^\perp$ and, hence, is the normal to $\mathcal{M}(\mathcal{A}_1, \mathcal{A}_2)$.

LEMMA 2.2. *Assume that, with respect to some inner product on* $\mathbb{R}^m$, π_1 *and* π_2 *are orthogonal projections onto subspaces* Σ_1 *and* Σ_2 *of* $\mathbb{R}^m$. *Let* π *be the orthogonal projection onto* $\Sigma = \Sigma_1 \cap \Sigma_2$. *Then*

(i) *both* $\pi_1\pi_2$ *and* $I-\pi_1\pi_2$ *map* $\Sigma^\perp$ *onto itself and* Σ *onto itself*;

(ii) *the restriction of* $\pi_1\pi_2$ *to* $\Sigma^\perp$ *has norm strictly less than* 1 *in the operator norm induced by the inner product vector norm on* $\Sigma^\perp$;

(iii) $\lim_{k\to\infty}(\pi_1\pi_2)^k = \pi$ *on* $\mathbb{R}^m$;

(iv) $\lim_{k\to\infty}\sum_{j=0}^{k}(\pi_1\pi_2)^j \equiv \sum_{j=0}^{\infty}(\pi_1\pi_2)^j = (I-\pi_1\pi_2)^{-1}$ *on* $\Sigma^\perp$;

(v) $(I-\pi_1\pi_2)^{-1}\pi_1\pi_2^\perp = \pi^\perp$ *on* Σ_1.

The limits in (iii) *and* (iv) *are taken in the operator norms induced by the inner-product vector norm over* $\mathbb{R}^m$ *on* Σ *and* $\Sigma^\perp$, *respectively.*

Proof. We prove (ii) and (v) only. (The proof of (i) follows immediately from $x = \pi_1\pi_2x+\pi_1^\perp\pi_2x+\pi_2^\perp x$ and (iii) and (iv) are immediate consequences of (i) and (ii).)

To prove (ii), it suffices to show that $\|\pi_1\pi_2 x\| < \|x\|$ for each nonzero $x \in \Sigma^\perp$ since $\Sigma^\perp$ is finite-dimensional and, hence, has a compact unit sphere. For any $x \in \mathbb{R}^m$, one has $\pi_2 x = \pi_1\pi_2 x + \pi_1^\perp \pi_2 x$, so

$$\|\pi_1\pi_2 x\|^2 = \langle \pi_2 x, \pi_1\pi_2 x\rangle \leqq \|\pi_2 x\| \|\pi_1\pi_2 x\|, \tag{2.8}$$

with equality if and only if either $\pi_2 x = \pi_1\pi_2 x$ or $\pi_1\pi_2 x = 0$. Now if $x \in \Sigma^\perp$ and $\pi_2 x = \pi_1\pi_2 x$, then $\pi_1\pi_2 x \in \Sigma \cap \Sigma^\perp = \{0\}$. Consequently, if $x \in \Sigma^\perp$, then equality holds in (2.8) if and only if $\pi_1\pi_2 x = 0$. One concludes that for nonzero $x \in \Sigma^\perp$, either $0 = \|\pi_1\pi_2 x\| < \|x\|$ or $0 < \|\pi_1\pi_2 x\| < \|\pi_2 x\| \leqq \|x\|$, and (ii) is proved.

To prove (v), note that on Σ_1, $I - \pi_1\pi_2 = \pi_1\pi_2^\perp$ so

$$\begin{aligned}(I - \pi_1\pi_2)^{-1}\pi_1\pi_2^\perp &= \lim_{k\to\infty}\left[\sum_{j=0}^{k} (\pi_1\pi_2)^j\right](I - \pi_1\pi_2)\\ &= \lim_{k\to\infty} [I - (\pi_1\pi_2)^{k+1}]\\ &= I - \pi = \pi^\perp.\end{aligned}$$

This completes the proof of the lemma.

To obtain an expression for A_+ from the general expression (2.5), note that $\mathcal{Q} = \mathcal{Q}(y, s)$ can be written as

$$\mathcal{Q} = \left\{\frac{ys^T}{s^Ts} + M : M \in \mathcal{N}(s)\right\},$$

where $\mathcal{N}(s) = \{M \in \mathbb{R}^{n\times n} : Ms = 0\}$ is the subspace of annihilators of s. Denoting $\mathcal{N}(s)$ by $\mathcal{N}$, one sees that

$$\mathcal{Q} = \left\{P_{\mathcal{N}}^\perp\left(\frac{ys^T}{s^Ts}\right) + M : M \in \mathcal{N}\right\}. \tag{2.9}$$

Similarly, one can write

$$\mathcal{A} = \{A_N + M : M \in \mathcal{S}\}, \tag{2.10}$$

where the "normal" $A_N \in \mathcal{S}^\perp$. Now (2.9) and (2.10) give the form (2.4) for $\mathcal{A}_1 = \mathcal{A}$ and $\mathcal{A}_2 = \mathcal{Q}$. We note for future reference that

$$P_{\mathcal{Q}}M = P_{\mathcal{N}}^\perp\left(\frac{ys^T}{s^Ts}\right) + P_{\mathcal{N}}M \quad \text{and} \quad P_{\mathcal{A}}M = A_N + P_{\mathcal{S}}M$$

for $M \in \mathbb{R}^{n\times n}$. Applying Lemma 2.1 in this case, one immediately obtains from (2.3) and (2.5) the desired expression

$$\begin{aligned}A_+ &= \lim_{k\to\infty} (P_{\mathcal{A}}P_{\mathcal{Q}})^k P_{\mathcal{A}}A\\ &= \left[\sum_{j=0}^{\infty} (P_{\mathcal{S}}P_{\mathcal{N}})^j\right]A_N + \left[\sum_{j=0}^{\infty} (P_{\mathcal{S}}P_{\mathcal{N}})^j\right]P_{\mathcal{S}}P_{\mathcal{N}}^\perp\left(\frac{ys^T}{s^Ts}\right) + P_{\mathcal{S}\cap\mathcal{N}}A \qquad (2.11)\\ &= (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}A_N + (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}P_{\mathcal{S}}P_{\mathcal{N}}^\perp\left(\frac{ys^T}{s^Ts}\right) + P_{\mathcal{S}\cap\mathcal{N}}A\end{aligned}$$

for $A \in \mathbb{R}^{n\times n}$. Note that the normal to $\mathcal{M}(\mathcal{A}, \mathcal{Q})$ is the sum of the first two terms on the right-hand side of (2.11).

At this point, we wish to introduce an example. Although the example is given here for the specific purpose of showing how formula (2.11) can be applied, we refer to it for illustrative purposes throughout the remainder of the paper. The reader is almost certainly acquainted with the very important nonlinear least-squares problem [9], [10], which can be viewed as

$$\min_{x \in \mathbb{R}^n} \tfrac{1}{2} R(x)^T R(x), \qquad R: \mathbb{R}^n \to \mathbb{R}^r. \tag{2.12}$$

In this case for $f(x) = \frac{1}{2} R(x)^T R(x)$, the system of equations to be solved is

$$F(x) \equiv \nabla f(x) = R'(x)^T R(x) = 0,$$

and the associated derivative matrix is

$$F'(x) = \nabla^2 f(x) = R'(x)^T R'(x) + \sum_{i=1}^{r} R_i(x) \nabla^2 R_i(x), \tag{2.13}$$

where $R(x) = (R_1(x), \cdots, R_r(x))^T$. It is usual to assume that $R'(x)$ is available either analytically or from finite differences but that the component Hessians $\nabla^2 R_i(x)$ are not. Hence (1.2) for this case has $C(x_{k+1}) = R'(x_{k+1})^T R'(x_{k+1})$, and A_{k+1} is an approximation to

$$\sum_{i=1}^{r} R_i(x_{k+1}) \nabla^2 R_i(x_{k+1}).$$

A reasonable set of approximators $\mathscr{A}$ for this case is $\mathscr{A} = \mathscr{S} = \{M \in \mathbb{R}^{n \times n} : M = M^T\}$. Setting $x_+ = x + s$ for a given point x and a step s of interest, one sees that a reasonable choice for $y \approx P_{\mathscr{S}}[F'(x_+) - C(x_+)]s$ is

$$y = R'(x_+)^T R(x_+) - R'(x)^T R(x_+), \tag{2.14}$$

since this corresponds to the approximations

$$\nabla^2 R_i(x_+)(x_+ - x) \approx \nabla R_i(x_+) - \nabla R_i(x)$$

for $i = 1, \cdots, r$.

If we take $\|\cdot\| = \|\cdot\|_{\mathscr{F}}$, then the update formula for $A \in \mathscr{A}$ resulting from (2.11) is a Powell symmetric Broyden augmentation [1], [9], [13] of the Gauss–Newton Hessian $R'(x_+)^T R'(x_+)$. To obtain it, we note that since $\mathscr{A} = \mathscr{S}$, we have $A_N = 0$; thus (2.11) yields

$$A_+ = (I - P_{\mathscr{S}} P_{\mathscr{N}})^{-1} P_{\mathscr{S}} P_{\mathscr{N}}^{\perp}\left(\frac{ys^T}{s^T s}\right) + P_{\mathscr{S} \cap \mathscr{N}} A. \tag{2.15}$$

One easily verifies that $P_{\mathscr{S}}(M) = \frac{1}{2}(M + M^T)$, $P_{\mathscr{N}}(M) = M[I - ss^T/s^T s]$, $P_{\mathscr{N}}^{\perp}(\mathscr{M}) = Mss^T/s^T s$ and

$$P_{\mathscr{S} \cap \mathscr{N}}(M) = \left[I - \frac{ss^T}{s^T s}\right]\left[\frac{1}{2}(M + M^T)\right]\left[I - \frac{ss^T}{s^T s}\right] \quad \text{for } M \in \mathbb{R}^{n \times n}.$$

The steps of this verification are as follows. For each operator and subspace in question: (1) show that the operator is an idempotent which is self-adjoint in the Frobenius inner product; (2) show that the range of the operator is contained in the subspace; and (3) show that the operator acts as the identity on the subspace. Since $A \in \mathscr{S}$, (2.15) simplifies to

$$A_+ = (I - P_{\mathscr{S}} P_{\mathscr{N}})^{-1} P_{\mathscr{S}} P_{\mathscr{N}}^{\perp}\left(\frac{ys^T}{s^T s}\right) + \left(I - \frac{ss^T}{s^T s}\right) A \left(I - \frac{ss^T}{s^T s}\right), \tag{2.16}$$

and it remains to determine

$$D \equiv (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right) = \frac{1}{2}(I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}\left(\frac{ys^T}{s^Ts} + \frac{sy^T}{s^Ts}\right), \tag{2.17}$$

the normal to $\mathcal{M}(\mathcal{A}, \mathcal{Q})$.

One sees from (2.16) that $D \in \mathcal{S}$. Hence,

$$\begin{aligned} \frac{1}{2}\left(\frac{ys^T}{s^Ts} + \frac{sy^T}{s^Ts}\right) &= (I - P_{\mathcal{S}}P_{\mathcal{N}})D = P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}D \\ &= \frac{1}{2}\left(D\frac{ss^T}{s^Ts} + \frac{ss^T}{s^Ts}D\right). \end{aligned} \tag{2.18}$$

Since D is also in $(\mathcal{S} \cap \mathcal{N})^{\perp}$, because it is the normal to $\mathcal{M}(\mathcal{A}, \mathcal{Q})$,

$$\begin{aligned} O = P_{\mathcal{S}\cap\mathcal{N}}D &= \left(I - \frac{ss^T}{s^Ts}\right)D\left(I - \frac{ss^T}{s^Ts}\right) \\ &= D - \frac{ss^T}{s^Ts}D - D\frac{ss^T}{s^Ts} + \frac{ss^T}{s^Ts}D\frac{ss^T}{s^Ts}. \end{aligned} \tag{2.19}$$

From (2.18) and (2.19), one obtains

$$D + \frac{ss^T}{s^Ts}D\frac{ss^T}{s^Ts} = \frac{ys^T + sy^T}{s^Ts}.$$

Pre- and post-multiplying this expression by ss^T/s^Ts yields

$$\frac{ss^T}{s^Ts}D\frac{ss^T}{s^Ts} = \frac{s^Tyss^T}{(s^Ts)^2},$$

and it follows that

$$D = \frac{ys^T + sy^T}{s^Ts} - \frac{s^Tyss^T}{(s^Ts)^2}.$$

Substituting this expression for D in (2.16), one obtains the PSB update formula for A_+, i.e.,

$$\begin{aligned} A_+ &= \left(I - \frac{ss^T}{s^Ts}\right)A\left(I - \frac{ss^T}{s^Ts}\right) + \frac{ys^T + sy^T}{s^Ts} - \frac{s^Tyss^T}{(s^Ts)^2} \\ &= A + \frac{(y - As)s^T + s(y - As)^T}{s^Ts} - \frac{s^T(y - As)ss^T}{(s^Ts)^2}. \end{aligned} \tag{2.20}$$

Later, we derive the analogous DFP update formula for A_+, which works better in practice than (2.20) (see [13]). This completes the discussion of the example for the present.

Elements of $\mathcal{M}(\mathcal{A}, \mathcal{Q})$ play an important role in both the statements and the proofs of the convergence theorems in the sequel. We conclude this section with Theorem 2.3 below, which is intended to be a compendium of the properties of elements of $\mathcal{M}(\mathcal{A}, \mathcal{Q})$ which are of interest here. Of particular interest is the inequality (2.24), which shows, in essence, that least-change secant updates exhibit a very general form of bounded deterioration (see [7] or [12]). The inequality (2.24) is used in the sequel in conjunction with the results of the appendix to obtain general local linear and superlinear convergence results for least-change secant update methods and rescaled least-change secant update methods.

THEOREM 2.3. *Let there be given vectors $s, y \in \mathbb{R}^n$ with $s \neq 0$, an affine subspace $\mathcal{A} \subseteq \mathbb{R}^{n\times n}$, and an inner-product norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$. Set $\mathcal{Q} = \mathcal{Q}(y, s)$ and $\mathcal{N} = \mathcal{N}(s)$. Then $\mathcal{M}(\mathcal{A}, \mathcal{Q})$ is an affine subspace of $\mathbb{R}^{n\times n}$ with parallel subspace $\mathcal{S} \cap \mathcal{N}$; in particular, $P_{\mathcal{M}(\mathcal{A},\mathcal{Q})}A = A_+$ for $A \in \mathbb{R}^{n\times n}$ and*

$$(2.21)\quad \mathcal{M}(\mathcal{A}, \mathcal{Q}) = \left\{(I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}A_N + (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right) + M : M \in \mathcal{S} \cap \mathcal{N}\right\}.$$

If $G, \bar{G} \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$, then $P_{\mathcal{N}}^{\perp}G = P_{\mathcal{N}}^{\perp}\bar{G}$, i.e., $Gs = \bar{G}s$. Furthermore, if $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$, then

$$(2.22)\quad P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}G = P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right)$$

and, if $A \in R^{n\times n}$, then

$$(2.23)\quad A_+ = P_{\mathcal{S}\cap\mathcal{N}}A + P_{\mathcal{S}\cap\mathcal{N}}^{\perp}G.$$

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

$$(2.24)\quad \|A_+ - M\| \leqq \|P_{\mathcal{S}\cap\mathcal{N}}(A - M)\| + \|P_{\mathcal{S}\cap\mathcal{N}}^{\perp}(G - M)\|.$$

Proof. The first part of the theorem through (2.21) follows directly from Lemma 2.1 with $\mathcal{A}_1 = \mathcal{A}$ and $\mathcal{A}_2 = \mathcal{Q}$. The second part follows from the fact that if G, $\bar{G} \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$, then $(G - \bar{G}) \in \mathcal{S} \cap \mathcal{N} \subseteq \mathcal{N}$ so $(G - \bar{G})s = 0$ and $P_{\mathcal{N}}^{\perp}(G - \bar{G}) = 0$.

To obtain (2.22), suppose that $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$. Since $P_{\mathcal{S}}P_{\mathcal{N}}^{\perp} = P_{\mathcal{S}}(I - P_{\mathcal{S}}P_{\mathcal{N}})$ and $G = G_+$, one sees from (2.11) that

$$\begin{aligned} P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}G &= P_{\mathcal{S}}(I - P_{\mathcal{S}}P_{\mathcal{N}})G_+ \\ &= P_{\mathcal{S}}(I - P_{\mathcal{S}}P_{\mathcal{N}})\left[(I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}A_N + (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right) + P_{\mathcal{S}\cap\mathcal{N}}G\right] \\ &= P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right). \end{aligned}$$

To obtain (2.23), note that it follows from (2.21) and $G = G_+$ that

$$(2.25)\quad P_{\mathcal{S}\cap\mathcal{N}}^{\perp}G = (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}A_N + (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}P_{\mathcal{S}}P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^Ts}\right)$$

for every $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$. One verifies (2.23) immediately from (2.11) and (2.25).

To obtain (2.24), let $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q})$ and $A, M \in \mathbb{R}^{n\times n}$. From (2.23), one has

$$A_+ - M = P_{\mathcal{S}\cap\mathcal{N}}(A - M) + P_{\mathcal{S}\cap\mathcal{N}}^{\perp}(G - M),$$

and (2.24) follows from the triangle inequality. This completes the proof of the theorem.

3. Fixed-scale least-change secant update methods. We now establish general local linear and superlinear convergence theorems for fixed-scale least-change secant update methods for solving (1.1). Theorem 3.1 below gives conditions sufficient to insure local q-linear convergence for methods which are basically least-change secant update methods but which offer the option of not updating either or both parts of the approximation to F' at each iteration. Theorem 3.3 shows that if the hypotheses of Theorem 3.1 are satisfied, then q-linearly convergent sequences of iterates produced by fixed-scale least-change secant update methods (in which updating both parts of the approximation to F' is required at each iteration) exhibit q-linear convergence which is asymptotically optimal in the sense of having the same associated q-linear rate constant as the idealized stationary iteration that takes $B_k \equiv P_{\mathscr{A}}[F'(x_*) - C(x_*)] + C(x_*)$, the closest matrix to $F'(x_*)$ in $\mathscr{A} + C(x_*)$. Furthermore, necessary and sufficient conditions are given in Theorem 3.3 for q-linearly convergent sequences produced by these methods to be q-superlinearly convergent. The section ends with convergence results for all of the example methods given in [14].

In methods of the type considered here, there are often several reasonable choices of $y_k \approx P_{\mathscr{A}}[F'(x_{k+1}) - C(x_{k+1})]s_k$. It is assumed in the following that there is associated with F and C a choice rule for determining admissible values of $y \in \mathbb{R}^n$, given points x, $x_+ \in \mathbb{R}^n$. By such a choice rule, we mean, strictly speaking, a function $\chi : \mathbb{R}^n \times \mathbb{R}^n \to 2^{\mathbb{R}^n}$, which determines a set $\chi(x, x_+) \subset \mathbb{R}^n$ of admissible values of y for x, $x_+ \in \mathbb{R}^n$. After k iterations of a method of interest for solving (1.1), one uses the choice rule to determine $\chi(x_k, x_{k+1})$ and picks $y_k \in \chi(x_k, x_{k+1})$. In the nonlinear least-squares example of § 2 the reader saw in (2.14) a specific example of a choice of y which profitably reflects problem structure. Another choice of y, given by Broyden and Dennis [9] for which only slightly poorer performance is reported in [13], is $s = x_+ - x$ and

$$y = R'(x_+)^T R(x_+) - R'(x)^T R(x) - R'(x_+)^T R'(x_+)s, \tag{3.1}$$

which is just a specific instance of the "default" condition given by

$$y = F(x_+) - F(x) - C(x_+)s, \qquad s = x_+ - x,$$

which is equivalent to requiring that

$$B_+ s = F(x_+) - F(x), \qquad s = x_+ - x,$$

as in the traditional case when $C(x) = 0$. A third choice of y tested in [13] and given originally by Betts [2] is

$$y = R'(x_+)^T R(x_+) - R'(x)^T R(x) - R'(x)^T R'(x)s, \qquad s = x_+ - x, \tag{3.2}$$

which corresponds to the condition

$$y = F(x_+) - F(x) - C(x)s, \qquad s = x_+ - x,$$

which is equivalent to requiring that

$$B_+ s = F(x_+) - F(x), \qquad s = x_+ - x,$$

where now $B_+ = A_+ + C(x)$, or to requiring that

$$[A_+ + C(x_+)]s = F(x_+) - F(x) + [C(x_+) - C(x)]s.$$

To allow some flexibility in the choice of y, one might take

$$\chi(x, x_+) = \{y^{(1)}, y^{(2)}, y^{(3)}\}, \tag{3.3}$$

where $y^{(1)}$, $y^{(2)}$ and $y^{(3)}$ are determined by (2.14), (3.1) and (3.2), respectively.

THEOREM 3.1. *Let F and C satisfy the standard hypothesis and let $\mathscr{A}$ have the properties that*

$$A_* = P_{\mathscr{A}}[F'(x_*) - C(x_*)] \quad \textit{and} \quad B_* = A_* + C(x_*), \tag{3.4}$$

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

$$|B_*^{-1} P_{\mathscr{A}}^{\perp}[F'(x_*) - C(x_*)]| \leqq r_* < 1. \tag{3.5}$$

Also assume that the choice rule χ for y has the property with $\mathscr{A}$ that there exists an $\alpha \geqq 0$ such that for any $x, x_+ \in \Omega$ and any $y \in \chi(x, x_+)$, one has

$$\|P^{\perp}_{\mathscr{S}\cap\mathscr{N}(s)}(G-A_*)\| \leqq \alpha\sigma(x, x_+)^p \tag{3.6}$$

for every $G \in \mathscr{M}(\mathscr{A}, \mathscr{Q}(y, s))$, where $\sigma(x, x_+) = \max\{|x-x_*|, |x_+-x_*|\}$. Under these hypotheses, if $r \in (r_*, 1)$, then there are positive constants ε_r, δ_r such that for $x_0 \in \mathbb{R}^n$ and $A_0 \in R^{n\times n}$ satisfying $|x_0 - x_*| < \varepsilon_r$ and $|A_0 - A_*| < \delta_r$, any sequence $\{x_k\}$ defined by $B_0 = A_0 + C(x_0)$ and

$$x_{k+1} = x_k - B_k^{-1}F(x_k), \qquad y_k \in \chi(x_k, x_{k+1}),$$

$$B_{k+1} \in \{B_k, A_k + C(x_{k+1}), (A_k)_+ + C(x_k), (A_k)_+ + C(x_{k+1})\},$$

satisfies $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ for $k = 0, 1, 2, \cdots$, where $(A_k)_+$ is the least-change secant update with respect to $s_k = x_{k+1} - x_k$, y_k, and the norm $\|\cdot\|$. Furthermore, $\{\|B_k\|\}$ and $\{\|B_k^{-1}\|\}$ are uniformly bounded.

Proof. The proof is a straightforward application of Theorem 2.3 and Theorem A2.1 of the appendix with condition (3.5) exactly the same as $|I - B_*^{-1}F'(x_*)| \leqq r_* < 1$. We begin with the definition of the update function U in a neighborhood $N = N_1 \times N_2$ of (x_*, B_*). Since B_* is invertible and (3.5) holds, there exist neighborhoods N_1 of x_* and N_2 of B_* such that $N_1 \subseteq \Omega$, N_2 contains only nonsingular matrices, and $x_+ = x - B^{-1}F(x) \in \Omega$ for any $x \in N_1$ and $B \in N_2$. (See the discussion of the inequality (3.5) following the proof.) We define U on $N = N_1 \times N_2$ as follows: For $(x, B) \in N$, set $A = [B - C(x)]$ and

$$U(x, B) = \{B, A + C(x_+)\} \cup \{A_+ + C(x), A_+ + C(x_+): y \in \chi(x, x_+)\},$$

where $x_+ = x - B^{-1}F(x)$ and A_+ is the least-change secant update of A in $\mathscr{A}$ with respect to $s = x_+ - x$, $y \in \chi(x, x_+)$ and the norm $\|\cdot\|$.

We now show that the bounded deterioration inequality

$$\|B_+ - B_*\| \leqq \|B - B_*\| + (\alpha + 3\beta\gamma_c)\sigma(x, x_+)^p, \tag{3.7}$$

holds for $(x, B) \in N$ and $B_+ \in U(x, B)$, where β is a constant such that $\|M\| \leqq \beta|M|$ for any $M \in \mathbb{R}^{n\times n}$. With the inequality established, the theorem follows from Theorem A2.1. We prove the inequality only in the case $B_+ = A_+ + C(x_+)$ for some $y \in \chi(x, x_+)$. The cases $B_+ = A_+ + C(x)$, $B_+ = A + C(x_+)$ and $B_+ = B$, follow more easily with respective smaller constants $(\alpha + \beta\gamma_c)$, $2\beta\gamma_c$ and 0 multiplying $\sigma(x, x_+)^p$. For convenience, set $C(x) = C$, $C(x_+) = C_+$ and $C(x_*) = C_*$. Letting $G \in \mathscr{M}(\mathscr{A}, \mathscr{Q}(y, s))$ and denoting $\mathscr{N} = \mathscr{N}(s)$, we apply (2.24) with $M = B_* - C_+$ to obtain

$$\begin{aligned}
\|B_+ - B_*\| &= \|A_+ + C_+ - B_*\| \\
&\leqq \|P_{\mathscr{S}\cap\mathscr{N}}(A + C_+ - B_*)\| + \|P^{\perp}_{\mathscr{S}\cap\mathscr{N}}(G + C_+ - B_*)\| \\
&\leqq \|A + C - B_* + (C_+ - C_*) - (C - C_*)\| + \|P^{\perp}_{\mathscr{S}\cap\mathscr{N}}(G - A_* + C_+ - C_*)\| \\
&\leqq \|B - B_*\| + \|C_+ - C_*\| + \|C - C_*\| + \|P^{\perp}_{\mathscr{S}\cap\mathscr{N}}(G - A_*)\| + \|P^{\perp}_{\mathscr{S}\cap\mathscr{N}}(C_+ - C_*)\| \\
&\leqq \|B - B_*\| + (\alpha + 3\beta\gamma_c)\sigma(x, x_+)^P.
\end{aligned}$$

The theorem now follows from Theorem A2.1.

Before discussing asymptotically optimal q-linear convergence and q-superlinear convergence, we would like to shed some light on the conditions imposed by the inequalities (3.5) and (3.6) of Theorem 3.1. Considering (3.5) first, assume that F is continuously differentiable in Ω and suppose that one desires an iteration $x_{k+1} = x_k - B_k^{-1}F(x_k)$ to produce iterates satisfying $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ for some $r \in (0, 1)$.

Since

$$x_{k+1}-x_* = \left\{I - B_k^{-1}\int_0^1 F'[x_* + \theta(x_k - x_*)]\, d\theta\right\}(x_k - x_*),$$

a condition which implies $|x_{k+1}-x_*| \leqq r|x_k - x_*|$ for x_k near x_* is that B_k be taken from a set

$$\mathcal{S}(r-\varepsilon) = \{B \in R^{n\times n} : |I - B^{-1}F'(x_*)| < r - \varepsilon\}$$

for some $\varepsilon > 0$. If $B_k = A_k + C(x_k)$ for $A_k \in \mathcal{A}$ and x_k near x_*, then B_k is near the affine subspace $\mathcal{A} + C(x_*)$. Thus in order to obtain $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ with $B_k = A_k + C(x_k)$, it is reasonable to require that $\mathcal{S}(r-\varepsilon) \cap [\mathcal{A} + C(x_*)] \neq \emptyset$ for some $\varepsilon > 0$. If $r_* < r < 1$, then (3.5) guarantees that $P_{\mathcal{A}+C(x_*)}[F'(x_*)] = B_* \in \mathcal{S}(r-\varepsilon) \cap [\mathcal{A} + C(x_*)]$ for $0 < \varepsilon < r - r_*$. Indeed, for $0 < \varepsilon < r - r_*$, (3.5) yields

$$|I - B_*^{-1}F'(x_*)| = |B_*^{-1}[B_* - F'(x_*)]| = |B_*^{-1}P_{\mathcal{A}}^{\perp}[F'(x_*) - C(x_*)]| \leqq r_* < r - \varepsilon.$$

The essential reasoning underlying Theorem 3.1 is that if (3.5) is satisfied and if $|x_0 - x_*| < \varepsilon_r$ and $|A_0 - A_*| = |A_0 + C(x_*) - B_*| < \delta_r$, then one can use the bounded deterioration inequality (3.7) to show that the matrices B_k remain in some set $N_\delta(B_*) = \{B \in R^{n\times n} : \|B - B_*\| < \delta\} \subseteq \mathcal{S}(r-\varepsilon)$. For clarification we offer Fig. 1.

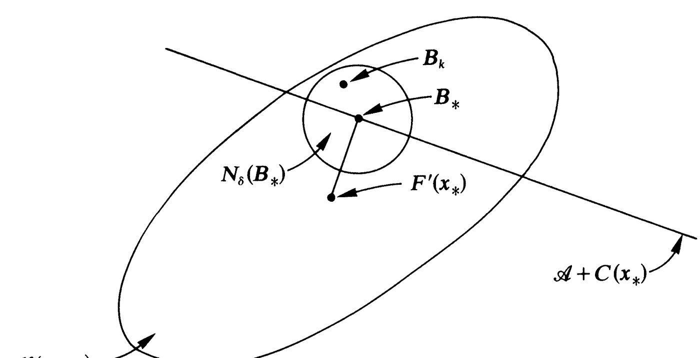

FIG. 1

We now turn to the condition imposed by the inequality (3.6) on the choice rule $\chi(x, x_+)$ for $y \approx P_{\mathcal{A}}[F'(x_+) - C(x_+)]s$. At first glance, the matrices $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$ seem to be a red herring in the matter of choosing y. On deeper consideration, however, it is seen that they embody concepts that have been around for some time. Implicit in a choice of y is a determination of the affine subspace $\mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$ containing A_+, all of the members of which have, by Theorem 2.3, the same action on s. In fact, it follows from Theorem 2.3 that if G, $\bar{G} \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$, then $P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(G - A_*) = P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(\bar{G} - A_*)$. Thus if an inequality of the form (3.6) holds for one member of $\mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$, then it holds for all members, including A_+. Now in passing from A to A_+, one hopes to "correct" the action of A on s to approximate that of $[F'(x_+) - C(x_+)]$ as well as possible among elements of $\mathcal{A}$. It seems reasonable, then, to require that y be such that A_+s approximate $A_*s = P_{\mathcal{A}}[F'(x_*) - C(x_*)]s$ within $O(\sigma(x, x_+)^p|s|)$. Since

$$\begin{aligned}(A_+ - A_*)s &= [P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(A_+ - A_*)]s + [P_{\mathcal{S}\cap\mathcal{N}(s)}(A_+ - A_*)]s \\ &= [P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(A_+ - A_*)]s = [P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(G - A_*)]s\end{aligned} \tag{3.8}$$

for any $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$, one sees that if an inequality (3.6) holds for members of $\mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$ and if κ is such that $|M| \leqq \kappa \|M\|$ for all $M \in \mathbb{R}^{n\times n}$, then

$$|(A_+ - A_*)s| \leqq \kappa\alpha\sigma(x, x_+)^p |s|. \tag{3.9}$$

In light of (3.8), it is doubtful that one can reasonably formulate a less restrictive condition than (3.6), which implies an inequality of the form (3.9).

In practice, a choice rule χ for y is usually suggested by the problem under consideration. To apply Theorem 3.1, one must then determine whether such a "natural" choice rule has the property that an inequality of the form (3.6) is satisfied. The lemma below can sometimes be helpful. Following the lemma, we discuss conditions which imply the existence of an inequality of the form (3.6) and which can be easily verified in most interesting situations.

LEMMA 3.2. *Given $s, y \in \mathbb{R}^n$ with $s \neq 0$, one has*

$$P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s)}(G - A_*) = (I - P_{\mathcal{S}}P_{\mathcal{N}(s)})^{-1} P_{\mathcal{S}} P^{\perp}_{\mathcal{N}(s)}\left[\frac{(y - A_* s)s^T}{s^T s}\right] \tag{3.10}$$

for every $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$.

Proof. Denoting $\mathcal{N}(s)$ by $\mathcal{N}$, one obtains from Lemma 2.2, part (v), (with $\Sigma_1 = \mathcal{A}$) and (2.22) that

$$\begin{aligned} P^{\perp}_{\mathcal{S}\cap\mathcal{N}}(G - A_*) &= (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1} P_{\mathcal{S}} P^{\perp}_{\mathcal{N}}(G - A_*) \\ &= (I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1} P_{\mathcal{S}} P^{\perp}_{\mathcal{N}}\left(\frac{ys^T}{s^T s} - A_*\right) \end{aligned}$$

for $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$. Since $A_*(I - ss^T/s^Ts) \in \mathcal{N}$, one has $P^{\perp}_{\mathcal{N}}A_* = P^{\perp}_{\mathcal{N}}(A_* ss^T/s^Ts)$, and (3.10) follows.

In most applications, one can determine without difficulty whether an inequality

$$|y - A_* s| \leqq \kappa\sigma(x, x_+)^p |s| \tag{3.11}$$

holds for $x, x_+ \in \Omega$ and $y \in \chi(x, x_+)$. In light of (3.10), it is apparent that an inequality (3.11) implies an inequality (3.6) if the operator $(I - P_{\mathcal{S}}P_{\mathcal{N}(s)})^{-1} P_{\mathcal{S}} P^{\perp}_{\mathcal{N}(s)}$ is bounded in norm uniformly in $s = x_+ - x$ for $x, x_+ \in \Omega$. Although this uniform bound might be difficult to verify in general, it is easily seen to be satisfied in two important cases.

The first case is that in which $\mathcal{A} = \mathcal{S} = \mathbb{R}^{n\times n}$. In this case, it follows from Lemma 2.2, part (v), that the operator norm induced by the inner product norm is not more than one, since

$$(I - P_{\mathcal{S}}P_{\mathcal{N}(s)})^{-1} P_{\mathcal{S}} P^{\perp}_{\mathcal{N}(s)} = P^{\perp}_{\mathcal{N}(s)}$$

on $\mathbb{R}^{n\times n}$.

The second case is that in which $\mathcal{A} = \mathcal{S} = \{M \in \mathbb{R}^{n\times n}: M = M^T\}$, and the norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$ is a weighted Frobenius norm $\|\cdot\|_W$ for some positive-definite symmetric weight matrix W. (This includes the case $W = I$ and $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$, of course.) Set $\mathcal{N} = \mathcal{N}(s)$; since $P_{\mathcal{S}}P^{\perp}_{\mathcal{N}}M \in \mathcal{S} \cap (\mathcal{S} \cap \mathcal{N})^{\perp}$ for all $M \in \mathbb{R}^{n\times n}$, it suffices to bound $(I - P_{\mathcal{S}}P_{\mathcal{N}})^{-1}$ on $\mathcal{S} \cap (\mathcal{S} \cap \mathcal{N})^{\perp}$. Setting $v = Ws$, one easily verifies in this case that $P_{\mathcal{S}}M = \frac{1}{2}(M + M^T)$,

$$P_{\mathcal{N}}M = M\left(I - \frac{sv^T}{v^Ts}\right), \quad P^{\perp}_{\mathcal{N}}M = M\frac{sv^T}{v^Ts}, \quad \text{and} \quad P_{\mathcal{S}\cap\mathcal{N}}M = \frac{1}{2}\left(I - \frac{vs^T}{v^Ts}\right)(M + M^T)\left(I - \frac{sv^T}{v^Ts}\right).$$

Suppose that $M \in \mathcal{S} \cap (\mathcal{S} \cap \mathcal{N})^{\perp}$ so that $P_{\mathcal{S}\cap\mathcal{N}}M = 0$, then

$$P_{\mathcal{S}}P_{\mathcal{N}}M = \frac{1}{2}\left[M\left(I - \frac{sv^T}{v^Ts}\right) + \left(I - \frac{vs^T}{v^Ts}\right)M\right]$$

and

$$(P_{\mathscr{S}}P_{\mathscr{N}})^2M = P_{\mathscr{S}}\left\{\frac{1}{2}\left[M\left(I-\frac{sv^T}{v^Ts}\right)+\left(I-\frac{vs^T}{v^Ts}\right)M\left(I-\frac{sv^T}{v^Ts}\right)\right]\right\}$$
$$= \frac{1}{2}[P_{\mathscr{S}}P_{\mathscr{N}}M + P_{\mathscr{S}\cap\mathscr{N}}M] = \tfrac{1}{2}P_{\mathscr{S}}P_{\mathscr{N}}M.$$

It follows, by induction, that $(P_{\mathscr{S}}P_{\mathscr{N}})^jM = 1/2^{j-1}P_{\mathscr{S}}P_{\mathscr{N}}M$ for $j \geqq 1$ and, hence, that

$$\begin{aligned}(I-P_{\mathscr{S}}P_{\mathscr{N}})^{-1}M &= \lim_{k\to\infty}\sum_{j=0}^{k}(P_{\mathscr{S}}P_{\mathscr{N}})^jM \\ &= M + \left(\sum_{j=0}^{\infty}\frac{1}{2^j}\right)P_{\mathscr{S}}P_{\mathscr{N}}M \\ &= (I+2P_{\mathscr{S}}P_{\mathscr{N}})M.\end{aligned}$$

It now follows that $(I-P_{\mathscr{S}}P_{\mathscr{N}})^{-1}P_{\mathscr{S}}P_{\mathscr{N}}^{\perp} = (I+2P_{\mathscr{S}}P_{\mathscr{N}})P_{\mathscr{S}}P_{\mathscr{N}}^{\perp}$, and one concludes that $(I-P_{\mathscr{S}}P_{\mathscr{N}})^{-1}P_{\mathscr{S}}P_{\mathscr{N}}^{\perp}$ is bounded in operator norm by 3 uniformly in s.

In the nonlinear least-squares example of § 2, the update (2.20) is that obtained for a given choice of y with $\|\cdot\| = \|\cdot\|_{\mathscr{F}}$ and $\mathscr{A} = \mathscr{S} = \{M \in R^{n\times n}: M = M^T\}$. It follows from the discussion here that for this choice of $\|\cdot\|$ and $\mathscr{A}$, an inequality of the form (3.6) holds if $y \in \chi(x, x_+)$ satisfies an inequality (3.11) for $x, x_+ \in \Omega$. It is easily verified that an inequality (3.11) holds if $\chi(x, x_+)$ is given by (3.3) and if $F(x) = R'(x)^TR(x)$ and $C(x) = R'(x)^TR'(x)$ satisfy the standard hypothesis.

A condition on χ which is slightly stronger than (3.11) but which can also be easily verified in most applications is that

$$y - A_*s = Es, \quad \text{where } E \in \mathscr{S} \quad \text{and} \quad \|P_{\mathscr{S}\cap\mathscr{N}(s)}^{\perp}E\| \leqq \kappa\sigma(x, x_+)^p \tag{3.12}$$

for $x, x_+ \in \Omega$ and $y \in \chi(x, x_+)$. (Since $Es = (P_{\mathscr{S}\cap\mathscr{N}(s)}^{\perp}E)s$, it is clear that (3.12) implies an inequality (3.11).) It follows from (3.12), (3.10) and Lemma 2.2, part (v), that

$$\begin{aligned}\|P_{\mathscr{S}\cap\mathscr{N}(s)}^{\perp}(G-A_*)\| &= \left\|(I-P_{\mathscr{S}}P_{\mathscr{N}(s)})^{-1}P_{\mathscr{S}}P_{\mathscr{N}(s)}^{\perp}\left(E\frac{ss^T}{s^Ts}\right)\right\| = \|(I-P_{\mathscr{S}}P_{\mathscr{N}(s)})^{-1}P_{\mathscr{S}}P_{\mathscr{N}(s)}^{\perp}E\| \\ &= \|P_{\mathscr{S}\cap\mathscr{N}(s)}^{\perp}E\| \leqq \kappa\sigma(x, x_+)^p\end{aligned}$$

for $G \in \mathscr{M}(\mathscr{A}, \mathscr{Q}(y, s))$. Thus (3.12) implies (3.6) with $\alpha = \kappa$. One can verify without difficulty that (3.12) is satisfied in the case of the nonlinear least-squares example if $\chi(x, x_+)$ is given by (3.3) and if $F(x) = R'(x)^TR(x)$ and $C(x) = R'(x)^TR'(x)$ satisfy the standard hypothesis. In general, under the standard hypothesis and the additional assumption that F' is continuous in Ω, a choice of y for which (3.12) is satisfied is

$$y = P_{\mathscr{A}}\left[\int_0^1 F'[x+t(x_+-x)]\,dt - C(x_+)\right]s. \tag{3.13}$$

While the choice (3.13) might appear somewhat artificial at first, the reader should keep in mind that $\mathscr{A}$ is presumably chosen to reflect the structure of $(F'-C)$. If $[F'(z)-C(x_+)] \in \mathscr{A}$ for all $x_+ \in \Omega$ and $z \in \Omega$, then (3.13) is just the default choice

$$y = F(x_+) - F(x) - C(x_+)s.$$

We now address asymptotically optimal linear convergence and superlinear convergence of fixed-scale least-change secant update methods, below in Theorem 3.3. It is interesting to note that for Fig. 1 in the case $F'(x_*) \in [\mathscr{A} + C(x_*)]$, Theorem 3.3. guarantees q-superlinear convergence.

It is worth pointing out that Theorem 3.3 applies to any sequence $\{x_k\}$ generated by a method of the type considered here and not just a sequence started from a sufficiently good x_0, B_0 as required by Theorem 3.1. It is also in order to remark that, as one would expect, much of the detail of the next proof is familiar to the specialist.

THEOREM 3.3. *Suppose that the hypotheses of Theorem* 3.1 *hold and that for some* $x_0 \in \mathbb{R}^n$ *and* $A_0 \in \mathbb{R}^{n\times n}$, $\{x_k\}$ *is a sequence defined by* $B_0 = A_0 + C(x_0)$ *and*

$$x_{k+1} = x_k - B_k^{-1}F(x_k), \quad y_k \in \chi(x_k, x_{k+1}), \quad B_{k+1} = (A_k)_+ + C(x_{k+1}),$$

that converges q-linearly to x_*, *where* $(A_k)_+$ *is the least-change secant update of* A_k *with respect to* $s_k = x_{k+1} - x_k$, y_k *and the norm* $\|\cdot\|$. *Set* $e_k = x_k - x_*$ *for* $k = 0, 1, 2, \cdots$. *Then*

$$\lim_{k\to\infty} \left| \frac{e_{k+1}}{|e_k|} + B_*^{-1} P_{\mathscr{A}}^{\perp}[F'(x_*) - C(x_*)] \frac{e_k}{|e_k|} \right| = 0,$$

where B_* *is given by* (3.4). *It follows that*

$$\overline{\lim_{k\to\infty}} \frac{|e_{k+1}|}{|e_k|} = \overline{\lim_{k\to\infty}} \left| B_*^{-1} P_{\mathscr{A}}^{\perp}[F'(x_*) - C(x_*)] \frac{e_k}{|e_k|} \right| \leqq r_*$$

and, hence, that $\{x_k\}$ *converges q-superlinearly to* x_* *if and only if*

$$\lim_{k\to\infty} \left| P_{\mathscr{A}}^{\perp}[F'(x_*) - C(x_*)] \frac{e_k}{|e_k|} \right| = 0.$$

In particular, $\{x_k\}$ *converges q-superlinearly to* x_* *if* $[F'(x_*) - C(x_*)] \in \mathscr{A}$.

Proof. In light of Theorem A3.1 of the appendix and the fact that $I - B_*^{-1}F'(x_*) = -B_*^{-1}P_{\mathscr{A}}^{\perp}[F'(x_*) - C(x_*)]$, it suffices to show that $\lim_{k\to\infty} |(B_k - B_*)s_k/|s_k|| = 0$. Now, it follows from Lemma 3.4 below that this is the case if and only if

$$\lim_{k\to\infty} \|P_{\mathscr{N}(s_k)}^{\perp}(B_k - B_*)\| = 0. \tag{3.14}$$

Thus we establish (3.14) to prove the theorem.

Since the iterates satisfy $x_k \in \Omega$ for k large enough we assume, without loss of generality, that all the iterates are in Ω.

For convenience, we again set $C(x_*) = C_*$ and let β be a constant such that $\|M\| \leqq \beta|M|$ for every $M \in \mathbb{R}^{n\times n}$. For each k, set $C(x_k) = C_k$, $C(x_{k+1}) = C_{k+1}$, $\mathscr{N}(s_k) = \mathscr{N}_k$ and $\sigma(x_k, x_{k+1}) = \sigma_k$, and let $G_k \in \mathscr{M}(\mathscr{A}, \mathscr{Q}(y_k, s_k))$. Applying (2.24) with $A = A_k$, $G = G_k$, $M = B_* - C_{k+1}$ and $\mathscr{N} = \mathscr{N}_k$, one obtains, as in the proof of Theorem 3.1,

$$\begin{aligned}
\|B_{k+1} - B_*\| &= \|(A_k)_+ + C_{k+1} - B_*\| \\
&\leqq \|P_{\mathscr{S}\cap\mathscr{N}_k}(A_k + C_{k+1} - B_*)\| + \|P_{\mathscr{S}\cap\mathscr{N}_k}^{\perp}(G_k + C_{k+1} - B_*)\| \\
&\leqq \|P_{\mathscr{S}\cap\mathscr{N}_k}(B_k - B_*)\| + \|(C_{k+1} - C_*)\| + \|C_k - C_*\| \\
&\quad + \|P_{\mathscr{S}\cap\mathscr{N}_k}^{\perp}(G_k - A_*)\| + \|P_{\mathscr{S}\cap\mathscr{N}_k}^{\perp}(C_{k+1} - C_*)\|.
\end{aligned}$$

Since $P_{\mathscr{S}\cap\mathscr{N}_k} = P_{\mathscr{S}\cap\mathscr{N}_k} \cdot P_{\mathscr{N}_k}$ it follows that

$$\|B_{k+1} - B_*\| \leqq \|P_{\mathscr{N}_k}(B_k - B_*)\| + \kappa\sigma_k^p, \tag{3.15}$$

where $\kappa = (\alpha + 3\beta\gamma_c)$.

For each k, set $\eta_k = \|B_k - B_*\|$ and $\psi_k = \|P^{\perp}_{\mathcal{N}_k}(B_k - B_*)\|$. Our goal is to show that $\lim_{k\to\infty} \psi_k = 0$. Note that for any $M \in \mathbb{R}^{n\times n}$, one has

$$\begin{aligned}\|P_{\mathcal{N}_k}M\| &= \|(I - P^{\perp}_{\mathcal{N}_k})M\| \\ &= \{\|M\|^2 - \|P^{\perp}_{\mathcal{N}_k}M\|^2\}^{1/2} \\ &\leqq \|M\| - (2\|M\|)^{-1}\|P^{\perp}_{\mathcal{N}_k}M\|^2.\end{aligned} \tag{3.16}$$

Applying (3.16) to (3.15) with $M = B_k - B_*$, one obtains

$$\eta_{k+1} \leqq \eta_k - (2\eta_k)^{-1}\psi_k^2 + \kappa\sigma_k^p. \tag{3.17}$$

It follows from (3.17)

$$\eta_{k+1} \leqq \eta_k + \kappa\sigma_k^p \leqq \eta_0 + \kappa \sum_{j=0}^{k} \sigma_j^p.$$

Since $\{x_k\}$ converges q-linearly to x_*, the sum on the right-hand side of this inequality converges to a finite limit. Consequently, there exists an η such that $\eta_k \leqq \eta$ for $k = 0, 1, 2, \cdots$, and one obtains from (3.17) that

$$(2\eta)^{-1}\psi_k^2 \leqq \eta_k - \eta_{k+1} + \kappa\sigma_k^p.$$

This inequality yields

$$(2\eta)^{-1}\sum_0^\infty \psi_k^2 \leqq \eta_0 + \kappa \sum_0^\infty \sigma_k^p,$$

from which one concludes that $\lim_{k\to\infty} \psi_k = 0$. This completes the proof of the theorem.

LEMMA 3.4. *Let $|\cdot|$ denote a given vector norm on $\mathbb{R}^n$ and the corresponding operator norm on $\mathbb{R}^{n\times n}$. There exist positive constants κ_1 and κ_2 such that*

$$\kappa_1\|P^{\perp}_{\mathcal{N}(s)}M\| \leqq \frac{|Ms|}{|s|} \leqq \kappa_2\|P^{\perp}_{\mathcal{N}(s)}M\|$$

for all $M \in \mathbb{R}^{n\times n}$ and all nonzero $s \in \mathbb{R}^n$.

Proof. Suppose that $M \in \mathbb{R}^{n\times n}$ and a nonzero $s \in \mathbb{R}^n$ are given. Denote $\mathcal{N} = \mathcal{N}(s)$ for convenience. Since $M = P^{\perp}_{\mathcal{N}}M + P_{\mathcal{N}}M$, one has

$$\frac{|Ms|}{|s|} = \frac{|(P^{\perp}_{\mathcal{N}}M)s|}{|s|} \leqq |P^{\perp}_{\mathcal{N}}M| \leqq \kappa_2\|P^{\perp}_{\mathcal{N}}M\|$$

for a constant κ_2 such that $|\bar{M}| \leqq \kappa_2\|\bar{M}\|$ for every $\bar{M} \in \mathbb{R}^{n\times n}$. On the other hand, since $M(I - ss^T/s^Ts) \in \mathcal{N}$, $P^{\perp}_{\mathcal{N}}M = P^{\perp}_{\mathcal{N}}(Mss^T/s^Ts)$ and

$$\begin{aligned}\|P^{\perp}_{\mathcal{N}}M\| &= \left\|P^{\perp}_{\mathcal{N}}\left(M\frac{ss^T}{s^Ts}\right)\right\| \leqq \left\|M\frac{ss^T}{s^Ts}\right\| \leqq \tilde{\kappa}\left\|M\frac{ss^T}{s^Ts}\right\|_{\mathcal{F}} \\ &= \tilde{\kappa}\frac{|Ms|_2}{|s|_2} \leqq \tilde{\kappa}\frac{\kappa''|Ms|}{\kappa'|s|}.\end{aligned} \tag{3.18}$$

In this expression, $\tilde{\kappa}$ is a constant such that $\|\bar{M}\| \leqq \tilde{\kappa}\|\bar{M}\|_{\mathcal{F}}$ for every $\bar{M} \in \mathbb{R}^{n\times n}$, and κ' and κ'' are constants such that

$$\kappa'|x| \leqq |x|_2 \leqq \kappa''|x|$$

for every $x \in \mathbb{R}^n$, where $|\cdot|_2$ is the l_2 norm on $\mathbb{R}^n$. It follows from (3.18) that $\kappa_1\|P^{\perp}_{\mathcal{N}}M\| \leqq Ms|/|s|$ for $\kappa_1 = \kappa'/\tilde{\kappa}\kappa''$.

There is a very good chance that the techniques of this section can be extended to obtain global theorems of the sort given by Powell [25]. We leave that and other more general results for future work and end the section with an easy corollary that contains all the known local convergence results for fixed-scale least change secant update methods and one apparently new result. We believe this is the first complete local q-superlinear convergence result for the Marwil-Toint sparse symmetric Broyden method as generalized and strengthened in [14]. In this connection, it should be mentioned that it has been shown by Toint [33] that (essentially) linear local convergence implies local q-superlinear convergence for this method.

For brevity we assume the reader knows the algorithms by name and we appeal to [14] for a proof that they are fixed-scale least-change secant update methods.

THEOREM 3.5. *Let F satisfy the standard hypothesis and assume that $F'(x_*)^{-1}$ exists. Let $F'(x_*) \in Z$, the set of matrices with a given fixed sparsity, and let S be the set of symmetric matrices. Then the following are true:*

(i) *The sparse Broyden-Schubert method is locally q-superlinearly convergent.*

(ii) *If $F'(x_*) \in S$ then the sparse symmetric Broyden method is locally q-superlinearly convergent.*

Remark. If $Z = \mathbb{R}^{n\times n}$ then i) and ii) guarantee the convergence of the Broyden and PSB methods.

Proof. Since $A_* = B_* = F'(x_*)$ and $r_* = 0$, we need only verify (3.6) for $\chi(x, x_+) = \{F(x_+) - F(x)\}$; but that is the content of the discussion between Theorems 3.1 and 3.3, and amounts to noting that $|F(x_+) - F(x) - F'(x_*)(x_+ - x)| \leqq \gamma\sigma(x, x_+)^p |s|$.

4. Rescaled least-change secant update methods. As stated in the introduction, (iteratively) rescaled least-change secant update methods are of interest when there is an unknown ideal scaling associated with the problem under consideration. In such a method, the norm on $\mathbb{R}^{n\times n}$ used to define least-change secant updates is itself updated at each iteration to reflect current information about the scaling. Throughout this section, the only norms which we consider on $\mathbb{R}^{n\times n}$ are weighted Frobenius norms. Theorems 4.2 and 4.3 below are analogues for the rescaled methods of Theorems 3.1 and 3.3 for fixed-scale methods respectively. The technical lemma preceding Theorem 4.2 is both of interest in its own right and of crucial importance in the proofs of Theorems 4.2 and 4.3. It allows us to translate the weighted Frobenius norm bounds on $B_{k+1} - B_*$, obtained so easily from Theorem 2.3 for each different norm, to obtain bounded deterioration in the Frobenius norm weighted by $F'(x_*)$, which is assumed to be positive definite and symmetric in this section.

Ideally we would choose $F'(x_*)$ to be the weight matrix at each iteration and the least-change secant updates would be defined with respect to the fixed norm $\|\cdot\|_{F'(x_*)}$. Of course, $F'(x_*)$ is unknown during the iteration and so we wish to choose a weight matrix which incorporates whatever information is currently available about $F'(x_*)$. After k iterations, currently available information about $F'(x_*)$ is usually contained in vectors $s_k = x_{k+1} - x_k$ and $v_k \approx [F(x_{k+1}) - F(x_k)]$. The idea is that if s_k is small and x_k is near x_*, then $v_k \approx F'(x_*)s_k$. Thus it is reasonable to choose a weight matrix W which is positive-definite and symmetric and which satisfies $v_k = Ws_k$. Note that there exists such a matrix W if and only if $v_k^T s_k > 0$.

We assume in this section that there is a given choice rule for determining admissible values not only of $y \approx P_{\mathscr{A}}[F'(x_+) - C(x_+)]s$ but also of $v \approx F'(x_*)s$ for x, $x_+ \in \mathbb{R}^n$ and $s = x_+ - x$. By such a choice rule, we mean a function $\chi: \mathbb{R}^n \times \mathbb{R}^n \to 2^{\mathbb{R}^n \times \mathbb{R}^n}$, which determines a set $\chi(x, x_+) \subseteq \mathbb{R}^n \times \mathbb{R}^n$ of admissible pairs $(v, y) \in \mathbb{R}^n \times \mathbb{R}^n$ for every x, $x_+ \in \mathbb{R}^n$. It is also assumed that χ is such that if $s = x_+ - x \neq 0$ and $(v, y) \in \chi(x, x_+)$, then $v^T s > 0$. This assumption insures that the set of positive-definite symmetric matrices sending s to v is nonempty whenever $s = x_+ - x \neq 0$ and v is an admissible value determined by $\chi(x, x_+)$. This set, which we denote by $\mathcal{Q}_+(v, s)$, can be regarded as the set of admissible weight matrices for defining norms on $\mathbb{R}^{n\times n}$ to be used in determining least-change secant updates. We remark that we have prescribed a joint choice rule for v and y, rather than two independent choice rules, for two reasons: first, a joint choice rule is more general; second, we see reason to anticipate in light of condition (4.18) below that v and y cannot always be chosen independently.

In order to illustrate the role played by the choice rule χ, suppose for the moment that $\mathcal{A} = \mathcal{S} = \{M \in \mathbb{R}^{n\times n} : M = M^T\}$. For $x, x_+ \in \mathbb{R}^n$ with $s = x_+ - x \neq 0$, let $(v, y) \in \chi(x, x_+)$ and $W \in \mathcal{Q}_+(v, s)$, and set $\mathcal{N} = \mathcal{N}(s)$. As remarked in § 3, one has $P_{\mathcal{S}} M = \frac{1}{2}(M + M^T)$, $P_{\mathcal{N}} M = M(I - sv^T/v^T s)$, $P_{\mathcal{N}}^{\perp} M = Msv^T/v^T s$, and

$$P_{\mathcal{S}\cap\mathcal{N}} M = \frac{1}{2}\left(I - \frac{vs^T}{s^T v}\right)(M + M^T)\left(I - \frac{sv^T}{v^T s}\right) \quad \text{for } M \in \mathbb{R}^{n\times n},$$

where all projections are orthogonal with respect to $\|\cdot\|_W$. If $A \in \mathcal{A} = \mathcal{S}$, then (2.11) yields

$$A_+ = (I - P_{\mathcal{S}} P_{\mathcal{N}})^{-1} P_{\mathcal{S}} P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^T s}\right) + \left(I - \frac{vs^T}{v^T s}\right) A \left(I - \frac{sv^T}{v^T s}\right),$$

and, to specify A_+, one must determine

$$D \equiv (I - P_{\mathcal{S}} P_{\mathcal{N}})^{-1} P_{\mathcal{S}} P_{\mathcal{N}}^{\perp}\left(\frac{ys^T}{s^T s}\right) = \frac{1}{2}(I - P_{\mathcal{S}} P_{\mathcal{N}})^{-1}\left(\frac{yv^T}{v^T s} + \frac{vy^T}{v^T s}\right) \tag{4.1}$$

in terms of s, v, y and A. Reasoning as in the nonlinear least-squares example of § 2, we observe from (4.1) that $D \in \mathcal{S} \cap (\mathcal{S} \cap \mathcal{N})^{\perp}$; hence

$$\frac{1}{2}\left(\frac{yv^T}{v^T s} + \frac{vy^T}{v^T s}\right) = \frac{1}{2}\left(D\frac{sv^T}{v^T s} + \frac{vs^T}{v^T s} D\right) \tag{4.2}$$

and

$$0 = \left(I - \frac{vs^T}{v^T s}\right) D \left(I - \frac{sv^T}{v^T s}\right) = D - \frac{vs^T}{v^T s} D - D\frac{sv^T}{v^T s} + \frac{vs^T}{v^T s} D \frac{sv^T}{v^T s}. \tag{4.3}$$

From (4.2) and (4.3), one obtains

$$D + \frac{vs^T}{v^T s} D \frac{sv^T}{v^T s} = \frac{yv^T + vy^T}{v^T s}.$$

Multiplying by $vs^T/v^T s$ on the left and by $sv^T/v^T s$ on the right yields

$$\frac{vs^T}{v^T s} D \frac{sv^T}{v^T s} = \frac{s^T y vv^T}{(v^T s)^2},$$

and it follows that

$$\begin{aligned} A_+ &= \left(I - \frac{vs^T}{v^T s}\right) A \left(I - \frac{sv^T}{v^T s}\right) + \frac{yv^T + vy^T}{v^T s} - \frac{s^T y vv^T}{(v^T s)^2} \\ &= A + \frac{(y - As)v^T + v(y - As)^T}{v^T s} - \frac{s^T (y - As) vv^T}{(v^T s)^2}. \end{aligned} \tag{4.4}$$

This expression for A_+ is also given in [12, Thm. 7.3] and in [13, Thm. 3.1].

It is apparent from (4.4) that A_+ is independent of the particular choice of $W \in \mathcal{Q}_+(v, s)$. (We explain later just why this is the case.) If $C(x) \equiv 0$ and $v = y = F(x_+) - F(x)$, then A_+ is just the usual DFP update of A, and the PSB update of A results if $v = s$, i.e., if I is an admissible weight matrix and $\|\cdot\|_{\mathcal{F}}$ is an admissible norm. Returning to the nonlinear least-squares example of § 2, one sees that if C and y are given as before and if $v = F(x_+) - F(x) = R'(x_+)^T R(x_+) - R'(x)^T R(x)$, then (4.4) is the DFP analogue of (2.20), i.e., A_+ is the DFP augmentation of the Gauss–Newton Hessian $R'(x)^T R'(x)$ considered in [13]. Also, (4.4) reduces to (2.20) if $v = s$.

LEMMA 4.1. *Let $W_* \in \mathbb{R}^{n\times n}$ be positive definite and symmetric, and let κ and ε be positive constants with $\varepsilon < 1$. Suppose that positive parameters σ, p and vectors $s, v \in \mathbb{R}^n$ with $s \neq 0$ satisfy the following*:

(i) $$\sigma^p \leqq \frac{(1-\varepsilon)}{\kappa |W_*^{-1}|_2},$$

(ii) $$|v - W_* s|_2 \leqq \kappa \sigma^p |s|_2,$$

where $|\cdot|_2$ denotes the l_2 norm on $\mathbb{R}^n$ and the corresponding operator norm on $\mathbb{R}^{n\times n}$. Then W, the BFGS *update of W_* sending s to v, is well defined by $W_* = J_* J_*^T$,*

$$w = \sqrt{\frac{v^T s}{s^T W_* s}}\, J_*^T s, \qquad J = J_* + \frac{(v - J_* w) w^T}{w^T w}, \qquad W = JJ^T,$$

and there exists a positive constant β_1, independent of σ, p, s and v, for which

$$\|M\|_{W_*} \leqq (1 + \beta_1 \sigma^p) \|M\|_W \tag{4.5}$$

for every $M \in \mathbb{R}^{n\times n}$. If, in addition,

(i)′ $$\sigma^p \leqq \frac{(1-\varepsilon)\varepsilon}{(1+\sqrt{\varepsilon})\kappa |W_*^{-1}|_2},$$

then there exists a positive constant β_2, independent of σ, p, s and v, for which

$$\|M\|_W \leqq (1 + \beta_2 \sigma^p) \|M\|_{W_*} \tag{4.6}$$

for every $M \in \mathbb{R}^{n\times n}$.

Remark. Note that

$$f(\varepsilon) \equiv \frac{(1-\varepsilon)\varepsilon}{1+\sqrt{\varepsilon}} < 1 - \varepsilon$$

for $0 < \varepsilon < 1$. Thus condition (i)′ is more restrictive than condition (i). Now (i)′ is least restrictive when $f(\varepsilon)$ is maximal, and one can verify that the unique value of ε in $(0, 1)$ at which f is maximized is $\varepsilon = \frac{4}{9}$. Since $f(\frac{4}{9}) = \frac{4}{27}$, conditions (i) and (i)′ in the statement of Lemma 4.1 can be replaced for convenience by the single condition

(i)″ $$\sigma^p \leqq \frac{4}{27\kappa |W_*^{-1}|_2}$$

and (4.5) and (4.6) remain valid with constants β_1 and β_2 independent of σ, p, s and v.

Proof. For convenience, $|\cdot|_2$ is denoted simply by $|\cdot|$ throughout the proof. To show that W is well-defined, we verify that $v^Ts>0$. Indeed,

$$\begin{aligned} v^Ts &= s^TW_*s+(v-W_*s)^Ts \\ &\geqq |W_*^{-1}|^{-1}|s|^2-\kappa\sigma^p|s|^2 \\ &\geqq |W_*^{-1}|^{-1}|s|^2[1-(1-\varepsilon)] \\ &= \varepsilon|W_*^{-1}|^{-1}|s|^2>0. \end{aligned}$$

For future reference, we note that

$$\frac{|s|^2}{v^Ts}\leqq\frac{1}{\varepsilon}|W_*^{-1}|. \tag{4.7}$$

Now let J_* be any matrix for which $W_*=J_*J_*^T$. Then W is given by $W=JJ^T$, where

$$\begin{aligned} J &= J_*+\frac{(v-J_*w)w^T}{|w|^2}, \\ w &= \sqrt{\frac{v^Ts}{|J_*^Ts|^2}}\,J_*^Ts. \end{aligned} \tag{4.8}$$

For any $M\in\mathbb{R}^{n\times n}$,

$$\begin{aligned} \|M\|_{W_*} &= \|J_*^{-1}M(J_*^T)^{-1}\|_{\mathcal{F}} \\ &= \|J_*^{-1}JJ^{-1}M(J^T)^{-1}(J^T)(J_*^T)^{-1}\|_{\mathcal{F}} \\ &\leqq |J_*^{-1}J|^2\|J^{-1}M(J^T)^{-1}\|_{\mathcal{F}} \\ &\leqq |J_*^{-1}J|^2\|M\|_W. \end{aligned}$$

Thus, to establish (4.5), it suffices to show

$$|J_*^{-1}J|^2\leqq(1+\beta_1\sigma^p) \tag{4.9}$$

for a constant β_1 independent of σ, p, s and v.

From (4.8), one obtains

$$J_*^{-1}J=I+\frac{J_*^{-1}(v-J_*w)w^T}{|w|^2}. \tag{4.10}$$

We claim that

$$\frac{|J_*^{-1}(v-J_*w)|}{|w|}\leqq\kappa|W_*^{-1}|\left(\frac{1+\sqrt{\varepsilon}}{\varepsilon}\right)\sigma^p. \tag{4.11}$$

Once this is established then it follows from (4.10) and (4.11) that

$$|J_*^{-1}J|\leqq 1+\kappa|W_*^{-1}|\left(\frac{1+\sqrt{\varepsilon}}{\varepsilon}\right)\sigma^p,$$

from which (4.9) follows easily.

To verify (4.11), note that

$$\begin{aligned} J_*^{-1}(v-J_*w) &= J_*^{-1}\left[(v-W_*s)+\left(1-\sqrt{\frac{v^Ts}{|J_*^Ts|^2}}\right)J_*J_*^Ts\right] \\ &= J_*^{-1}(v-W_*s)+\left(\sqrt{\frac{(W_*s)^Ts}{v^Ts}}-1\right)w. \end{aligned}$$

Since $|w|^2 = v^T s$ and

$$\left|\sqrt{\frac{(W_*s)^T s}{v^T s}}-1\right| = \left|\sqrt{1-\frac{(v-W_*s)^T s}{v^T s}}-1\right| \leqq \left|\frac{(v-W_*s)^T s}{v^T s}\right|,$$

it follows that

$$\begin{aligned}\frac{|J_*^{-1}(v-J_*w)|}{|w|} &\leqq \frac{|J_*^{-1}||v-W_*s|}{(v^Ts)^{1/2}}+\frac{|v-W_*s||s|}{v^Ts} \\ &\leqq \kappa\left\{\frac{|W_*^{-1}|^{1/2}|s|}{(v^Ts)^{1/2}}+\frac{|s|^2}{v^Ts}\right\}\sigma^p.\end{aligned} \tag{4.12}$$

Using (4.7), one immediately obtains (4.11) from (4.12).

Reasoning as above, one sees that to establish (4.6), it suffices to show

$$|J^{-1}J_*|^2 \leqq (1+\beta_2\sigma^p) \tag{4.13}$$

for a constant β_2 independent of σ, p, s and v. Using the Sherman–Morrison–Woodbury formula [22], one sees from (4.10) that

$$J^{-1}J_* = I-\left[1+\frac{w^TJ_*^{-1}(v-J_*w)}{|w|^2}\right]^{-1}\frac{J_*^{-1}(v-J_*w)w^T}{|w|^2}. \tag{4.14}$$

If $\sigma^p \leqq \varepsilon(1-\varepsilon)/(1+\sqrt{\varepsilon})\kappa|W_*^{-1}|$, then it follows from (4.11) that

$$\frac{|J_*^{-1}(v-J_*w)|}{|w|} \leqq \kappa|W_*^{-1}|\left(\frac{1+\sqrt{\varepsilon}}{\varepsilon}\right)\sigma^p \leqq (1-\varepsilon).$$

In light of this inequality and (4.11), one verifies from (4.14) that

$$|J^{-1}J_*| \leqq 1+\kappa|W_*^{-1}|\left(\frac{1+\sqrt{\varepsilon}}{\varepsilon^2}\right)\sigma^p,$$

and (4.13) follows easily. This completes the proof of Lemma 4.1.

Theorems 4.2 and 4.3 below are the counterparts for rescaled least-change secant update methods of Theorems 3.1 and 3.3 for fixed-scale least-change secant update methods. The discussion between Theorems 3.1 and 3.3 is valid here, mutatis mutandis, and we do not repeat it. We remark that Theorems 4.2 and 4.3 together imply the local superlinear convergence of, not only the method of Pearson [23], [7] and the Davidon-Fletcher-Powell method, but also the nonlinear least-squares methods of [13] employing the update (4.4), when $v = F(x_+)-F(x)$ and y is given by (3.3).

Before stating Theorems 4.2 and 4.3, we introduce some notation and offer an explanation of the assumption concerning projections onto $\mathcal{S}$ in Theorem 4.2. The norms of interest here are weighted Frobenius norms defined with respect to a variety of weight matrices. To avoid confusion, we indicate the weighted norm with respect to which a particular projection is orthogonal by writing the weight matrix as a subscript to the projection symbol. Thus, for example, if W is a positive-definite, symmetric weight matrix, then the projection onto $\mathcal{A}$ which is orthogonal with respect to the norm $\|\cdot\|_W$ is denoted by $P_{\mathcal{A},W}$. Given $x, x_+ \in \mathbb{R}^n$ with $s = x_+ - x \neq 0$ and given $(v, y) \in \chi(x, x_+)$, our interest is in the least-change secant update A_+ of $A \in \mathbb{R}^{n\times n}$, defined with respect to s, y and a norm $\|\cdot\|_W$ for $W \in \mathcal{Q}_+(v, s)$. Now there are many possible choices of $W \in \mathcal{Q}_+(v, s)$, and making a particular choice of W and using it explicitly in determining

A_+ seems likely to be somewhat difficult. Thus it seems desirable that A_+ be independent of any particular choice of $W \in \mathcal{Q}_+(v, s)$. In light of (2.11) and the facts that $P^{\perp}_{\mathcal{N}(s),W} = (I - P_{\mathcal{N}(s),W})$ and

$$P_{\mathcal{S}\cap\mathcal{N}(s),W} = \lim_{k\to\infty} (P_{\mathcal{S},W}P_{\mathcal{N}(s),W})^k,$$

this is certainly the case if $P_{\mathcal{S},W}$ and $P_{\mathcal{N}(s),W}$ are independent of W. Now

$$P_{\mathcal{N}(s),W}M = M\left(I - \frac{sv^T}{v^Ts}\right) \quad \text{for } M \in \mathbb{R}^{n\times n},$$

and so $P_{\mathcal{N}(s),W}$ is independent of $W \in \mathcal{Q}_+(v, s)$. One concludes that A_+ is independent of $W \in \mathcal{Q}_+(v, s)$ if $\mathcal{S}$ is such that $P_{\mathcal{S},W}$ is independent of $W \in \mathcal{Q}_+(v, s)$.

We assume the independence of $P_{\mathcal{S},W}$, $W \in \mathcal{Q}_+(v, s)$, in the remainder of this section and in the relevant parts of § 5. This is a valid assumption for the important case of symmetric matrices since $P_{\mathcal{S},W}M = \frac{1}{2}(M + M^T)$ is independent of W, but there is a very important instance of $\mathcal{A}$ in which it is not valid. When $\mathcal{A} = \mathcal{S} = Z$, the set of matrices of a given sparsity, $P_{\mathcal{S},W}M$ is not independent of $W \in \mathcal{Q}_+(v, s)$. This really complicates the search for iteratively rescaled sparse updates, and it is related to the fact that for the scalings derived from factoring elements of $\mathcal{Q}_+(v, s)$, $Z \neq \hat{Z}$. The reader will find a complete discussion in [14, § 4].

THEOREM 4.2. *Let F and C satisfy the standard hypothesis. Let $\mathcal{S}$ have the property that for any $s, v \in \mathbb{R}^n$ with $s^Tv > 0$, the projection $P_{\mathcal{S},W}$ is independent of $W \in \mathcal{Q}_+(v, s)$. In addition, let $\mathcal{A}$ have the properties that*

$$A_* = P_{\mathcal{A},F'(x_*)}[F'(x_*) - C(x_*)] \quad \text{and} \quad B_* = A_* + C(x_*) \tag{4.15}$$

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

$$|B_*^{-1}P^{\perp}_{\mathcal{A},F'(x_*)}[F'(x_*) - C(x_*)]| \leqq r_* < 1. \tag{4.16}$$

Also assume that the choice rule χ for v and y has the property, with respect to $\mathcal{A}$, that there exist $\alpha_1, \alpha_2 \geqq 0$ such that for any distinct pair $x, x_+ \in \Omega$ determining $s = x_+ - x$ and $(v, y) \in \chi(x, x_+)$, one has

$$|v - F'(x_*)s| \leqq \alpha_1\sigma(x, x_+)^p|s| \tag{4.17}$$

and

$$\|P^{\perp}_{\mathcal{S}\cap\mathcal{N}(s),W}(G - A_*)\|_W \leqq \alpha_2\sigma(x, x_+)^p \tag{4.18}$$

for every $G \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(y, s))$, where $\sigma(x, x_+) = \max\{|x - x_*|, |x_+ - x_*|\}$ and $W \in \mathcal{Q}_+(v, s)$. Under these hypotheses, if $r \in (r_*, 1)$, then there are positive constants ε_r, δ_r such that for $x_0 \in \mathbb{R}^n$ and $A_0 \in \mathbb{R}^{n\times n}$ satisfying $|x_0 - x_*| < \varepsilon_r$ and $|A_0 - A_*| < \delta_r$, a sequence $\{x_k\}$ defined by $B_0 = A_0 + C(x_0)$ and

$$x_{k+1} = x_k - B_k^{-1}F(x_k), \qquad (v_k, y_k) \in \chi(x_k, x_{k+1})$$

$$B_{k+1} \in \{B_k, A_k + C(x_{k+1}), (A_k)_+ + C(x_k), (A_k)_+ + C(x_{k+1})\},$$

satisfies $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ for $k = 0, 1, 2, \cdots$, where $(A_k)_+$ is the least-change secant update of A_k with respect to $s_k = x_{k+1} - x_k$, y_k, and any norm $\|\cdot\|_W$, $W \in \mathcal{Q}_+(v_k, s_k)$. Furthermore, $\{\|B_k\|_{F'(x_*)}\}$ and $\{\|B_k^{-1}\|_{F'(x_*)}\}$ are uniformly bounded.

Proof. The proof very closely parallels that of Theorem 3.1. Since B_* is invertible and (4.16) holds, there exist neighborhoods N_1 of x_* and N_2 of B_* which are sufficiently small that $N_1 \subseteq \Omega$, N_2 contains only nonsingular matrices and $x_+ = x - B^{-1}F(x) \in \Omega$ for every $(x, B) \in N = N_1 \times N_2$. One sees from (4.17) that there exists a constant κ for which

$$|v - F'(x_*)s|_2 \leqq \kappa\sigma(x, x_+)^p |s|_2 \tag{4.19}$$

for any distinct $x, x_+ \in \Omega$, $s = x_+ - x$ and $(v, y) \in \chi(x, x_+)$. If necessary, one can further restrict the size of N_1 and N_2 so that if $(x, B) \in N$ and $x_+ = x - B^{-1}F'(x)$, then

$$\sigma(x, x_+)^p \leqq \frac{4}{27\kappa|F'(x_*)^{-1}|_2}. \tag{4.20}$$

Define an update function U on N as follows: For $(x, B) \in N$, set $A = [B - C(x)]$ and

$$U(x, B) = \{B, A + C(x_+)\} \cup \{A_+ + C(x), A_+ + C(x_+) \colon (v, y) \in \chi(x, x_+)\},$$

where $x_+ = x - B^{-1}F(x)$ and A_+ is the least-change secant update of A in $\mathscr{A}$ with respect to $s = x_+ - x$, y and a norm $\|\cdot\|_W$ for $W \in \mathscr{Q}_+(v, s)$.

In order to apply Theorem A2.1, we now show that there exist constants κ_1 and κ_2 for which a bounded deterioration inequality

$$\|B_+ - B_*\|_{F'(x_*)} \leqq [1 + \kappa_1\sigma(x, x_+)^p]\|B - B_*\|_{F'(x_*)} + \kappa_2\sigma(x, x_+)^p, \tag{4.21}$$

holds for $(x, B) \in N$ and $B_+ \in U(x, B)$. As in the proof of Theorem 3.1, it suffices to consider the case $B_+ = A_+ + C(x_+)$ for a choice $(v, y) \in \chi(x, x_+)$. In light of (4.19), (4.20) and the remark after Lemma 4.1, one sees from Lemma 4.1, with $W_* = F'(x_*)$ and $W = \overline{F'(x_*)}$, that there exist constants β_1 and β_2 independent of x, B, y and v for which

$$\|M\|_{F'(x_*)} \leqq [1 + \beta_1\sigma(x, x_+)^p]\|M\|_{\overline{F'(x_*)}} \tag{4.22}$$

and

$$\|M\|_{\overline{F'(x_*)}} \leqq [1 + \beta_2\sigma(x, x_+)^p]\|M\|_{F'(x_*)} \tag{4.23}$$

for all $M \in \mathbb{R}^{n \times n}$, where $\overline{F'(x_*)}$ denotes the BFGS update of $F'(x_*)$ sending s to v. From (4.22), one obtains

$$\|B_+ - B_*\|_{F'(x_*)} \leqq [1 + \beta_1\sigma(x, x_+)^p]\|B_+ - B_*\|_{\overline{F'(x_*)}}. \tag{4.24}$$

Since $\overline{F'(x_*)} \in \mathscr{Q}_+(v, s)$, one can use (2.24) to estimate $\|B_+ - B_*\|_{\overline{F'(x_*)}}$. Letting $G \in \mathcal{M}(\mathscr{A}, \mathscr{Q}(y, s))$, apply (2.24) as in the proof of Theorem 3.1 to obtain

$$\begin{aligned}\|B_+ - B_*\|_{\overline{F'(x_*)}} \leqq{}& \|B - B_*\|_{\overline{F'(x_*)}} + 2\|C(x_+) - C(x_*)\|_{\overline{F'(x_*)}} \\ &+ \|C(x) - C(x_*)\|_{\overline{F'(x_*)}} + \|P^{\perp}_{\mathscr{S} \cap \mathcal{N}(s), F'(x_*)}(G - A_*)\|_{\overline{F'(x_*)}}.\end{aligned} \tag{4.25}$$

It follows from (4.18), (4.23) and (4.25) that

$$\begin{aligned}\|B_+ - B_*\|_{\overline{F'(x_*)}} \leqq{}& [1 + \beta_2\sigma(x, x_+)^p]\|B - B_*\|_{F'(x_*)} \\ &+ \{\alpha_2 + 3\beta\gamma_c[1 + \beta_2\sigma(x, x_+)^p]\}\sigma(x, x_+)^p,\end{aligned} \tag{4.26}$$

where β is a constant such that $\|M\|_{F'(x_*)} \leqq \beta|M|$ for every $M \in \mathbb{R}^{n \times n}$. Combining (4.24) and (4.26) yields

$$\begin{aligned}\|B_+ - B_*\|_{F'(x_*)} \leqq{}& \{1 + [\beta_1 + \beta_2 + \beta_1\beta_2\sigma(x, x_+)^p]\sigma(x, x_+)^p\}\|B - B_*\|_{F'(x_*)} \\ &+ [1 + \beta_1\sigma(x, x_+)^p]\{\alpha_2 + 3\beta\gamma_c[1 + \beta_2\sigma(x, x_+)^p]\}\sigma(x, x_+)^p.\end{aligned} \tag{4.27}$$

From (4.20) and (4.27), one obtains (4.21) with

$$\kappa_1 = \beta_1 + \beta_2 + \frac{\beta_1\beta_2}{5\kappa|F'(x_*)^{-1}|_2}$$

and

$$\kappa_2 = \left[1+\frac{\beta_1}{5\kappa|F'(x_*)^{-1}|_2}\right]\left\{\alpha_2+3\beta\gamma_c\left[1+\frac{\beta_2}{5\kappa|F'(x_*)^{-1}|_2}\right]\right\}.$$

With (4.21) established, the theorem follows from Theorem A2.1.

THEOREM 4.3. *Suppose that the hypotheses of Theorem* 4.2 *hold and that for some* $x_0 \in \mathbb{R}^n$ *and* $A_0 \in \mathbb{R}^{n\times n}$, $\{x_k\}$ *is a sequence defined by* $B_0 = A_0 + C(x_0)$ *and*

$$x_{k+1} = x_k - B_k^{-1}F(x_k), \qquad (v_k, y_k) \in \chi(x_k, x_{k+1}),$$
$$B_{k+1} = (A_k)_+ + C(x_{k+1}),$$

which converges q-linearly to x_*, *where* $(A_k)_+$ *is the least-change secant update of* A_k *with respect to* $s_k = x_{k+1} - x_k$, y_k *and a norm* $\|\cdot\|_W$, $W \in \mathcal{Q}_+(v_k, s_k)$. *Set* $e_k = x_k - x_*$ *for* $k = 0, 1, 2, \cdots$. *Then*

$$\lim_{k\to\infty}\left|\frac{e_{k+1}}{|e_k|} + B_*^{-1}P^{\perp}_{\mathcal{A},F'(x_*)}[F'(x_*) - C(x_*)]\frac{e_k}{|e_k|}\right| = 0,$$

where B_* *is given by* (4.15). *It follows that*

$$\overline{\lim_{k\to\infty}}\frac{|e_{k+1}|}{|e_k|} = \overline{\lim_{k\to\infty}}\left|B_*^{-1}P^{\perp}_{\mathcal{A},F'(x_*)}[F'(x_*) - C(x_*)]\frac{e_k}{|e_k|}\right| \leqq r_*$$

and, hence, that $\{x_k\}$ *converges q-superlinearly to* x_* *if and only if*

$$\lim_{k\to\infty}\left|P^{\perp}_{\mathcal{A},F'(x_*)}[F'(x_*) - C(x_*)]\frac{e_k}{|e_k|}\right| = 0.$$

In particular, $\{x_k\}$ *converges q-superlinearly to* x_* *if* $[F'(x_*) - C(x_*)] \in \mathcal{A}$.

Proof. As in the proof of Theorem 3.3, it suffices to show that

$$\lim_{k\to\infty}\frac{|(B_k - B_*)s_k|}{|s_k|} = 0, \tag{4.28}$$

in light of Theorem A3.1 of the appendix. For convenience, set $C(x_*) = C_*$ and for each k, set $C(x_k) = C_k$, $C(x_{k+1}) = C_{k+1}$, $\mathcal{N}(s_k) = \mathcal{N}_k$ and $\sigma(x_k, x_{k+1}) = \sigma_k$, and let $G_k \in \mathcal{M}(\mathcal{A}, \mathcal{Q}(v_k, s_k))$. It is understood throughout the proof that for each k, all projections are orthogonal with respect to $\|\cdot\|_W$, $W \in \mathcal{Q}_+(y_k, s_k)$; thus we denote $P^{\perp}_{\mathcal{N}_k,W}$ simply by $P^{\perp}_{\mathcal{N}_k}$, etc. Since $\{x_k\}$ converges to x_*, Lemma 4.1 implies the following: For each k, the BFGS update $\overline{F'(x_*)}$ of $F'(x_*)$ is well defined in $2_+(v_k, s_k)$ and we denote $\|\cdot\|_{\overline{F'(x_*)}}$ by $\|\cdot\|_k$; furthermore, there are constants β_1 and β_2 independent of k for which

$$\|M\|_{F'(x_*)} \leqq (1+\beta_1\sigma_k^p)\|M\|_k \quad \text{and} \quad \|M\|_k \leqq (1+\beta_2\sigma_k^p)\|M\|_{F'(x_*)} \tag{4.29}$$

for every $M \in \mathbb{R}^{n\times n}$. Since the convergence of $\{x_k\}$ to x_* is at least q-linear, we also have that $\sigma_0 \geqq \sigma_1 \geqq \sigma_2 \cdots$.

We observe that

$$\frac{|(B_k - B_*)s_k|}{|s_k|} = \frac{|P^{\perp}_{\mathcal{N}_k}(B_k - B_*)s_k|}{|s_k|} \leqq |P^{\perp}_{\mathcal{N}_k}(B_k - B_*)|$$
$$\leqq \beta'\|P^{\perp}_{\mathcal{N}_k}(B_k - B_*)\|_{F'(x_*)},$$

where β' is a constant such that $|M| \leqq \beta'\|M\|_{F'(x_*)}$ for every $M \in \mathbb{R}^{n\times n}$. Thus (4.28) is implied by

$$\lim_{k\to\infty}\|P^{\perp}_{\mathcal{N}_k}(B_k - B_*)\|_{F'(x_*)} = 0, \tag{4.30}$$

and we establish (4.30) to prove the theorem. (Not surprisingly, it can be shown, in the spirit of Lemma 3.4, that (4.28) and (4.30) are equivalent; however, showing this is not worth the trouble for the present purposes.) Apply (2.24) as in the proof of Theorem 3.3 to obtain

$$\|B_{k+1}-B_*\|_k \leqq \|P_{\mathcal{S}\cap\mathcal{N}_k}(B_k-B_*)\|_k+2\|C_{k+1}-C_*\|_k+\|C_k-C_*\|_k+\|P^{\perp}_{\mathcal{S}\cap\mathcal{N}_k}(G_k-A_*)\|_k$$

for $k=0, 1, 2, \cdots$. Since $P_{\mathcal{S}\cap\mathcal{N}_k}=P_{\mathcal{S}\cap\mathcal{N}_k}P_{\mathcal{N}_k}$, it follows from this inequality and (4.29), together with the hypotheses of Theorem 4.2, that

$$\|B_{k+1}-B_*\|_k \leqq \|P_{\mathcal{N}_k}(B_k-B_*)\|_k+\kappa\sigma_k^p, \tag{4.31}$$

where $\kappa=[\alpha_2+3\beta\gamma_c(1+\beta_2\sigma_0^p)]$, in which β is a constant such that $\|M\|_{F'(x_*)}\leqq\beta|M|$ for every $M\in\mathbb{R}^{n\times n}$. Using (3.16) with $M=B_k-B_*$ and $\|\cdot\|=\|\cdot\|_k$, one obtains from (4.31) that

$$\|B_{k+1}-B_*\|_k \leqq \|B_k-B_*\|_k-[2\|B_k-B_*\|_k]^{-1}\|P^{\perp}_{\mathcal{N}_k}(B_k-B_*)\|_k^2+\kappa\sigma_k^p. \tag{4.32}$$

Setting $\psi_k=\|P^{\perp}_{\mathcal{N}_k}(B_k-B_*)\|_{F'(x_*)}$ and $\eta_k=\|B_k-B_*\|_{F'(x_*)}$, one verifies from (4.32) and (4.29) that

$$\begin{aligned}\eta_{k+1}\leqq{}&(1+\beta_1\sigma_k^p)(1+\beta_2\sigma_k^p)\eta_k\\ &-[2(1+\beta_1\sigma_k^p)(1+\beta_2\sigma_k^p)\eta_k]^{-1}\psi_k^2+(1+\beta_1\sigma_k^p)\kappa\sigma_k^p.\end{aligned} \tag{4.33}$$

Now, (4.33) yields

$$\eta_{k+1}\leqq(1+\beta_1\sigma_k^p)(1+\beta_2\sigma_k^p)\eta_k+(1+\beta_1\sigma_k^p)\kappa\sigma_k^p,$$

from which one obtains, by induction, the somewhat generous bound

$$\eta_{k+1}\leqq\left[\prod_{j=1}^{k}(1+\beta_1\sigma_j^p)(1+\beta_2\sigma_j^p)\right]\left(\eta_0+\kappa\sum_{j=0}^{k}\sigma_j^p\right).$$

Since $\{x_k\}$ converges q-linearly to x_*, it follows that there is an η such that $\eta_k\leqq\eta$ for $k=0, 1, 2, \cdots$. One sees from (4.33) that

$$[2(1+\beta_1\sigma_0^p)(1+\beta_2\sigma_0^p)\eta]^{-1}\psi_k^2\leqq\eta_k-\eta_{k+1}+\kappa'\sigma_k^p,$$

where $\kappa'=(\beta_1+\beta_2+\beta_1\beta_2\sigma_0^p)\eta+(1+\beta_1\sigma_0^p)\kappa$. Consequently,

$$[2(1+\beta_1\sigma_0^p)(1+\beta_2\sigma_0^p)\eta]^{-1}\sum_{k=0}^{\infty}\psi_k^2\leqq\eta_0+\kappa'\sum_{k=0}^{\infty}\sigma_k^p,$$

which implies that $\lim_{k\to\infty}\psi_k=0$. This completes the proof.

5. Least-change inverse-secant update methods. In this concluding section, we state analogues of the theorems of §§ 3 and 4 which are appropriate for fixed-scale least-change inverse-secant update methods and (iteratively) rescaled least-change inverse-secant update methods. Theorems 5.1, 5.2, 5.3 and 5.4 below correspond to Theorems 3.1, 3.3, 4.2 and 4.3, respectively. Because the proofs of the theorems in this section so closely parallel those of their counterparts in §§ 3 and 4, with Theorems A2.2 and A3.2 of the appendix used in place of Theorems A2.1 and A3.1, respectively, we omit them here. Theorems 5.1 and 5.2 imply the local superlinear convergence of G. McCormick's method (see [23]) and the Broyden–Fletcher–Goldfarb–Shanno method [4], [5], [16], [18], [28], [7], [26].

We consider here iterative procedures for solving (1.1) which employ approximations of the form

$$F'(x_k)^{-1}\approx K_k=C(x_k)+A_k, \tag{5.1}$$

at the kth iteration, where $C:\mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a given function which determines a "computed part" of $F'(x)^{-1}$ for every x of interest and $A_k \approx [F'(x_k)^{-1} - C(x_k)]$ is an "approximated part" of $F'(x_k)^{-1}$. In Theorems 5.1 and 5.2, it is understood that a fixed inner-product norm $\|\cdot\|$ is specified on $\mathbb{R}^{n\times n}$. In addition, we assume in these theorems that there is associated with F and C a choice rule $\chi:\mathbb{R}^n\times\mathbb{R}^n \to 2^{\mathbb{R}^n\times\mathbb{R}^n}$ which determines admissible pairs $(w, y)\in\chi(x, x_+)$ for $x, x_+\in\mathbb{R}^n$. In accordance with the introduction, our point of view is that $w \approx P_{\mathscr{A}}[F'(x_+)^{-1} - C(x_+)]y$ and $\{P_{\mathscr{A}}[F'(x_+)^{-1} - C(x_+)] + C(x_+)\}y \approx s = x_+ - x$. We also assume that the choice rule is such that if $x_+ \neq x$, then $y \neq 0$ for every $(w, y)\in\chi(x, x_+)$.

THEOREM 5.1. *Let F and C satisfy the standard hypothesis and assume that $F'(x_*)$ is invertible. Let $\mathscr{A}$ have the property that $A_* = P_{\mathscr{A}}[F'(x_*)^{-1} - C(x_*)]$ and $K_* = [A_* + C(x_*)]$ are such that there exists an r_* for which*

$$|I - K_*F'(x_*)| = |\{P_{\mathscr{A}}^{\perp}[F'(x_*)^{-1} - C(x_*)]\}F'(x_*)| \leqq r_* < 1.$$

Also assume that the choice rule χ for w and y has the property with $\mathscr{A}$ that there exists an $\alpha \geqq 0$ such that for any distinct pair $x, x_+\in\Omega$ determining $(w, y)\in\chi(x, x_+)$, one has

$$\|P_{\mathscr{S}\cap\mathscr{N}(y)}^{\perp}(G - A_*)\| \leqq \alpha\sigma(x, x_+)^p$$

for every $G\in\mathscr{M}(\mathscr{A}, \mathscr{Q}(w, y))$, where $\sigma(x, x_+) = \max\{|x - x_*|, |x_+ - x_*|\}$. Under these hypotheses, if $r\in(r_*, 1)$, then there are positive constants ε_r, δ_r such that for $x_0\in\mathbb{R}^n$ and $A_0\in\mathbb{R}^{n\times n}$ satisfying $|x_0 - x_*| < \varepsilon_r$ and $|A_0 - A_*| < \delta_r$, a sequence $\{x_k\}$ defined by $K_0 = A_0 + C(x_0)$ and

$$x_{k+1} = x_k - K_kF(x_k), \qquad (w_k, y_k)\in\chi(x_k, x_{k+1}),$$
$$K_{k+1}\in\{K_k, A_k + C(x_{k+1}), (A_k)_+ + C(x_k), (A_k)_+ + C(x_{k+1})\},$$

satisfies $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ for $k = 0, 1, 2, \cdots$, where $(A_k)_+$ is the least-change inverse-secant update of A_k as given by (2.11) with $s = y_k$, $y = w_k$, and $\mathscr{N} = \mathscr{N}(y_k)$. Furthermore, $\{\|K_k\|\}$ and $\{\|K_k^{-1}\|\}$ are uniformly bounded.

THEOREM 5.2. *Suppose that the hypotheses of Theorem 5.1 hold and that for some $x_0\in\mathbb{R}^n$ and $A_0\in\mathbb{R}^{n\times n}$, $\{x_k\}$ is a sequence defined by $K_0 = A_0 + C(x_0)$ and*

$$x_{k+1} = x_k - K_kF(x_k), \qquad (w_k, y_k)\in\chi(x_k, x_{k+1}),$$
$$K_{k+1} = (A_k)_+ + C(x_{k+1}),$$

which converges q-linearly to x_*, where $(A_k)_+$ is the least-change inverse-secant update of A_k as given by (2.11) with $s = y_k$, $y = w_k$, and $\mathscr{N} = \mathscr{N}(y_k)$. Suppose further that $\{\|K_k\|\}$ and $\{\|K_k^{-1}\|\}$ are uniformly bounded and that $\{y_k\}$ satisfies $|K_*y_k - s_k| \leqq \alpha_k|s_k|$, where $s_k = x_{k+1} - x_k$ and $\lim_{k\to\infty}\alpha_k = 0$. Set $e_k = x_k - x_*$ for $k = 0, 1, 2, \cdots$. Then

$$\lim_{k\to\infty}\left|\frac{e_{k+1}}{|e_k|} - \{P_{\mathscr{A}}^{\perp}[F'(x_*)^{-1} - C(x_*)]\}F'(x_*)\frac{e_k}{|e_k|}\right| = 0.$$

It follows that

$$\overline{\lim_{k\to\infty}}\frac{|e_{k+1}|}{|e_k|} = \overline{\lim_{k\to\infty}}\left|\{P_{\mathscr{A}}^{\perp}[F'(x_*)^{-1} - C(x_*)]\}F'(x_*)\frac{e_k}{|e_k|}\right| \leqq r_*$$

and, hence, that $\{x_k\}$ converges q-superlinearly to x_* if and only if

$$\lim_{k\to\infty}\left|\{P_{\mathscr{A}}^{\perp}[F'(x_*)^{-1} - C(x_*)]\}F'(x_*)\frac{e_k}{|e_k|}\right| = 0.$$

In particular, $\{x_k\}$ *converges q-superlinearly to* x_* *if* $[F'(x_*)^{-1}-C(x_*)]\in\mathcal{A}$.

The requirement in Theorem 5.2 that $|K_*y_k-s_k|\leqq\alpha_k|s_k|$, where $s_k=x_{k+1}-x_k$ and $\lim_{k\to\infty}\alpha_k=0$, is one of the hypotheses of Theorem A3.2 of the appendix and essentially guarantees that the approximation $\{P_{\mathcal{A}}[F'(x_{k+1})^{-1}-C(x_{k+1})]+C(x_{k+1})\}y_k\approx s_k$ is a good one. It is interesting to note that no such requirement is necessary in Theorem 5.1. It is also naturally of interest to ask when the usual choice $y_k=F(x_{k+1})-F(x_k)$ meets this requirement. We observe that if $[F'(x_*)^{-1}-C(x_*)]\in\mathcal{A}$, then

$$K_*y_k=[P_{\mathcal{A}}[F'(x_*)^{-1}-C(x_*)]+C(x_*)]y_k=F'(x_*)^{-1}y_k.$$

It follows easily, under the assumptions of Theorems 5.1 and 5.2, that $y_k=F(x_{k+1})-F(x_k)$ satisfies the requirement in the case $[F'(x_*)^{-1}-C(x_*)]\in\mathcal{A}$. Note also that the sequence $\{x_k\}$ generated by the iteration of Theorem 5.2 converges superlinearly in this case.

Theorems 5.3 and 5.4 below are analogues for rescaled least-change inverse-secant update methods of Theorems 5.1 and 5.2 respectively. As always in rescaled methods, the norm on $\mathbb{R}^{n\times n}$, used to define least-change inverse-secant updates, is itself updated at each iteration to reflect current information about the ideal scaling associated with the problem at hand. We assume here that current information about the ideal scaling after k iterations is incorporated in vectors y_k and $u_k\approx F'(x_{k+1})^{-1}y_k$ satisfying $u_k^Ty_k>0$ and that the norm used to define least-change inverse-secant updates is at each iteration a weighted Frobenius norm $\|\cdot\|_W$, $W\in\mathcal{Q}_+(u_k,y_k)$. Specifically, it is assumed in Theorems 5.3 and 5.4 that there is given a choice rule for determining admissible values not only of w and y but also of $u\approx F'(x_+)^{-1}y$ for every $x, x_+\in\mathbb{R}^n$. By such a choice rule, we mean a function $\chi:\mathbb{R}^n\times\mathbb{R}^n\to 2^{\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^n}$ which determines admissible triples $(u,w,y)\in\chi(x,x_+)$ for $x, x_+\in\mathbb{R}^n$. We assume that χ is such that if $x_+\neq x$, then $y\neq 0$ and $u^Ty>0$ for every $(u,w,y)\in\chi(x,x_+)$. In the case $[F'(x_*)^{-1}-C(x_*)]\in\mathcal{A}$, one sees, as before, that the sequence $\{x_k\}$ generated by the iteration of Theorem 5.4 converges q-superlinearly to x_* if one chooses $y=F(x_+)-F(x)$ for x, $x_+\in\mathbb{R}^n$. It is also interesting to note that for this choice of y, the choice $u=s=x_+-x$ satisfies the condition $|u-F'(x_*)^{-1}y|\leqq\alpha_1\sigma(x,x_+)^p|y|$ of Theorem 5.3 for an appropriate α_1.

THEOREM 5.3. *Let F and C satisfy the standard hypothesis. Let* $\mathcal{S}$ *have the property that for any* $y, u\in\mathbb{R}^n$ *with* $y^Tu>0$, *the projection* $P_{\mathcal{S},W}$ *is independent of* $W\in\mathcal{Q}_+(u,y)$. *In addition, assume that* $F'(x_*)$ *is invertible and let* $\mathcal{A}$ *have the property that* $A_*=P_{\mathcal{A},F'(x_*)^{-1}}[F'(x_*)^{-1}-C(x_*)]$ *and* $K_*=A_*+C(x_*)$ *are such that there exists an* r_* *for which*

$$|I-K_*F'(x_*)|=|\{P^{\perp}_{\mathcal{A},F'(x_*)^{-1}}[F'(x_*)^{-1}-C(x_*)]\}F'(x_*)|\leqq r_*<1.$$

Also assume that the choice rule χ *for u, w and y has the property with respect to* $\mathcal{A}$ *that there exist* $\alpha_1, \alpha_2\geqq 0$ *such that for any distinct pair* $x, x_+\in\Omega$ *determining* $(u,w,y)\in\chi(x,x_+)$, *one has*

$$|u-F'(x_*)^{-1}y|\leqq\alpha_1\sigma(x,x_+)^p|y|$$

and

$$\|P^{\perp}_{\mathcal{S}\cap\mathcal{N}(y),W}(G-A_*)\|_W\leqq\alpha_2\sigma(x,x_+)^p$$

for every $G\in\mathcal{M}(\mathcal{A},\mathcal{Q}(w,y))$, *where* $\sigma(x,x_+)=\max\{|x-x_*|,|x_+-x_*|\}$ *and* $W\in\mathcal{Q}_+(u,y)$. *Under these hypotheses, if* $r\in(r_*,1)$, *then there are positive constants* ε_r, δ_r *such that for* $x_0\in\mathbb{R}^n$ *and* $A_0\in\mathbb{R}^{n\times n}$ *satisfying* $|x_0-x_*|<\varepsilon_r$ *and* $|A_0-A_*|<\delta_r$, *a sequence* $\{x_k\}$

defined by $K_0 = A_0 + C(x_0)$ *and*

$$x_{k+1} = x_k - K_k F(x_k), \qquad (u_k, w_k, y_k) \in \chi(x_k, x_{k+1})$$
$$K_{k+1} \in \{K_k, A_k + C(x_{k+1}), (A_k)_+ + C(x_k), (A_k)_+ + C(x_{k+1})\}$$

satisfies $|x_{k+1} - x_*| \leqq r|x_k - x_*|$ *for* $k = 0, 1, 2, \cdots$, *where* $(A_k)_+$ *is the least-change inverse-secant update of* A_k *as given by* (2.11) *with* $s = y_k$, $y = w_k$, $\mathcal{N} = \mathcal{N}(y_k)$ *and* $\|\cdot\| = \|\cdot\|_W$ *for* $W \in \mathcal{Q}_+(u_k, y_k)$. *Furthermore,* $\{\|K_k\|_{F'(x_*)^{-1}}\}$ *and* $\{\|K_k^{-1}\|_{F'(x_*)^{-1}}\}$ *are uniformly bounded.*

THEOREM 5.4. *Suppose that the hypotheses of Theorem* 5.3 *hold and that for some* $x_0 \in \mathbb{R}^n$ *and* $A_0 \in \mathbb{R}^{n \times n}$, $\{x_k\}$ *is a sequence defined by* $K_0 = A_0 + C(x_0)$ *and*

$$x_{k+1} = x_k - K_k F(x_k), \qquad (u_k, w_k, y_k) \in \chi(x_k, x_{k+1}),$$
$$K_{k+1} = (A_k)_+ + C(x_{k+1}),$$

which converges q-linearly to x_*, *where* $(A_k)_+$ *is the least-change inverse-secant update of* A_k *as given by* (2.11) *with* $s = y_k$, $y = w_k$, $\mathcal{N} = \mathcal{N}(y_k)$ *and* $\|\cdot\| = \|\cdot\|_W$ *for* $W \in \mathcal{Q}_+(u_k, y_k)$. *Suppose further that* $\{\|K_k\|_{F'(x_*)^{-1}}\}$ *and* $\{\|K_k^{-1}\|_{F'(x_*)^{-1}}\}$ *are uniformly bounded and that* $\{y_k\}$ *satisfies* $|K_* y_k - s_k| \leqq \alpha_k |s_k|$, *where* $s_k = x_{k+1} - x_k$ *and* $\lim_{k\to\infty} \alpha_k = 0$. *Set* $e_k = x_k - x_*$ *for* $k = 0, 1, 2, \cdots$. *Then*

$$\lim_{k\to\infty} \left| \frac{e_{k+1}}{|e_k|} - \{P^{\perp}_{\mathcal{A}, F'(x_*)^{-1}}[F'(x_*)^{-1} - C(x_*)]\} F'(x_*) \frac{e_k}{|e_k|} \right| = 0.$$

It follows that

$$\overline{\lim_{k\to\infty}} \frac{|e_{k+1}|}{|e_k|} = \overline{\lim_{k\to\infty}} \left| \{P^{\perp}_{\mathcal{A}, F'(x_*)^{-1}}[F'(x_*)^{-1} - C(x_*)]\} F'(x_*) \frac{e_k}{|e_k|} \right| \leqq r_*$$

and, hence, that $\{x_k\}$ *converges q-superlinearly to* x_* *if and only if*

$$\lim_{k\to\infty} \left| \{P^{\perp}_{\mathcal{A}, F'(x_*)^{-1}}[F'(x_*)^{-1} - C(x_*)]\} F'(x_*) \frac{e_k}{|e_k|} \right| = 0.$$

In particular, $\{x_k\}$ *converges q-superlinearly to* x_* *if* $[F'(x_*)^{-1} - C(x_*)] \in \mathcal{A}$.

To illustrate the potential applications of the methods considered in this section, we again turn to the nonlinear least-squares problem. If $f(x) = \frac{1}{2}R(x)^T R(x)$ is the functional to be minimized and R is small near a minimizer x_* of f, then one can expect the Hessian of f, given by (2.13), to be dominated by the term $R'(x)^T R'(x)$ for x near x_*. (Equivalently, one can expect the inverse Hessian $\nabla^2 f(x)^{-1}$ to be dominated by $[R'(x)^T R'(x)]^{-1}$ for x near x_*.) With this in mind, one often wishes to proceed, at the kth step of an iteration for determining x_*, from x_k to a better approximation x_{k+1} of x_* by initially using the Gauss–Newton step, i.e., by initially defining

$$x_{k+1} = x_k - [R'(x_k)^T R'(x_k)]^{-1} F(x_k), \tag{5.2}$$

where $F(x) \equiv \nabla f(x)$ as before. If this initial x_{k+1}, or some standard modification of it, is found to be unsatisfactory, then one might reasonably redefine x_{k+1} by

$$x_{k+1} = x_k - K_k F(x_k), \tag{5.3}$$

where K_k is of the form (5.1) for some augmentation A_k of the inverse Gauss–Newton Hessian $C(x_k) \equiv [R'(x_k)^T R'(x_k)]^{-1}$. The inverse-augmentation method of proceeding from the initial Gauss–Newton determination (5.2) to the final determination (5.3) has the advantage over the direct-augmentation methods, discussed earlier, of requiring for each k only one matrix factorization, namely that necessary to determine x_{k+1} by (5.2). The direct-augmentation methods require this factorization to determine the Gauss–Newton step and, if this step proves unsatisfactory, another factorization to determine the step obtained using the directly augmented Gauss–Newton Hessian.

How might one obtain a least-change inverse-secant update of the augmentation A_k of the inverse Gauss–Newton Hessian $C(x_k)$, which will yield a procedure (5.3) having desirable convergence properties? Suppose that one has distinct points $x, x_+ \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n\times n}$ and that one wants a least-change inverse-secant update $A_+ \approx [F'(x_+)^{-1} - C(x_+)]$ of A. It is reasonable to take as before $\mathcal{A} = \mathcal{S} = \{M \in \mathbb{R}^{n\times n} : M = M^T\}$ and to assume that A is symmetric. Since $[F'(x_*)^{-1} - C(x_*)] \in \mathcal{A}$ with this choice of $\mathcal{A}$, a satisfactory choice of y for the theorems in this section is

$$y = F(x_+) - F(x), \tag{5.4}$$

according to the remarks between Theorems 5.2 and 5.3. It appears to us that the only safe choices of $w \approx P_{\mathcal{A}}[F'(x_+)^{-1} - C(x_+)]y$ are the "default" choices

$$w^{(1)} = s - C(x_+)y \quad \text{and} \quad w^{(2)} = s - C(x)y, \tag{5.5}$$

where $s = x_+ - x$. If one makes the choice of norm $\|\cdot\| = \|\cdot\|_{\mathcal{F}}$ and defines the choice rule χ for w and y by $\chi(x, x_+) = \{(w^{(1)}, y), (w^{(2)}, y)\}$, where $w^{(1)}$ and $w^{(2)}$ are given by (5.5) and y is given by (5.4), then the least-change inverse-secant update A_+ of A for $(w, y) \in \chi(x, x_+)$ is

$$\begin{aligned} A_+ &= \left(I - \frac{yy^T}{y^Ty}\right) A \left(I - \frac{yy^T}{y^Ty}\right) + \frac{wy^T + yw^T}{y^Ty} - \frac{y^Twyy^T}{(y^Ty)^2} \\ &= A + \frac{(w - Ay)y^T + y(w - Ay)^T}{y^Ty} - \frac{y^T(w - Ay)yy^T}{(y^Ty)^2}. \end{aligned} \tag{5.6}$$

The update (5.6) is, of course, the Greenstadt augmentation-update analogue of the PSB augmentation-update formula (2.20). Theorems 5.1 and 5.2 imply the local q-superlinear convergence of the fixed-scale least-change inverse-secant update method (5.3) with the successive augmentation matrices A_k obtained using the update (5.6), whenever $F(x) = R'(x)^T R(x)$ and $C(x) = [R'(x)^T R'(x)]^{-1}$ satisfy the hypotheses of Theorem 5.1. On the other hand, since the unsuccessful methods of Broyden and Greenstadt result from $C(x) = 0$, we don't expect (5.6) to define a successful numerical method.

If one desires a rescaled least-change inverse-secant update method, then $u = s = x_+ - x$ is a satisfactory choice of u for Theorems 5.3 and 5.4, according to the remarks between Theorems 5.2 and 5.3. If one defines the choice rule χ for u, w, and y by $\chi(x, x_+) = \{(s, w^{(1)}, y)(s, w^{(2)}, y)\}$, where $w^{(1)}$ and $w^{(2)}$ are given by (5.5) and y is given by (5.4), then the least-change inverse-secant update of A is

$$\begin{aligned} A_+ &= \left(I - \frac{sy^T}{s^Ty}\right) A \left(I - \frac{ys^T}{s^Ty}\right) + \frac{ws^T + sw^T}{s^Ty} - \frac{y^Twss^T}{(s^Ty)^2} \\ &= A + \frac{(w - Ay)s^T + s(w - Ay)^T}{s^Ty} - \frac{y^T(w - Ay)ss^T}{(s^Ty)^2} \end{aligned} \tag{5.7}$$

for $(s, w, y) \in \chi(x, x_+)$ and $\|\cdot\| = \|\cdot\|_W$, $W \in \mathcal{Q}_+(s, y)$. The update (5.7) is the BFGS augmentation-update analogue of the DFP augmentation-update formula (4.4). Note that if $C(x)$ were 0, then w would be s and (5.7) would be the usual BFGS update formula. Theorems 5.3 and 5.4 imply the local q-superlinear convergence of the rescaled least-change inverse-secant update method (5.3), with the successive augmentation matrices A_k obtained using the update (5.7) whenever F and C satisfy the hypotheses of Theorem 5.3.

We feel that (5.7) is of great potential value and that computational testing on the nonlinear least-squares problem is needed.

Appendix: Local convergence theorems for quasi-Newton methods.

A1. Introduction. Our interest here is in general *quasi-Newton* or *Newton-like* methods:

$$x_{k+1} = x_k - B_k^{-1}F(x_k) = x_k - K_kF(x_k), \qquad B_k \in \mathbb{R}^{n\times n}, \quad K_k = B_k^{-1} \tag{A1.1}$$

for solving (1.1). It is assumed in the following that the standard hypothesis given in the introduction to the main body of the paper is in force, although we have no explicit interest here in a computed part C of F'.

The usual procedure for analyzing the iteration (A1.1) when it reduces to one of the familiar least-change secant update methods (cf. Broyden–Dennis–Moré [7], Powell [26], Sorensen [30]) is first to establish the local existence and q-linear convergence of the iteration sequence $\{x_k\}$ and then to show q-superlinear convergence by the use of the characterization theorem of Dennis and Moré [11]. The technique used for proving q-linear convergence is generally based on some variant of the principle of bounded deterioration, which states that while the approximate partial derivative matrices B_k need not get nearer $F'(x_*)$, they should only get worse in a certain controlled way as the iteration proceeds.

Our intention here is to show how to extend this method of analysis to the case in which the iteration (A1.1) uses a sequence $\{B_k\}$ which is taken to have some desirable property not necessarily shared by $F'(x)$ at any x. A familiar example to illustrate this case is the nonlinear Jacobi iteration in which $B_k = \text{diag}\,(F'(x_k))$ even though $F'(x_k)$ is not a diagonal matrix. Certainly, we know for this iteration that no matter how near x_0 is to x_*, we can't reasonably expect convergence unless there is some diagonal matrix B_* (perhaps $B_* = \text{diag}\,(F'(x_*))$ for which $B_k \equiv B_*$ would yield a convergent iteration (A1.1).

In § A2, the bounded-deterioration theorems of Broyden–Dennis–Moré [7] are generalized to show that if $\{B_k\}$ or $\{B_k^{-1}\}$ is of bounded deterioration as a sequence of approximants to some B_* or B_*^{-1}, then the iteration (A1.1) has the same local convergence properties and arbitrarily nearly the same linear rate as would be achieved by the stationary iteration which uses $B_k \equiv B_*$. Then in § A3, the characterization of superlinear convergence given by Dennis and Moré [11] is generalized to give necessary and sufficient conditions on $\{B_k\}$ for a linearly convergent iteration sequence $\{x_k\}$ to have the same q-linear rate constant as that of a sequence produced by the stationary iteration which uses $B_k \equiv B_*$. In case the convergence of the stationary sequence is q-superlinear, then the theorems of § A3 reduce to those of [11].

In formulating the results of this appendix, our primary purpose has been to provide the tools necessary for the analysis of least-change secant update methods carried out in the main body of the paper. However, we feel that the theorems here are likely to prove useful beyond the present context. In support of this position, we refer the reader to Dennis and Walker [15], in which the results given here are applied to the convergence analysis of a computationally convenient modification of the Jacobi secant method of Ortega and Rheinboldt [22] and Wegge [34] and to the analysis of the rate of convergence of the general class of Newton iterative methods studied by Ortega and Rheinboldt [22] and Sherman [29].

A2. Convergence results. The results of this section are direct generalizations along the lines mentioned above, of the results of Broyden–Dennis–Moré [7, § 3]. We also use their notion of an updating function here, and any reader who desires more discussion of this useful abstraction is referred to the original paper.

In our theorems we find it convenient to use two norms. As in the main body of the paper, it is useful to denote a vector norm by $|v|$ for $v \in \mathbb{R}^n$ and the subordinate matrix operator norm by $|A|$ for $A \in \mathbb{R}^{n\times n}$. The notation $\|A\|$ for $A \in \mathbb{R}^{n\times n}$ stands for any arbitrary but fixed norm on $\mathbb{R}^{n\times n}$ which may not be subordinate to a vector norm. We make strong use of the equivalence of all norms on $\mathbb{R}^{n\times n}$; in particular for $|\cdot|$ and $\|\cdot\|$ we assume for some μ, $\eta > 0$ and any $A \in \mathbb{R}^{n\times n}$, that

$$\mu\|A\| \leqq |A| \leqq \eta\|A\|.$$

THEOREM A2.1. *Let F satisfy the standard hypothesis and let $B_* \in \mathbb{R}^{n\times n}$ have the property that B_*^{-1} exists and for some operator norm*

$$|I - B_*^{-1}F'(x_*)| \leqq r_* < 1.$$

Let $U : \mathbb{R}^n \times \mathbb{R}^{n\times n} \to 2^{\mathbb{R}^{n\times n}}$ be defined in a neighborhood $N = N_1 \times N_2$ of (x_*, B_*) where $N_1 \subset \Omega$ and N_2 contains only nonsingular matrices. Assume that there are nonnegative constants α_1 and α_2 such that for each $(x, B) \in N$, and for $x_+ = x - B^{-1}F(x)$, every $B_+ \in U(x, B)$ satisfies

$$\|B_+ - B_*\| \leqq [1 + \alpha_1\sigma(x, x_+)^p] \cdot \|B - B_*\| + \alpha_2\sigma(x, x_+)^p$$

for $\sigma(x, x_+) = \max\{|x - x_*|, |x_+ - x_*|\}$.

Under these hypotheses for any $r \in (r_*, 1)$, there exist constants ε_r, δ_r such that if $|x_0 - x_*| < \varepsilon_r$ and $|B_0 - B_*| < \delta_r$, then any iteration sequence $\{x_k\}$ defined by

$$x_{k+1} = x_k - B_k^{-1}F(x_k), \qquad B_{k+1} \in U(x_k, B_k),$$

$k = 0, 1, \cdots$, exists, converges q-linearly to x_* with

$$|x_{k+1} - x_*| \leqq r \cdot |x_k - x_*|,$$

and has the property that $\{|B_k|\}$ and $\{|B_k^{-1}|\}$ *are uniformly bounded.*

Proof. Let $r \in (r_*, 1)$ and choose δ, ε_r so small that for $\beta \geqq |B_*^{-1}|$ and $\psi \geqq |F'(x_*)|$, one has $2\beta\eta\delta < 1$,

$$r \geqq r_* + \frac{\beta}{1 - 2\beta\eta\delta}(\gamma\varepsilon_r^p + 2\beta\eta\psi\delta) \quad \text{and} \quad (2\alpha_1\delta + \alpha_2)\frac{\varepsilon_r^p}{1 - r^p} \leqq \delta.$$

Now select δ_r small enough so that $\|B - B_*\| < \delta$ whenever $|B - B_*| < \delta_r$. If necessary further restrict ε_r, δ_r so that $(x, B) \in N$ whenever $|B - B_*| \leqq 2\eta\delta$ and $|x - x_*| < \varepsilon_r$. Let $|B_0 - B_*| < \delta_r$ and $|x_0 - x_*| < \varepsilon_r$.

It follows from the Banach perturbation lemma [22, p. 45], since $|B_*^{-1}| \cdot |B_0 - B_*| \leqq \beta\eta\|B_0 - B_*\| < \beta\eta\delta < 2\beta\eta\delta < 1$, that B_0^{-1} exists and that $|B_0^{-1}| \leqq \beta/(1 - 2\beta\eta\delta)$. Thus, from standard arguments,

$$\begin{aligned}
|x_1 - x_*| &\leqq |B_0^{-1}|\,|F(x_0) - F(x_*) - F'(x_*)(x_0 - x_*)| + |I - B_0^{-1}F'(x_*)|\,|x_0 - x_*| \\
&\leqq [|B_0^{-1}|\gamma\varepsilon_r^p + |I - B_*^{-1}F'(x_*)| + |B_*^{-1} - B_0^{-1}| \cdot |F'(x_*)|]\,|x_0 - x_*| \\
&\leqq [|B_0^{-1}|(\gamma\varepsilon_r^p + |B_*^{-1}| \cdot |B_0 - B_*| \cdot \psi) + r_*] \cdot |x_0 - x_*| \\
&\leqq \left[\frac{\beta}{1 - 2\beta\eta\delta}(\gamma\varepsilon_r^p + 2\beta\eta\delta\psi) + r_*\right] \cdot |x_0 - x_*| \leqq r|x_0 - x_*|.
\end{aligned}$$

Assume by way of induction that for $k=0,1,\cdots,m-1$, $\|B_k-B_*\|\leqq 2\delta$ and $|x_{k+1}-x_*|\leqq r|x_k-x_*|$. Then, $\|B_{k+1}-B_*\|-\|B_k-B_*\|\leqq 2\alpha_1\delta\varepsilon_r^p r^{pk}+\alpha_2\varepsilon_r^p r^{pk}$. We can sum both sides from $k=0$ to $m-1$ to obtain

$$\|B_m-B_*\|\leqq\|B_0-B_*\|+(2\alpha_1\delta+\alpha_2)\frac{\varepsilon_r^p}{1-r^p}\leqq 2\delta,\quad \text{so } |B_m-B_*|\leqq 2\eta\delta$$

and again by the Banach lemma, B_m^{-1} exists and $|B_m^{-1}|\leqq\beta/(1-2\beta\eta\delta)$. To complete the induction we proceed as for $m=0$:

$$\begin{aligned}|x_{m+1}-x_*|&\leqq[|B_m^{-1}|\,(\gamma\varepsilon_r^p+|B_*^{-1}|\cdot|B_m-B_*|\cdot\psi)+r_*]\cdot|x_m-x_*|\\&\leqq\left[\frac{\beta}{1-2\beta\eta\delta}(\gamma\varepsilon_r^p+2\beta\eta\delta\psi)+r_*\right]\cdot|x_m-x_*|\leqq r\cdot|x_m-x_*|.\end{aligned}$$

Note that we have easily that $|B_k^{-1}|\leqq\beta/1-2\beta\eta\delta$ and that $|B_k|\leqq 2\eta\delta+|B_*|$, and this completes the proof.

Sometimes it is useful to have conditions directly on $\{B_k^{-1}\}$ rather than on $\{B_k\}$.

THEOREM A2.2. *Let F satisfy the standard hypothesis and let K_* be an invertible matrix with $|I-K_*F'(x_*)|\leqq r_*<1$.*

Let $U:\mathbb{R}^n\times\mathbb{R}^{n\times n}\to 2^{\mathbb{R}^{n\times n}}$ be defined in a neighborhood $N=N_1\times N_2$ of (x_*,K_*), where $N_1\subset\Omega$. Assume that there are nonnegative constants α_1, α_2 such that for each (x,K) in N, and for $x_+=x-KF(x)$, the function U satisfies

$$\|K_+-K_*\|\leqq[1+\alpha_1\sigma(x,x_+)^p]\|K-K_*\|+\alpha_2\sigma(x,x_+)^p$$

for each $K_+\in U(x,K)$. Then for each $r\in(r_*,1)$ there exist positive constants ε_r, δ_r such that for $|x_0-x_*|<\varepsilon_r$ and $|K_0-K_*|<\delta_r$, any sequence $\{x_k\}$ defined by

$$x_{k+1}=x_k-K_kF(x_k),\qquad K_{k+1}\in U(x_k,K_k)$$

$k=0,1,\cdots$, exists, converges q-linearly to x_* with $|x_{k+1}-x_*|\leqq r\,|x_k-x_*|$, and has the property that $\{|K_k|\}$ and *$\{|K_k^{-1}|\}$ are uniformly bounded.*

Proof. Let $r\in(r_*,1)$ and choose ε_r, δ so that

$$(2\alpha_1\delta+\alpha_2)\frac{\varepsilon_r^p}{1-r^p}\leqq\delta\quad\text{and}\quad|F'(x_*)|\cdot 2\eta\delta+r_*+(|K_*|+2\eta\delta)\gamma\varepsilon_r^p\leqq r.$$

Now select δ_r small enough so that $|K-K_*|<\delta_r$ implies that $\|K-K_*\|<\delta$. If necessary, further restrict ε_r, δ_r so that $(x,K)\in N$ whenever $|K-K_*|<2\eta\delta$ and $|x-x_*|<\varepsilon_r$.

Let x_0, K_0 be chosen to satisfy $|x_0-x_*|<\varepsilon_r$ and $|K_0-K_*|<\delta_r$. Then

$$\begin{aligned}|x_1-x_*|&\leqq|K_0|\,|F(x_0)-F(x_*)-F'(x_*)(x_0-x_*)|+|I-K_0F'(x_*)|\,|x_0-x_*|\\&\leqq[(|K_*|+|K_0-K_*|)\gamma\varepsilon_r^p+|I-K_*F'(x_*)|+|K_*-K_0|\cdot|F'(x_*)|]\cdot|x_0-x_*|\\&\leqq[(|K_*|+\eta\delta)\gamma\varepsilon_r^p+r_*+\eta\delta\cdot|F'(x_*)|]\cdot|x_0-x_*|\\&\leqq r|x_0-x_*|.\end{aligned}$$

Now assume by way of induction that

$$\|K_k-K_*\|\leqq 2\delta\quad\text{and}\quad|x_{k+1}-x_*|\leqq r\cdot|x_k-x_*|$$

for $k=0,1,\cdots,m-1$. It follows that

$$\|K_{k+1}-K_*\|-\|K_k-K_*\|\leqq 2\alpha_1\delta\varepsilon_r^p r^{pk}+\alpha_2\varepsilon_r^p r^{pk}$$

and, again as in Theorem A2.1, by summing from $k=0$ to $m-1$, we obtain $\|K_m-K_*\|\leqq$

$\|K_0-K_*\|+(2\alpha_1\delta+\alpha_2)\varepsilon_r^p/1-r^p \leqq 2\delta$. Thus,

$$\begin{aligned}|x_{m+1}-x_*| &\leqq [|K_m|\gamma\varepsilon_r^p+|I-K_mF'(x_*)|]\cdot|x_m-x_*|\\ &\leqq [(|K_*|+2\eta\delta)\gamma\varepsilon_r^p+r_*+2\eta\delta\cdot|F'(x_*)|]\cdot|x_m-x_*|\\ &\leqq r\cdot|x_m-x_*|,\end{aligned}$$

and the induction is complete.

In order to finish the proof we need to derive the bounds for $\{|K_k|\}$ and $\{|K_k^{-1}|\}$. These follow readily from the induction relations; in fact we already have $|K_k|\leqq |K_*|+\eta\|K_k-K_*\|\leqq|K_*|+2\eta\delta$. Furthermore, $|I-K_*F'(x_*)|\leqq r_*<1$, implies that $|F'(x_*)^{-1}|$ exists and $|F'(x_*)^{-1}|\leqq|K_*|/(1-r_*)$. Thus we have $|I-K_kF'(x_*)|< r_*+2\eta\delta\cdot|F'(x_*)|\leqq r<1$, and so K_k^{-1} exists and $|K_k^{-1}|\leqq|F'(x_*)|/(1-r)$.

A3. Speed of convergence. In this section we will present theorems which give necessary and sufficient conditions for the iteration (A1.1) to have the same q-linear rate of convergence as some idealized stationary iteration $x_{k+1}=x_k-B_*^{-1}F(x_k)$. When this stationary iteration is q-superlinear, our theorems reduce to the Dennis–Moré results [11].

Some remarks are in order about q-linear convergence and the use of different norms. Given any vector norm, Ortega and Rheinboldt [22, p. 281] define the linear q-factor of $\{x_k\}$ as

$$Q_1\{x_k\}=\begin{cases}0 & \text{if } x_k=x^*,\quad k\geqq \text{some } k_0,\\ \overline{\lim\limits_{k\to\infty}}\dfrac{|x_{k+1}-x_*|}{|x_k-x_*|} & \text{if } x_k\neq x_*,\quad k\geqq k_0,\\ +\infty & \text{otherwise.}\end{cases}$$

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 $Q_1\{x_k\}=0$. Since all norms are equivalent, the condition that $Q_1\{x_k\}=0$ is clearly norm-independent. On the other hand $Q_1\{x_k\}<1$ in one norm only ensures that $Q_1\{x_k\}<+\infty$ in any other norm.

In this terminology, the following theorems give norm-invariant necessary and sufficient conditions for any sequence $\{x_k\}$ generated by (A1.1), which is q-linearly convergent to x_* in some norm, to have

$$Q_1\{x_k\}=\overline{\lim_{k\to\infty}}\left|[I-B_*^{-1}F'(x_*)]\frac{x_k-x_*}{|x_k-x_*|}\right|,$$

in every norm. With these remarks in mind, perhaps the reader will be patient with the attention given to norm independence in the statements of the following theorems.

THEOREM A3.1. *Suppose that F satisfies the standard hypothesis and that $\{x_k\}$ is a sequence generated by* (A1.1) *which converges to x_* with $x_k\neq x_*$ for all but finitely many k and that for some norm $|\cdot|_1$ and some $r\in(0,1)$,*

$$|x_{k+1}-x_*|_1\leqq r|x_k-x_*|_1,\qquad k=0,1,2,\cdots. \tag{A3.1}$$

If $s_k=x_{k+1}-x_k$ and $B_*\in\mathbb{R}^{n\times n}$ is any invertible matrix, then the norm-independent condition

$$\lim_{k\to\infty}\frac{|(B_k-B_*)s_k|}{|s_k|}=0, \tag{A3.2}$$

holds if and only if the norm-independent condition

$$\text{(A3.3)} \qquad \lim_{k\to\infty}\left|[I-B_*^{-1}F'(x_*)]\frac{(x_k-x_*)}{|x_k-x_*|}-\frac{(x_{k+1}-x_*)}{|x_k-x_*|}\right|=0,$$

holds. In particular, if (A3.2) *holds in some norm, then for any vector norm* $|\cdot|$,

$$\text{(A3.4)} \qquad Q_1\{x_k\}=\overline{\lim_{k\to\infty}}\frac{|x_{k+1}-x_*|}{|x_k-x_*|}=\overline{\lim_{k\to\infty}}\left|[I-B_*^{-1}F'(x_*)]\frac{(x_k-x_*)}{|x_k-x_*|}\right|\leqq|I-B_*^{-1}F'(x_*)|,$$

and $\{x_k\}$ *converges q-superlinearly to* x_* *if and only if*

$$\text{(A3.5)} \qquad \lim_{k\to\infty}\left|[I-B_*^{-1}F'(x_*)]\frac{(x_k-x_*)}{|x_k-x_*|}\right|=0.$$

Proof. Notice that (A3.2), (A3.3) and (A3.5) hold in every norm if and only if they hold in some norm. Now

$$(B_k-B_*)s_k=[B_*-F'(x_*)](x_k-x_*)-B_*(x_{k+1}-x_*)+F'(x_*)(x_k-x_*)-F(x_k),$$

and since an inequality $|F'(x)-F'(x_*)|_1\leqq\gamma_1|x-x_*|_1^p$ can be shown to hold in Ω for a constant γ_1, one has

$$\lim_{k\to\infty}\frac{|F'(x_*)(x_k-x_*)-F(x_k)|_1}{|s_k|_1}\leqq\lim_{k\to\infty}\frac{\gamma_1\sigma_k^p}{1-r}=0,$$

where $\sigma_k=\max\{|x_k-x_*|_1,|x_{k+1}-x_*|_1\}$. It follows that (A3.2) holds if and only if

$$\lim_{k\to\infty}\frac{|[B_*-F'(x_*)](x_k-x_*)-B_*(x_{k+1}-x_*)|_1}{|s_k|_1}=0.$$

Since $(1-r)|x_k-x_*|_1\leqq|s_k|_1\leqq(1+r)|x_k-x_*|_1$, one has

$$\frac{|[B_*-F'(x_*)](x_k-x_*)-B_*(x_{k+1}-x_*)|_1}{|s_k|_1}\leqq\frac{|B_*|_1}{(1-r)}\left|[I-B_*^{-1}F'(x_*)]\frac{(x_k-x_*)}{|x_k-x_*|_1}-\frac{(x_{k+1}-x_*)}{|x_k-x_*|_1}\right|_1$$

and

$$\frac{|[B_*-F'(x_*)](x_k-x_*)-B_*(x_{k+1}-x_*)|_1}{|s_k|_1}\geqq\frac{1}{|B_*^{-1}|_1(1+r)}\left|[I-B_*^{-1}F'(x_*)]\frac{(x_k-x_*)}{|x_k-x_*|_1}-\frac{(x_{k+1}-x_*)}{|x_k-x_*|_1}\right|.$$

Thus (A3.2) holds if and only if (A3.3) holds, and the proof is complete since only norm-independent "zero" limits have been used.

It is easy to see from Theorem (A3.1) that condition (A3.2) and hence (A3.3) and (A3.4) follow from $\lim_{k\to\infty}B_k=B_*$. This is not so easy to see from the following theorem, because the sequence $\{y_k\}$ in condition (A3.6) is unfamiliar. In fact if $\lim_{k\to\infty}K_k=K_*$, then $\{y_k\}=\{B_*s_k\}$ will certainly do, since with $\alpha_k=0$ and any norm, (A3.6) holds. We hope these remarks will make the statement of Theorem A3.2 easier to understand.

THEOREM A3.2. *Suppose that the hypotheses of Theorem* A3.1 *hold. Suppose further that* $\{\|K_k\|\}$ *and* $\{\|K_k^{-1}\|\}$ *are bounded and that* $\{y_k\}$ *is a sequence satisfying the* *norm-independent condition*

$$|K_* y_k - s_k| \leqq \alpha_k |s_k|, \tag{A3.6}$$

where $s_k = x_{k+1} - x_k$, K_* *is some invertible matrix, and* $\lim_{k\to\infty} \alpha_k = 0$. *Then the norm-independent condition*

$$\lim_{k\to\infty} \frac{|(K_k - K_*)y_k|}{|y_k|} = 0, \tag{A3.7}$$

holds if and only if the norm-independent condition

$$\lim_{k\to\infty} \left| [I - K_* F'(x_*)] \frac{(x_k - x_*)}{|x_k - x_*|} - \frac{(x_{k+1} - x_*)}{|x_k - x_*|} \right| = 0,$$

holds. In particular, if (A3.7) *holds in some norm, then for any norm,*

$$\overline{\lim_{k\to\infty}} \frac{|x_{k+1} - x_*|}{|x_k - x_*|} = \overline{\lim_{k\to\infty}} \left| [I - K_* F'(x_*)] \frac{(x_k - x_*)}{|x_k - x_*|} \right| \leqq |I - K_* F'(x_*)|,$$

and $\{x_k\}$ *converges q-superlinearly to* x_* *if and only if the norm-independent condition*

$$\lim_{k\to\infty} \left| [I - K_* F'(x_*)] \frac{(x_k - x_*)}{|x_k - x_*|} \right| = 0,$$

holds.

Proof. Set $B_* = K_*^{-1}$ and $B_k = K_k^{-1}$ for $k = 0, 1, 2, \cdots$, and note that

$$(B_k - B_*)s_k = (B_* - B_k)(K_* y_k - s_k) - B_k(K_k - K_*)y_k.$$

It follows that

$$\frac{|(B_k - B_*)s_k|}{|s_k|} \leqq |B_* - B_k| \frac{|K_* y_k - s_k|}{|s_k|} + \frac{|B_k||y_k|}{|s_k|} \frac{|(K_k - K_*)y_k|}{|y_k|} \tag{A3.8}$$

and, since $|B_k v| \geqq (1/|K_k|)\, |v|$ for $v \in \mathbb{R}^n$,

$$\frac{|y_k|}{|K_k||s_k|} \frac{|(K_k - K_*)y_k|}{|y_k|} - |B_* - B_k| \frac{|K_* y_k - s_k|}{|s_k|} \leqq \frac{|(B_k - B_*)s_k|}{|s_k|}. \tag{A3.9}$$

Now (A3.6) yields

$$\begin{aligned} |y_k| &\leqq |B_*||K_* y_k| \leqq |B_*|(|K_* y_k - s_k| + |s_k|) \\ &\leqq |B_*|(1 + \alpha_k)|s_k| \end{aligned} \tag{A3.10}$$

and

$$|y_k| \geqq \frac{|K_* y_k|}{|K_*|} \geqq \frac{1}{|K_*|} (|s_k| - |K_* y_k - s_k|) \geqq \frac{1}{|K_*|} (1 - \alpha_k)|s_k|, \tag{A3.11}$$

and since $\{\|K_k\|\}$ and $\{\|B_k\|\}$ are bounded and $\lim_{k\to\infty} \alpha_k = 0$, one sees from (A3.8) (A3.9), (A3.10) and (A3.11) that (A3.7) holds if and only if

$$\lim_{k\to\infty} \frac{|(B_k - B_*)s_k|}{|s_k|} = 0.$$

The theorem then follows from Theorem A3.1.

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