Local and Superlinear Convergence
of Structured Secant Methods
from the Convex Class[1]

by

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Abstract. In this paper we develop a unified theory for establishing the local and q-superlinear convergence of the secant methods from the convex class that take advantage of the structure present in the Hessian in constructing approximate Hessians.

As an application of this theory, we show the local and q-superlinear convergence of any structured secant method from the convex class for the constrained optimization problem and the nonlinear least-squares problem. Particular cases of these methods are the SQP augmented scale BFGS and DFP secant methods for constrained optimization problems introduced by Tapia. Another particular case, for which local and q-superlinear convergence is proved for the first time here, is the Al-Baali and Fletcher modification of the structured BFGS secant method considered by Dennis, Gay and Welsch for the nonlinear least-squares problem and implemented in the current version of the NL2SOL code.

Key words. secant, quasi-Newton, least-squares, superlinear convergence, bounded deterioration, constrained optimization.

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1. Introduction.

Our goal is to develop a unified theory which can be used to establish the local and q-superlinear convergence of the secant methods from the convex class studied by Broyden [1967] and Fletcher [1970] that take advantage of the structure present in the Hessian in constructing approximate Hessians.

The theory we will give can be seen either as a generalization of the result for the structured DFP secant method given by Dennis and Walker [1981] to any structured secant method in the convex class or as an extension of the results for the (unstructured) secant methods from the convex class obtained by Griewank and Toint [1982] to the structured secant methods in the same class. Indeed, our approach is similar to the one used in both of these papers.

As a surprising consequence of our careful computation of the constants in the bounded deterioration principle, we obtain a stronger bounded deterioration inequality for the BFGS secant method.

1.1. The Secant Method.

By a *secant method* for the optimization problem

$$\underset{x}{minimize}\ f(x) \tag{1.1}$$

where $f: \mathbb{R}^n \longrightarrow \mathbb{R}$, we mean the iterative procedure

$$\begin{aligned} x_+ &= x + s \\ B_+ &= \mathbb{B}(x, s, y, B). \end{aligned} \tag{1.2}$$

Here y is an approximation to $\nabla^2 f(x_+)s$, s is the quasi-Newton step defined by

$$Bs = -\nabla f(x)\ , \tag{1.3}$$

and B_+ is required to satisfy the secant equation

$$B_+ s = y \ . \tag{1.4}$$

One way of defining y, and the most often used, is

$$y = \nabla f(x_+) - \nabla f(x) \ . \tag{1.5}$$

A large class of this type of methods has been studied by Broyden [1967], Fletcher [1970], Greenstadt [1970], Huang [1970], Dennis [1972], Schnabel [1977], and numerous other authors.

1.1.1. The Broyden Class of Secant Updates.

We will call the set of "exact", "stable", and symmetric rank-2 secant updates suggested by Broyden [1967] *the Broyden class of secant updates.* In the literature, this class is also referred to as the Broyden β-class of secant updates because, initially, it was parametrized by a real scalar β. Fletcher [1970] shows that this class of secant updates can be written as

$$B_+ = B + \Delta_1(s, y, B, \phi) \tag{1.6}$$

where the parameter $\phi \in \mathbb{R}$, and the update correction $\Delta_1(s, y, B, \phi)$ is given by

$$\Delta_1(s, y, B, \phi) = \frac{yy^T}{y^T s} - \frac{Bss^T B}{s^T Bs} + \phi \, s^T Bs \, uu^T \tag{1.7a}$$

$$u = \frac{y}{y^T s} - \frac{Bs}{s^T Bs} \ . \tag{1.7b}$$

The following are well-known choices of the parameter ϕ:

Convex Class	$\phi \in [0,1]$	(1.8a)
DFP	$\phi = 1$	(1.8b)
BFGS	$\phi = 0$	(1.8c)

$$SR1 \qquad \phi = \frac{y^T s}{y^T s - s^T Bs}. \tag{1.8d}$$

Another important class of secant updates, suggested by Greenstadt [1970] is the set of all the symmetric secant updates which minimize a weighted Frobenius norm of $B_+ - B$ (see Dennis and Walker [1981] for more details). Dennis [1972] derived a larger class of symmetric secant updates as the limit of an iterative process and showed that this larger class can be written as

$$B_+ = B + \Delta_2(s, y, B, v) \tag{1.9}$$

where the vector $v \in \mathbb{R}^n$ is called *the scale* (see Dennis and Walker [1981]), and the update correction $\Delta_2(s, y, B, v)$ is given by

$$\Delta_2(s, y, B, v) = \frac{(y - Bs)v^T + v(y - Bs)^T}{v^T s} - \frac{(y - Bs)^T s}{(v^T s)^2} vv^T. \tag{1.10}$$

The scale v is often a function of s, y, and B, as is the case for the following well-known members of this class:

$$PSB \qquad v = s \tag{1.11a}$$

$$DFP \qquad v = y \tag{1.11b}$$

$$BFGS \qquad v = y + [\frac{y^T s}{s^T Bs}]^{1/2} Bs \tag{1.11c}$$

$$SR1 \qquad v = y - Bs. \tag{1.11d}$$

Dennis [1972] also pointed out that a member in his class was a member of the Broyden class only if the scale v is a linear combination of y and Bs. Schnabel [1977] proved that there exists an onto mapping from

$$\{\Delta_2(s, y, B, v) : v = y + \sigma(y - Bs), \sigma \in \mathbb{R}, \sigma \neq y^T s/(s^T Bs - y^T s)\} \tag{1.12a}$$

to

$$\{\Delta_1(s,y,B,\phi): \phi \in \mathbb{R}: (1-\phi)\frac{y^T s}{s^T Bs} + \phi > 0\}. \tag{1.12b}$$

Three remarks are important here. First of all, set (1.12b) is the set of rank-2 matrices that has the form given by (1.7) and can be written as $ww^T - zz^T$ for some nonzero vectors $w, z \in \mathbb{R}^n$. Secondly, if B is positive definite and $y^T s > 0$, set (1.12b) contains the convex class of secant updates. Finally, this mapping will be crucial to extend the bounded deterioration principle for the (unstructured) secant methods to the corresponding structured ones (see Theorem 2.5).

1.1.2. The Structured Secant Method.

Often, in practice, a part of $\nabla^2 f(x)$ is available and we need only to approximate the remaining part. Suppose that

$$\nabla^2 f(x) = C(x) + S(x) \tag{1.13}$$

where $C: \mathbb{R}^n \longrightarrow \mathbb{R}^{n \times n}$ is the available part of $\nabla^2 f$. In several important applications, e.g. nonlinear least-squares, $C(x)$ is composed of first-order information and $S(x)$ requires second-order information.

By a structured approximation of $\nabla^2 f(x)$ we mean an approximation of the form

$$B = A + C(x) \tag{1.14}$$

where A is an approximation to $S(x)$. Moreover, if B is updated according to the formula $B_+ = A_+ + C(x_+)$ where

$$A_+ = A + \Delta_2(s, y^\#, A, v), \tag{1.15}$$

$v = v(s, y, B)$, and $y^\#$ and y are approximations to $S(x_+)s$ and $\nabla^2 f(x_+)s$ respectively, we call B_+ a structured secant approximation of $\nabla^2 f(x_+)$. Observe that the structured update (1.15) satisfies the secant equation

$$A_+ s = y^\# \ . \tag{1.16}$$

We obtain a *structured secant method* for problem (1.1) if we use $B_+ = A_+ + C(x_+)$ instead of $B_+ = \mathbb{B}(x, s, y, B)$ in (1.2), where A_+ is given by (1.15).

Historically, a primary example of the use of structure has been the nonlinear least-squares problem, e.g., Brown and Dennis [1971], Dennis [1973], Betts [1976], Dennis [1976], Dennis [1977], Bartholomew-Biggs [1977], Dennis [1978], Dennis and Welsch [1978], Gill and Murray [1978], Dennis, Gay and Welsch [1978], Dennis and Walker [1981], Dennis and Schnabel [1983], Al-Baali and Fletcher [1985], Xu [1986], Fletcher and Xu [1987], and Toint [1987] (see Martinez [1988], Section 4.1.1.2, for more details about these works).

Initially, the structure was not carried into the calculation of the scale. It was Al-Baali and Fletcher [1985] who first suggested using structure also in the scale v. Independently, Tapia [1984] employed a structured scale in his work on structured updates for constrained optimization problems.

Dennis and Walker [1981] developed a convergence theory that includes the structured PSB and DFP secant methods. It also includes the *inverse—structured* BFGS secant method, i.e., the case when $\nabla^2 f(x)^{-1}$ instead of $\nabla^2 f(x)$ is assumed to be of the form given by (1.13). As an application of this theory, the local and q-superlinear convergence for the structured PSB and DFP secant methods for the nonlinear least-squares problem was established (see Chapter 10 of Dennis and Schnabel [1983]).

Xu [1986] (see Fletcher and [1987]) showed that the global and local properties proved by Powell [1976] for the BFGS secant method with an inexact linesearch carries over for the partial-structured BFGS secant method for nonlinear least squares problems suggested by Al-Baali and Fletcher [1985].

Another important application of structured secant methods was given by Tapia [1984]. He used the well-known bounded deterioration of the DFP and the inverse form of the BFGS secant updates as a basis for establishing bounded deterioration of the structured DFP and the inverse of the structured BFGS secant updates. Then he proved local and q-superlinear convergence for the structured DFP and BFGS secant version of his algorithms for equality constrained optimization problems. We will give more details about these algorithms in Section 4.2.1.

1.2 Standard Assumptions.

In our analysis, we will use several different matrix norms. The Frobenius norm will be denoted by $\|\cdot\|_F$, the Frobenius norm weighted by $\nabla^2 f(x_*)$ will be denoted by $\|\cdot\|_*$, i.e. $\|\cdot\|_* = \|\nabla^2 f(x_*)^{-1/2}(\cdot)\nabla^2 f(x_*)^{-1/2}\|_F$, and the l_2 operator norm will be denoted by $\|\cdot\|$. The only vector norm that will be used is the l_2 or Euclidean norm, and it will be denoted by $\|\cdot\|$.

The standard assumptions for problem (1.1) are:

A1: Problem (1.1) has a solution x_*.

A2: The function $f \in C^2$, and $\nabla^2 f$ and C (see (1.13)) are locally Lipschitz continuous at x_*, i.e., there exist positive constants L, L_C and ϵ_1 such that

$$\|\nabla^2 f(x) - \nabla^2 f(x_*)\| \leq L\, \|x - x_*\| \tag{1.17}$$

and

$$\|C(x) - C(x_*)\| \leq L_C\, \|x - x_*\| \tag{1.18}$$

for $x \in D_1 = \{x \colon \|x - x_*\| < \epsilon_1\}$.

A3: The matrix $\nabla^2 f(x_*)$ is positive definite, i.e., there exist positive constants m and M such that

$$m\, \|z\|^2 \leq z^T \nabla^2 f(x_*)\, z \leq M\, \|z\|^2 \tag{1.19}$$

for all $z \in \mathbb{R}^n$.

1.3. Local Convergence for Secant Methods.

The technique used for proving local convergence for secant methods for problem (1.1) is generally based on the bounded deterioration principle introduced by Dennis [1971] and popularized by Broyden, Dennis and Moré [1973]. Indeed, Dennis [1971] introduced the bounded deterioration principle as a majorization technique for analyzing the class of "Newton-like" methods which includes the secant methods.

Initially this principle was stated in terms of the approximations to the Hessian and expressed the fact that, while the sequence $\{B_k\}$ of approximations to the Hessian need not converge to $\nabla^2 f(x_*)$, it should deteriorate only in a controlled way. In mathematical terms, we can express this principle as follows: there exist non-negative constants α_1, α_2 such that for $x \in N_1$ and $B \in N_2$, B_+ satisfies

$$\|B_+ - B_*\|_* \leq [1+\alpha_1 \sigma(x,x_+)] \, \|B - B_*\|_* + \alpha_2 \sigma(x, x_+) \tag{1.20}$$

where $B_* = \nabla^2 f(x_*)$, N_1 and N_2 are neighborhoods of x_* and B_* respectively, and $\sigma(x_1, x_2) = \max\{\|x_1 - x_*\|, \|x_2 - x_*\|\}$. Here B_+ stands for B_{k+1} and B for B_k.

Broyden, Dennis and Moré [1973] used this principle of bounded deterioration as a sufficient condition for local convergence of the secant methods. As an application of their theory, they showed the local convergence of the DFP secant methods.

Since it was considered to be more convenient to work with approximations to $\nabla^2 f(x_*)^{-1}$ instead of approximations to $\nabla^2 f(x_*)$, they also stated the principle of bounded deterioration in terms of the approximations to the inverse of the Hessian. In mathematical terms it is expressed in the following way. There exist non-negative constants $\overline{\alpha}_1$, $\overline{\alpha}_2$ such that for $x \in \overline{N}_1$ and $B^{-1} \in \overline{N}_2$, B_+^{-1} satisfies

$$\|B_+^{-1} - B_*^{-1}\|_* \leq [1+\bar{\alpha}_1\sigma(x, x_+)]\, \|B^{-1} - B_*^{-1}\|_* + \bar{\alpha}_2\sigma(x, x_+) \qquad (1.21)$$

where $\bar{N}_1$ and $\bar{N}_2$ are neighborhoods of x_* and B_*^{-1} respectively.

This *inverse* form of the bounded deterioration inequality allowed them to prove that the BFGS secant method was locally convergent.

Based on the Broyden-Dennis-Moré theory, Dennis and Walker [1981] developed a general local convergence theory for structured secant methods which includes the *inverse—structured* BFGS and the structured DFP secant methods. Clearly, while the structured DFP proof uses the *direct* form of bounded deterioration inequality (1.20), the inverse-structured BFGS proof uses the *inverse* form of bounded deterioration inequality (1.21).

Ritter [1979] extended the Broyden-Dennis-Moré result to a subclass of Broyden's secant methods, the subclass of positive definite secant updates. His convergence results use

$$\psi = trace(B_*^{1/2}B^{-1}B_*^{1/2} + B_*^{-1/2}B\, B_*^{-1/2}) \qquad (1.22)$$

as the measure of a good approximation to B_* instead of the weighted Frobenius norm of $B - \nabla^2 f(x_*)$ used in the bounded deterioration principle (1.20). Indeed, the local convergence proof follows from a principle of bounded deterioration in terms of ψ, i.e.,

$$\psi_+ \leq \psi + \delta\sigma(x, x_+) \qquad \delta > 0 \qquad (1.23)$$

(see expressions (3.23) and (3.24) in Ritter [1979]).

Independently, Stachurski [1981] also extended the same result to Broyden's bounded ϕ-class of secant methods, which allows the parameter ϕ to change at each iteration. His approach is a generalization of the Broyden-Dennis-Moré proof for the BFGS secant method. In fact, the inverse bounded deterioration inequality (1.21) appears implicitly in his proof. He also proved that the Broyden bounded ϕ-class of secant updates includes the subclass considered by Ritter [1979]. An interesting fact about Stachurski's results is that his estimate for the radius of convergence decreases as the absolute value of ϕ, the parameter of the secant update formula (1.7), increases.

It was Griewank and Toint [1982] who first gave a unified direct bounded deterioration principle for all the members in the convex class (1.7 with 1.8a). They also showed that the inverse form of these secant updates satisfies the inverse form of the bounded deterioration inequality (1.21). In the same paper, they gave sufficient conditions for a member of this subclass of secant methods to have a q-superlinear rate of convergence. However, mainly due to their non-restrictive assumptions and their *big O* notation, it was not obvious how to extend this result to the structured secant methods described in Section **1.1.2.** It also was not clear how to obtain the direct form of the bounded deterioration principle for the structured secant methods, except DFP, from other approaches in the literature.

1.4. Material to Follow.

In this paper we will consider only the structured secant methods from the convex class. However, all our results are valid for some negative values of the parameter ϕ and for some values of it greater than one as well.

In Section 2 we prove that the structured secant approximations to the Hessian defined in Section 1.1.2 satisfy the bounded deterioration inequality (1.20) for $\phi \in [0,1]$. Moreover, we prove that a surprising and stronger form of this bounded deterioration is valid for the structured BFGS secant method.

In Section 3 we establish the local and q-superlinear convergence for all of the structured secant methods in the convex class using the Broyden, Dennis and Moré [1973] and Griewank and Toint [1982] theories.

Finally, in Section 4 we use this theory to prove the local and q-superlinear convergence of any structured secant method from the convex class for the constrained optimization problem and the nonlinear least-squares problem.

Particular cases of these methods are the SQP augmented scale BFGS and DFP secant methods for constrained optimization problems introduced by Tapia [1984]. Another particular case, for which local and q-superlinear convergence is proved for the first time here, is the Al-Baali and Fletcher [1985] modification of the structured BFGS secant method considered by Dennis, Gay and Welsch [1981] for the nonlinear least-squares problem and implemented in the current version of the NL2SOL code.

2. Bounded Deterioration.

Our objective in this section is to demonstrate that the structured secant approximations to the Hessian from the convex class satisfy the *direct* form of the bounded deterioration principle, i.e., for x sufficiently close to x_*, these approximations satisfy

$$\|B_+ - \nabla^2 f(x_*)\|_* \leq [1+\alpha_1\sigma(x,x_+)]\,\|B - \nabla^2 f(x_*)\|_* + \alpha_2\sigma(x,x_+) \quad (2.1)$$

where α_1 and α_2 are positive constants and $\sigma(x_1, x_2) = \max\{\|x_1 - x_*\|, \|x_2 - x_*\|\}$. Moreover, we will show that the structured BFGS secant approximations satisfy a surprising and stronger form of bounded deterioration. Specifically they satisfy inequality (2.1) with $\alpha_1 = 0$.

This bounded deterioration inequality will allow us to use the Broyden-Dennis-Moré theory to establish that under the standard assumptions the sequence $\{x_k\}$ generated by a structured secant method from the convex class is q-linearly convergent to x_*. The q-superlinear convergence will then follow from Proposition 4 of Griewank and Toint [1982]. This proposition is based on the well-known Dennis-Moré characterization (see Proposition 3.1).

2.1. Important Bounds.

The bounds needed to prove inequality (2.1) when the structure in the Hessian is not used, follow from Assumption A3 and the fact that y is a "good" approximation to $\nabla^2 f(x_*)s$. We formalize this fact in the following proposition.

PROPOSITION 2.1. *Suppose that Standard Assumption A3 holds and let D be a neighborhood of x_*. For $x_1, x_2 \in D$ define $s = x_2 - x_1$ and let y be an approximation to $\nabla^2 f(x_*)s$. If there exists $K_1 > 0$ such that*

$$\|y - \nabla^2 f(x_*)s\| \le K_1 \sigma(x_1, x_2) \|s\| \tag{2.2}$$

for all $x_1, x_2 \in D$, then the following inequalities hold:

$$\|y\| \le (M + K_1 \sigma(x_1, x_2)) \|s\| \tag{2.3a}$$

$$y^T s \le (M + K_1 \sigma(x_1, x_2)) \|s\|^2 \tag{2.3b}$$

where M is given in Assumption A3 (see (1.19)). Moreover, there exist positive constants ϵ_2, and *β such that the following inequalities hold:*

$$y^T s \ge \beta \|s\|^2 \tag{2.4a}$$

$$\frac{\|y\| \|s\|}{y^T s} \le \frac{M}{\beta} + \frac{K_1}{\beta} \sigma(x_1, x_2), \quad s \ne 0 \tag{2.4b}$$

for $x_1, x_2 \in D_2 = \{x : \|x - x_*\| \le \epsilon_2\} \subset D$.

Proof. Let $z = y - \nabla^2 f(x_*)s$ and $x_1, x_2 \in D$. Then (2.3) follows directly from inequality (2.2) and Assumption A3 (see (1.19)). To define D_2, choose ϵ_2 so that $K_1 \epsilon_2 < m$ and $D_2 \subset D$, where m is given in Assumption A3. If $x_1, x_2 \in D_2$, (2.4a) follows from Assumption A3 with $\beta = m - K_1 \epsilon_2$. Finally, notice that for $s \ne 0$

$$\frac{\|y\| \|s\|}{y^T s} = \frac{\|y\|}{\|s\|} \frac{\|s\|^2}{y^T s};$$

so that (2.4b) follows from inequalities (2.3a) and (2.4a). ●

Similarly, when the structure in the Hessian is used, the bounds needed to establish bounded deterioration (2.1) follow from Assumptions A2 and A3, and the fact that $y^{\#}$ is a "good" approximation to $S(x_*)s$, where S is given in (1.13). We formulate this fact in the next proposition.

PROPOSITION 2.2. *Suppose that Standard Assumption A2 holds and let D be a neighborhood of x_*. For $x_1, x_2 \in D$ define $s = x_2 - x_1$ and let $y^{\#}$ be an approximation to $S(x_*)s$. If there exists $K_2 > 0$ such that*

$$\|y^{\#} - S(x_*)s\| \leq K_2 \sigma(x_1, x_2) \|s\| \tag{2.5}$$

for all $x_1, x_2 \in D$, then there exists $K_3 > 0$ such that $y = y^{\#} + C(\overline{x})s$ for any $\overline{x} \in [x_1, x_2]$ satisfies

$$\|y - \nabla^2 f(x_*)s\| \leq K_3 \sigma(x_1, x_2) \|s\| \tag{2.6}$$

for all $x_1, x_2 \in D_1 \cap D$ where D_1 is given in Assumption A2.

Proof. Let $x_1, x_2 \in D_1 \cap D$. Taking advantage of the structure in y and in the Hessian, we can write

$$\begin{aligned} \|y - \nabla^2 f(x_*)s\| &\leq \|y^{\#} - S(x_*)s\| + \|[C(\overline{x}) - C(x_*)]s\| \\ &\leq K_2 \sigma(x_1, x_2) \|s\| + L_C \|\overline{x} - x_*\| \|s\| \\ &\leq (K_2 + L_C) \sigma(x_1, x_2) \|s\| . \qquad \bullet \end{aligned}$$

2.2. Basic Lemma

The next lemma is very useful when dealing with weighted Frobenius norms. Particular cases of it were established by Powell [1978] and by Griewank and Toint [1982].

LEMMA 2.3. *Consider a symmetric matrix $\overline{B} \in \mathbb{R}^{n \times n}$, vectors $u, z, w \in \mathbb{R}^n$, and scalars $\alpha, \phi \in \mathbb{R}$. Suppose that*

$$\alpha = u^T z, \quad w = \alpha u - z, \quad u^T \bar{B} z = z^T z, \tag{2.7a}$$

$$u^T u = 1 \quad \text{and} \quad u^T \bar{B} u = (u^T z)^2 . \tag{2.7b}$$

If we define

$$\bar{B}' = \bar{B} + uu^T - zz^T + \phi ww^T, \tag{2.8}$$

then

$$\|\bar{B}' - I\|^2_F = \|\bar{B} - I\|^2_F - \{p + 2q\phi - r\phi^2\} \tag{2.9}$$

where

$$\begin{aligned} p &= (1 - z^T z)^2 + 2[z^T \bar{B} z - (z^T z)^2] \\ q &= (z^T z)^2 + z^T z - (\alpha^2 + z^T \bar{B} z) \\ r &= (z^T w)^2 . \end{aligned} \tag{2.10}$$

Moreover, if $\bar{B}$ *is symmetric and positive definite,* $u = \dfrac{v}{\|v\|}$ *and* $z = \dfrac{\bar{B}v}{\sqrt{v^T \bar{B} v}}$ *for some nonzero vector* $v \in \mathbb{R}^n$*, then*

$$p, r \geq 0 \quad \text{and} \quad p + 2q - r \geq 0 \tag{2.11a}$$

which imply

$$\|\bar{B}' - I\|_F \leq \|\bar{B} - I\|_F \qquad \text{for } \phi \in [0,1] . \tag{2.11b}$$

Proof. To prove (2.9), observe that using definition (2.8) we can write

$$(\bar{B}'-I)^T(\bar{B}'-I) = (\bar{B}-I)^T(\bar{B}-I) + (\bar{B}-I)\,uu^T + uu^T(\bar{B}-I)$$
$$-(\bar{B}-I)\,zz^T - zz^T(\bar{B}-I) + (u^Tu)\,uu^T$$
$$+(z^Tz)\,zz^T - (u^Tz)\,uz^T - (z^Tu)\,zu^T$$
$$+\ \phi[(\bar{B}-I)ww^T + ww^T(\bar{B}-I) + (u^Tw)uw^T$$
$$+\ (w^Tu)wu^T - (z^Tw)zw^T - (w^Tz)wz^T]$$
$$+\ \phi^2(w^Tw)ww^T\ .$$

Therefore, using $trace\ (A+B) = trace\ (A) + trace\ (B)$, $trace\ (xy^T) = x^Ty$, and $\|A\|^2{}_F = trace\ (A^TA)$ we can write

$$trace\ (\bar{B}'-I)^T(\bar{B}'-I) = trace\ (\bar{B}-I)^T(\bar{B}-I)\ +\ 2u^T(\bar{B}-I)\,u$$
$$-2z^T(\bar{B}-I)\,z + (u^Tu)^2 + (z^Tz)^2 - 2(u^Tz)^2$$
$$+\ 2\phi[w^T(\bar{B}-I)w\ +\ (u^Tw)^2 - (z^Tw)^2]$$
$$+\ \phi^2(w^Tw)^2$$
$$= trace\ (\bar{B}-I)^T(\bar{B}-I)\ \ -\ \ \{p\ + 2q\phi - r\phi^2\}$$

where

$$p\ = 2z^T(\bar{B}-I)\,z - 2u^T(\bar{B}-I)\,u - (u^Tu)^2 - (z^Tz)^2 + 2(u^Tz)^2$$
$$q\ = (z^Tw)^2 - w^T(\bar{B}-I)w\ -\ (u^Tw)^2$$
$$r\ = (w^Tw)^2.$$

Finally, using (2.7), these expressions can be reduced to the ones given by (2.10).

To demonstrate (2.11a), notice that the given u and z satisfy (2.7) for any vector $v \neq 0$. Therefore, notice that from (2.10) $r \geq 0$ is obviously true, $p \geq 0$ will be true if $z^T\bar{B}z - (z^Tz)^2 \geq 0$, and since

$$p\ + 2q\ - r\ = (1-\alpha^2)^2 + 2\alpha^2(z^Tz - \alpha^2)\,,$$

$p\ + 2q\ - r \geq 0$ will be true if $z^Tz - \alpha^2 \geq 0$.

Using the definition of u, z and α we can write

$$z^T \bar{B} z - (z^T z)^2 = \frac{v^T \bar{B}^3 v}{v^T \bar{B} v} - \left(\frac{v^T \bar{B}^2 v}{v^T \bar{B} v} \right)^2 = \frac{v^T \bar{B}^3 v \;\; v^T \bar{B} v - [v^T \bar{B} v]^2}{[v^T \bar{B} v]^2},$$

and

$$(z^T z - \alpha^2) = \frac{v^T \bar{B}^2 v}{v^T \bar{B} v} - \frac{v^T \bar{B} v}{v^T v} = \frac{v^T \bar{B}^2 v \;\; v^T v - [v^T \bar{B} v]^2}{v^T \bar{B} v \;\; v^T v}.$$

We will now show that the numerators of these expressions are positive. From the Cauchy-Schwarz inequality we have

$$\begin{aligned} v^T \bar{B}^3 v \;\; v^T \bar{B} v &= \| \bar{B}^{3/2} v \|^2 \, \| \bar{B}^{1/2} v \|^2 = [\, \| \bar{B}^{3/2} v \| \, \| \bar{B}^{1/2} v \| \,]^2 \\ &\geq [\, (\bar{B}^{3/2} v)^T (\bar{B}^{1/2} v) \,]^2 = [v^T \bar{B}^2 v]^2, \end{aligned}$$

and

$$\begin{aligned} v^T \bar{B}^2 v \;\; v^T v &= \| \bar{B} v \|^2 \, \| v \|^2 = [\, \| \bar{B} v \| \, \| v \| \,]^2 \\ &\geq [(\bar{B} v)^T v]^2 = [v^T \bar{B} v]^2. \quad \bullet \end{aligned}$$

2.3. Bounded Deterioration for the Secant Approximations.

Now we establish the bounded deterioration inequality for the (unstructured) secant approximations from the convex class. The proof is based on the approach used by Griewank and Toint [1982]. However, our result is stronger than the specialization to the BFGS of their result (we obtain a sharper bounded deterioration inequality). Moreover, in order to fully expose the ideas involved, we will not assume that the problem has been transformed so that the Hessian at x_* is the identity matrix.

THEOREM 2.4. *Suppose that Standard Assumption A3 holds. Let B_+ be an (unstructured) secant update from the convex class, i.e.*

$$B_+ = B + \Delta_1(s, y, B, \phi) \tag{2.12}$$

where $s = x_+ - x$, $\Delta_1(s,y,B,\phi)$ *is given by (1.7) with the parameter* $\phi \in [0,1]$, *and* y *is an approximation to* $\nabla^2 f(x_*)s$. *If there exist* D, *a neighborhood of* x_*, *and* K_1, *a positive constant, such that*

$$\| y - \nabla^2 f(x_*)s \| \le K_1 \sigma(x, x_+) \| s \| , \tag{2.13}$$

for $x, x_+ \in D$, *then the bounded deterioration inequality (2.1) holds whenever* $x, x_+ \in D_2$, *where* D_2 *is given in Proposition 2.1.*

Proof. Let $B_* = \nabla^2 f(x_*)$ and $x, x_+ \in D_2$, and define

$$B' = B + \Delta_1(s, B_* s, B, \phi) . \tag{2.14}$$

The idea of the proof is to determine bounds on $\| B_+ - B' \|_*$ and $\| B' - B_* \|_*$ in terms of $\| B - B_* \|_*$ and then use the triangle inequality to obtain the bounded deterioration inequality (2.1).

The bound on $\| B' - B_* \|_*$ follows from (2.11) in Lemma 2.3. If $\overline{B}' = B^{*-1/2} B' B^{*-1/2}$, $\overline{B} = B^{*-1/2} B B^{*-1/2}$ and $v = B^{*1/2} s$ we can write

$$\begin{aligned}
\| B' - B_* \|_* &= \| B^{*-1/2}(B' - B_*) B^{*-1/2} \|_F = \| \overline{B}' - I \|_F \\
&= \| B^{*-1/2} [\, B - B_* + \Delta_1(s, B_* s, B, \phi) \,] \, B^{*-1/2} \|_F \\
&= \| B^{*-1/2}(B - B_*) B^{*-1/2} + B^{*-1/2} [\, \Delta_1(s, B_* s, B, \phi) \,] \, B^{*-1/2} \|_F \\
&= \| \overline{B} - I + uu^T - zz^T + \phi w w^T \|_F
\end{aligned}$$

where u, z, and w are defined, in terms of $\overline{B}$ and v given above, by (2.7) in Lemma 2.3. Therefore, by (2.11)

$$\| B' - B_* \|_* \le \| B - B_* \|_* \quad \text{for} \ \ \phi \in [0,1] . \tag{2.15}$$

To derive a bound on $\| B_+ - B' \|_*$, observe that

$$B_+ - B' = E_1 + \phi \, (E_2 + E_2^T + E_3) \tag{2.16}$$

where

$$E_1 = \frac{yy^T}{y^T s} - \frac{B_* ss^T B_*}{s^T B_* s}$$

$$E_2 = [\ \frac{B_* s}{s^T B_* s} - \frac{y}{y^T s}\ ]\ s^T B$$

$$E_3 = [\ \frac{yy^T}{(y^T s)^2} - \frac{B_* ss^T B_*}{(s^T B_* s)^2}\ ]\ s^T Bs\ .$$

Adding and subtracting the appropriate terms, and using Assumption A3, $\|xy^T\|_F = \|x\|\,\|y\|$, and inequalities (2.3) and (2.4) which follow from condition (2.13) and Lemma 2.1, the Frobenius norm of these matrices can be bounded as follows:

$$\begin{aligned}
\|E_1\|_F &= \|\frac{y(y-B_*s)^T}{y^T s} + ys^T B_*\ [\ \frac{1}{y^T s} - \frac{1}{s^T B_* s}\ ] + \frac{(y-B_*s)s^T B_*}{s^T B_* s}\|_F \\
&\le \frac{\|y\|\,\|y-B_*s\|}{y^T s} + \frac{\|y\|\,\|B_*s\|\,\|y-B_*s\|\,\|s\|}{y^T s\ s^T B_* s} + \frac{\|y-B_*s\|\,\|B_*s\|}{s^T B_* s} \\
&\le \frac{\|y\|\,\|s\|}{y^T s}\ \frac{\|y-B_*s\|}{\|s\|} + \frac{\|y\|\,\|s\|}{y^T s}\ \frac{\|B_*s\|\,\|s\|}{s^T B_* s}\ \frac{\|y-B_*s\|}{\|s\|} + \\
&\quad + \frac{\|y-B_*s\|}{\|s\|}\ \frac{\|B_*s\|\,\|s\|}{s^T B_* s} \\
&\le [\ \frac{M+K_1\sigma(x,x_+)}{\beta} + \frac{M+K_1\sigma(x,x_+)}{\beta}\ \frac{M}{m} + \frac{M}{m}\ ]\ K_1\ \sigma(x,x_+) \\
&\le \{[\ \frac{M+K_1\epsilon_2}{\beta} + \frac{M+K_1\epsilon_2}{\beta}\ \frac{M}{m} + \frac{M}{m}\ ]\ K_1\ \}\ \sigma(x,x_+)\ . \\
&= \gamma_1\,\sigma(x,x_+)\ ,
\end{aligned}$$

$$\|E_2\|_F = \| \frac{(B_* s - y)s^T B}{sB^*s} + ys^T B \left[\frac{1}{sB^*s} - \frac{1}{y^T s} \right] \|_F$$

$$\leq \frac{\|y - B_* s\| \, \|Bs\|}{sB^*s} + \frac{\|y\| \, \|Bs\| \, \|y - B_* s\| \, \|s\|}{sB^*s \quad y^T s}$$

$$\leq \|B\| \frac{\|y - B_* s\|}{\|s\|} \frac{\|s\|^2}{sB^*s} + \|B\| \frac{\|y\| \, \|s\|}{y^T s} \frac{\|y - B_* s\|}{\|s\|} \frac{\|s\|^2}{sB^*s}$$

$$\leq \|B\| \left[\frac{1}{m} + \frac{M + K_1 \sigma(x, x_+)}{\beta} \frac{1}{m} \right] K_1 \, \sigma(x, x_+)$$

$$\leq \|B\| \left\{ \left[1 + \frac{M + K_1 \epsilon_2}{\beta} \right] \frac{K_1}{m} \right\} \sigma(x, x_+)$$

$$= \gamma_2 \, \|B\| \, \sigma(x, x_+),$$

and

$$
\begin{aligned}
\|E_3\|_F &\le s^TBs \, \| \frac{y(y-B_*s)^T}{(y^Ts)^2} + ys^TB_*[\frac{1}{(y^Ts)^2} - \frac{1}{(sB^*s)^2}] \\
&\quad + \frac{(y-B_*s)s^TB_*}{(sB^*s)^2} \|_F \\
&\le s^TBs \, [\frac{\|y\|\,\|y-B_*s\|}{(y^Ts)^2} + \frac{\|y\|\,\|B_*s\|\,\|y-B_*s\|\,\|s\|\,\|y+B_*s\|\,\|s\|}{(y^Ts)^2\,(sB^*s)^2} \\
&\quad + \frac{\|y-B_*s\|\,\|B_*s\|}{(sB^*s)^2}] \\
&\le \frac{s^TBs}{y^Ts}\,\frac{\|y-B_*s\|}{\|s\|}\,\frac{\|s\|\|y\|}{y^Ts}\left[1 + \frac{\|B_*s\|\|s\|}{sB^*s}\,\frac{\|s\|^2}{sB^*s}\,\frac{\|y+B_*s\|}{\|s\|}\right] \\
&\quad + \frac{s^TBs}{sB^*s}\,\frac{\|y-B_*s\|}{\|s\|}\,\frac{\|B_*s\|\,\|s\|}{sB^*s} \\
&\le \|B\|[\frac{1}{\beta}\frac{M+K_1\sigma(x,x_+)}{\beta}\left[1+\frac{M}{m}\frac{1}{m}(2M+K_1\sigma(x,x_+))\right] \\
&\quad + \frac{1}{m}\frac{M}{m}]\,K_1\,\sigma(x,x_+) \\
&\le \|B\|\{[\frac{M+K_1\epsilon_2}{\beta^2}\left[1+\frac{M}{m^2}(2M+K_1\epsilon_2)\right] + \frac{M}{m^2}]\,K_1\}\,\sigma(x,x_+) \\
&= \gamma_3\,\|B\|\,\sigma(x,x_+).
\end{aligned}
$$

Now, using (2.16), and the bounds on $\|E_1\|_F$, $\|E_2\|_F$, and $\|E_3\|_F$, we have

$$
\begin{aligned}
\|B_+ - B'\|_F &\le [\,\gamma_1 + \phi(2\gamma_2+\gamma_3)\,\|B\|\,]\,\sigma(x,x_+) \\
&\le [\gamma_1 + \phi\gamma_4(\,\|B-B_*\| + \|B_*\|)]\,\sigma(x,x_+) \\
&\le [(\gamma_1 + \phi\gamma_4 M) + \phi\gamma_4\,\|B-B_*\|_F\,]\,\sigma(x,x_+)
\end{aligned}
$$

where $\gamma_4 = 2\gamma_2 + \gamma_3$; hence,

$$\|B_+ - B'\|_* \leq \|B_*^{-1/2}\|^2 \; \|B_+ - B'\|_F \\ \leq [\,\alpha_1 \|B - B'\|_* + \alpha_2\,]\,\sigma(x, x_+) \tag{2.18a}$$

where

$$\alpha_1 = \frac{\phi\gamma_4 M}{m} \quad \text{and} \quad \alpha_2 = \frac{\gamma_1 + \phi\gamma_4 M}{m}. \tag{2.18b}$$

Finally, the triangle inequality and inequalities (2.15) and (2.18) give us the bounded deterioration inequality (2.1) as follows:

$$\|B_+ - B_*\|_* \leq \|B_+ - B'\|_* + \|B' - B_*\|_* \\ \leq [\,\alpha_1 \|B - B_*\|_* + \alpha_2\,]\,\sigma(x, x_+) + \|B - B_*\|_* \tag{2.19} \\ = [\,1 + \alpha_1\sigma(x, x_+)\,]\,\|B - B_*\| + \alpha_2\,\sigma(x, x_+). \quad \bullet$$

Notice that the stronger form of bounded deterioration for the BFGS secant update is a consequence of the fact that the difference between B_+ and B' does not depend on B, i.e., $\alpha_1 = 0$ if $\phi = 0$.

2.4. Bounded Deterioration for the Structured Secant Approximations.

Finally, we prove an analogous result for the structured secant approximations from the convex class defined in Section 1.1.2.

THEOREM 2.5. *Suppose that Standard Assumptions A2 and A3 hold. Let B_+ be a structured secant update defined in Section 1.1.2, i.e.,*

$$B_+ = A_+ + C(x_+) \tag{2.20a}$$

where

$$A_+ = A + \Delta_2\,(s, y^{\#}, A, v), \tag{2.20b}$$

$s = x_+ - x$, $\Delta_2\,(s, y^{\#}, A, v)$ is given by (1.10), the scale $v = v(s, y, B)$ is chosen such that $\Delta_2(s, y, B, v)$ can be written as $\Delta_1(s, y, B, \phi)$ for some $\phi \in [0, 1]$, and y and $y^{\#}$ are approximations to $\nabla^2 f\,(x_*)s$ and $S(x_*)s$ respectively such that

$y - y^{\#} = C(\bar{x})s$ for some $\bar{x} \in [x, x_+]$. If there exist D, a neighborhood of x_* and K_2, a positive constant, such that

$$\| y^{\#} - S(x_*)s \| \leq K_2 \sigma(x, x_+) \| s \| , \tag{2.21}$$

for $x, x_+ \in D$, then the bounded deterioration inequality (2.1) holds whenever $x, x_+ \in D_3 = D_1 \cap D_2$, where D_1 and D_2 are given in Assumption A2 and Proposition 2.1 (and Theorem 2.4) respectively.

Proof. Let $B_* = \nabla^2 f(x_*)$, and $B1 = A + C(\bar{x})$. Using (2.20) and the following simple observation

$$\Delta_2 (s, y^{\#}, A, v) = \Delta_2 (s, y, B1, v)$$

we have for $x, x_+ \in D_3$

$$\begin{aligned} B_+ &= A_+ + C(x_+) \\ &= A + \Delta_2 (s, y^{\#}, A, v) + C(x_+) \\ &= A + \Delta_2 (s, y, B1, v) + C(x_+) \\ &= B1 - C(\bar{x}) + \Delta_2 (s, y, B1, v) + C(x_+) \\ &= B1 + \Delta_2 (s, y, B1, v) + C(x_+) - C(\bar{x}) . \end{aligned} \tag{2.22}$$

Since Proposition 2.2 with condition (2.21) allows us to use Theorem 2.4, and $B1 = B + C(\bar{x}) - C(x)$, we can write

$$
\begin{aligned}
\|B_+ - B_*\|_* &\le \|B1 + \Delta_2(s, y, B1, v) - B_*\|_* + \|C(x_+) - C(\bar{x})\|_* \\
&\le [1 + \alpha_1\sigma(x, x_+)] \, \|B1 - B_*\|_* + \alpha_2\sigma(x, x_+) \\
&\qquad + \sqrt{n}\; L_C \, \|B_*^{-1/2}\|^2 (\|x_+ - x_*\| + \|\bar{x} - x_*\|) \\
&\le [1 + \alpha_1\sigma(x, x_+)] \, [\, \|B - B_*\|_* + \|C(\bar{x}) - C(x)\|_* \,] + \alpha_2\sigma(x, x_+) \\
&\qquad + \frac{2\sqrt{n}\; L_C}{m} \sigma(x, x_+) \\
&\le [1 + \alpha_1\sigma(x, x_+)] \, \|B - B_*\|_* + \alpha_2\sigma(x, x_+) \\
&\qquad + [2 + \alpha_1\epsilon_1] \frac{2\sqrt{n}\; L_C}{m} \sigma(x, x_+) \\
&= [1 + \alpha_1\sigma(x, x_+)] \, \|B - B_*\|_* + \alpha_3\sigma(x, x_+),
\end{aligned}
$$

which is (2.1) with $\alpha_3 = \alpha_2 + \dfrac{2\sqrt{n}\; L_C}{m} [2 + \alpha_1\epsilon_1]$, and α_1, α_2 are given by (2.18b) in Theorem 2.4.

3. Local Convergence Theory.

In this section we will establish the local and q-superlinear convergence of the structured secant methods from the convex class defined in Section **1.1.2.** Our approach will be to use the results of Section 2 and the Broyden-Dennis-Moré theory to prove the locally q-linear convergence. Then, we will use (2.22) and Proposition 4 of Griewank and Toint [1982] to obtain the q-superlinear convergence. For completeness we restate the Griewank-Toint proposition as follows.

PROPOSITION 3.1 (Griewank and Toint [1982]). *Suppose that Standard Assumptions A1, A2 and A3 hold. Let* $\{x_k\}$ *be a sequence which converges to* x_* *and satisfies*

$$\sum_{k>0} \|x_k - x_*\| < \infty . \tag{3.1}$$

Also, for an arbitrary sequence of ϕ's in $[0,1]$ let $\{B_k\}$, the approximations to the Hessian, be generated by

$$B_+ = B + \Delta_1(s,y,B,\phi) \tag{3.2}$$

where $\Delta_1(s,y,B,\phi)$ is the secant update correction given by (1.7), starting with a symmetric positive definite matrix B_0. Then, $\{x_k\}$ converges q-superlinearly to x_*; equivalently, $\{B_k\}$ satisfies the Dennis-Moré characterization

$$\lim_k \frac{\| [B_k - \nabla^2 f(x_*)] s_k \|}{\|s_k\|} = 0 . \tag{3.3}$$

The next theorem gives sufficient conditions to insure local and q-superlinear convergence for any structured secant method from the convex class.

THEOREM 3.2. *Suppose that Standard Assumptions A1, A2 and A3 hold. If $s = x_1 - x_2$ and $y^{\#}$ is an approximation to $S(x_*)s$ satisfying*

$$\|y^{\#} - S(x_*)s\| \le K_2 \sigma(x_1, x_2) \|s\| \tag{3.4}$$

for $x_1, x_2 \in D$ and some $K_2 > 0$, then there exist positive constants ϵ, δ such that, for $x_0 \in \mathbb{R}^n$ and symmetric $A_0 \in \mathbb{R}^{n \times n}$ satisfying $\|x_0 - x_*\| < \epsilon$ and $\|A_0 - S(x_*)\| < \delta$, the sequence $\{x_k\}$ generated by any structured secant method from the convex class for problem (1.1) is q-superlinearly convergent to x_*.

Proof. As was the case in Dennis and Walker [1981], the local q-linear convergence is a straightforward application of bounded deterioration (Theorem 2.5 in this case) and the standard Broyden-Dennis-Moré theory.

Let $B_* = \nabla^2 f(x_*)$ and $A_* = S(x_*)$. Since B_* is positive definite, there exist neighborhoods N_1 of x_* and N_2 of B_* which are sufficiently small so that $N_1 \subset D_3$ (see Theorem 2.5), N_2 contains only positive definite matrices and $x_+ \in D_3$ for every $(x, B) \in N_1 \times N_2$. Now, choose a neighborhood N_3 of A_* and restrict N_1 as needed so that $(x, A) \in N = N_1 \times N_3$ implies that $A + C(x) \in N_2$.

Theorem 2.5 allows us to use Theorem 3.2 of Broyden, Dennis and Moré [1973] to prove that $\{x_k\}$ converges q-linearly to x_*. Finally, (2.22) allows us to use Proposition 3.1 to prove the theorem. •

4. Applications.

In this section we use the results of Sections 2 and 3 to establish the local and q-superlinear convergence of any structured secant method from the convex class for the constrained optimization problem and the nonlinear least-squares problem. Particular cases of these methods are the SQP augmented scale BFGS and DFP secant methods for constrained optimization problems suggested by Tapia [1984]. Another particular case, for which local and q-superlinear convergence is proved for the first time here, is the Al-Baali and Fletcher [1985] modification of the structured BFGS secant method considered by Dennis, Gay and Welsch [1981] for the nonlinear least-squares problem and implemented in the current version of the NL2SOL code.

4.1. Nonlinear Least Squares.

Our presentation of the nonlinear least-squares problem follows Chapter 10 of Dennis and Schnabel [1983]. The nonlinear least-squares problem is

$$\underset{x}{minimize}\, f(x) = \frac{1}{2} R(x)^T R(x) = \frac{1}{2} \sum_{i=1}^{m} r_i(x)^2 \tag{4.1}$$

where $m \geq n$, the residual function $R : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is nonlinear and $r_i(x)$ denotes the i^{th} component function of $R(x)$. Straightforward calculations show that the gradient of f is given by

$$\nabla f(x) = J(x)^T R(x) \tag{4.2}$$

where $J(x)$ denotes the Jacobian of R at x, and the Hessian of f is given by

$$\nabla^2 f(x) = C(x) + S(x) \tag{4.3}$$

where

$$C(x) = J(x)^T J(x),$$
$$S(x) = \sum_{i=1}^{m} r_i(x) \nabla^2 r_i(x), \tag{4.4}$$

and $\nabla^2 r_i(x)$ is the Hessian of r_i at x.

4.1.1. The Structured Secant Method.

By a structured secant method for the nonlinear least-squares problem (4.1) we mean the iterative procedure

$$x_+ = x + s$$
$$A_+ = A + \Delta_2(s, y^{\#}, A, v) \tag{4.5}$$
$$B_+ = A_+ + C(x_+)$$

where s is the quasi-Newton step defined by

$$Bs = -\nabla f(x) . \tag{4.6}$$

In (4.5), A is an approximation to $S(x)$, $\Delta_2(s, y^{\#}, A, v)$ is the secant update correction given by (1.10) with $v = v(s, y, B)$, and y and $y^{\#}$ are approximations to $\nabla^2 f(x_*)s$ and $S(x^*)s$ respectively.

The choice for $y^{\#}$

$$y^{\#} = [\, J(x_+) - J(x) \,]^T R(x_+) \tag{4.7}$$

was suggested independently by Dennis (1976) and Bartholomew-Biggs (1977) and is currently used in the algorithms given by Dennis, Gay and Welsch (1981) and Al-Baali and Fletcher (1985). Initially, Dennis, Gay and Welsh (1981) used in the NL2SOL code

$$y = \nabla f(x_+) - \nabla f(x) \tag{4.8}$$

to compute the scale v. It was Al-Baali and Fletcher (1985) who first suggested using

$$y = y^{\#} + J(x_+)^T J(x_+)s \tag{4.9}$$

instead of (4.8) to compute v, introducing, in this way, the structure of the problem into the scale of the update formula. This modification improved the numerical performance of the NL2SOL code (Dennis [1987]).

4.1.2. Standard Assumptions.

Consider the following standard assumptions for problem (4.1).

A1: Problem (4.1) has a solution x_*.

A2: The function $f \in C^2$, and J and $\nabla^2 f$ are locally Lipschitz continuous at x_*, i.e., there exist L_1, L_2, and ϵ such that

$$\| J(x) - J(x_*) \| \leq L_1 \| x - x_* \| \tag{4.10a}$$

and

$$\| \nabla^2 f(x) - \nabla^2 f(x_*) \| \leq L_2 \| x - x_* \| \tag{4.10b}$$

for $x \in D = \{x: \| x - x_* \| < \epsilon\}$.

A3: The matrix $\nabla^2 f(x_*)$ is nonsingular.

4.1.3. Local Convergence Theory.

The following lemma will serve as the foundation of our convergence result for the nonlinear least-squares problem (4.1).

LEMMA 4.1. *Suppose that the standard assumptions for problem (4.1) hold. Then there exists a positive constant K such that*

$$\|y^{\#} - S(x_*)s\| \le K\sigma(x, x_+)\|s\| \tag{4.11}$$

where $y^{\#}$ *is given by (4.7),* $x, x_+ \in D$, *and* $s = x_+ - x$.

Proof. Observe that by adding and subtracting the appropriate terms we have

$$\begin{aligned} y^{\#} - S(x_*)s &= J(x_+)^T R(x_+) - J(x)^T R(x_+) - S(x_*)s \\ &= \nabla f(x_+) - \nabla f(x) - J(x)^T [R(x_+) - R(x) - J(x_*)s] \\ &\qquad - [J(x) - J(x_*)]^T J(x_*)s - \nabla^2 f(x_*)s \,. \end{aligned} \tag{4.12}$$

From (4.10) and Lemma 4.1.15 in Dennis and Schnabel [1983] we have

$$\|\nabla f(x_+) - \nabla f(x) - \nabla^2 f(x_*)s\| \le L_2\sigma(x, x_+)\|s\| \tag{4.13a}$$

and

$$\|R(x_+) - R(x) - J(x_*)s\| \le L_1\sigma(x, x_+)\|s\| . \tag{4.13b}$$

Therefore, using (4.12) and (4.13)

$$\begin{aligned} \|y^{\#} - S(x_*)s\| &\le L_2\sigma(x, x_+)\|s\| + \|J(x)\| L_1\sigma(x, x_+)\|s\| \\ &\qquad + \|J(x_*)\| L_1 \|x - x_*\| \|s\| \\ &\le [L_2 + (L_1\epsilon + L_*)L_1 + L_* L_1]\,\sigma(x, x_+)\|s\| \end{aligned}$$

where $L_* = \|J(x_*)\|$. •

THEOREM 4.2. *Suppose that the standard assumptions for problem (4.1) hold. Then, there exist positive constants* ϵ, δ *such that, for* $x_0 \in \mathbb{R}^n$ *and symmetric* $A_0 \in \mathbb{R}^n$ *satisfying* $\|x_0 - x_*\| < \epsilon$ *and* $\|A_0 - S(x_*)\| < \delta$, *the iteration sequence* $\{x_k\}$ *generated by any structured secant method from the convex class for problem (4.1) is* q*-superlinearly convergent to* x_*.

Proof. The proof of this theorem is a straightforward application of Theorem 3.2 and Lemma 4.1. •

4.2. Constrained Optimization.

We will consider the special case of the nonlinear programming problem where we only have equality constraints. Namely,

$$\begin{array}{ll} \underset{x}{\textit{minimize}} & f(x) \\ \textit{subject to} & g(x) = 0 \end{array} \tag{4.14}$$

where $f:\mathbb{R}^n \rightarrow \mathbb{R}$, and $g:\mathbb{R}^n \rightarrow \mathbb{R}^m$ are smooth nonlinear functions ($m \leq n$).

Associated with problem (4.14) is the Lagrangian function

$$l(x,\lambda) = f(x) + g(x)^T \lambda . \tag{4.15}$$

Straightforward calculations show that the gradient of l with respect to x is given by

$$\nabla_x l(x,\lambda) = \nabla f(x) + \nabla g(x)^T \lambda , \tag{4.16}$$

and the Hessian of l with respect to x by

$$\nabla_x^2 l(x,\lambda) = \nabla^2 f(x) + \sum_{i=1}^{m} \lambda_i \nabla^2 g_i(x) , \tag{4.17}$$

where $g_i:\mathbb{R}^n \rightarrow \mathbb{R}$ denotes the i^{th} component function of g.

4.2.1. The SQP Augmented Scale Secant Method.

Following Tapia [1984], by the SQP augmented scale secant method for the constrained optimization problem (4.14), we mean the iterative process

$$\begin{aligned} x_+ &= x + s \\ \lambda_+ &= \lambda + \Delta\lambda \\ B_+ &= B + \Delta_2(s, y, B, v_L) \end{aligned} \tag{4.18}$$

where s and $\Delta\lambda$ are respectively the solution and the multiplier associated with the solution of the quadratic programming problem

$$\begin{aligned} &\underset{s}{minimize} \quad \nabla_x l(x,\lambda)^T s + \frac{1}{2} s^T B s \\ &subject\ to \quad \nabla g(x)^T s + g(x) = 0 . \end{aligned} \tag{4.19}$$

In (4.18), B is a symmetric approximation to $\nabla_x^2 l(x,\lambda)$, and $\Delta_2(s, y, B, v_L)$ is the secant update correction given by (1.10), where

$$\begin{aligned} v_L &= v(s, y_L, B_L) , \\ y &= \nabla_x l(x_+,\lambda_+) - \nabla_x l(x,\lambda_+) , \\ y_L &= y + \rho \nabla g(x_+) \nabla g(x_+)^T s , \\ B_L &= B + \rho \nabla g(x_+) \nabla g(x_+)^T \end{aligned} \tag{4.20}$$

and ρ is the penalty constant in the augmented Lagrangian function

$$L(x, \lambda; \rho) = l(x,\lambda) + \frac{1}{2}\rho g(x)^T g(x) \qquad \rho \geq 0 . \tag{4.21}$$

Observe that B_L is a structured approximation to the Hessian of the augmented Lagrangian at the solution, i.e.,

$$B_L \approx \nabla_x^2 L(x_*,\lambda_*; \rho) = \nabla_x^2 l(x_*,\lambda_*) + \rho \nabla g(x_*) \nabla g(x_*)^T \tag{4.22a}$$

since the last term of

$$\nabla_x^2 L(x, \lambda; \rho) = \nabla_x^2 l(x,\lambda) + \rho \nabla g(x) \nabla g(x)^T + \rho \sum_{i=1}^{m} g_i(x) \nabla^2 g_i(x) \tag{4.22b}$$

vanishes at the solution x_*. Moreover, Tapia [1984] gave strong arguments to blame this second-order term for the poor numerical performance of the SQP augmented Lagrangian secant method for large values of ρ.

Three issues are important in the derivation of the SQP augmented scale secant method. First of all, consider the augmented Lagrangian instead of the standard Lagrangian to compensate the lack of positive definiteness of $\nabla_x^2 l(x_*,\lambda_*)$. Secondly, use the structure of $\nabla_x^2 L(x_*,\lambda_*; \rho)$ as much as possible. Finally, observe that the penalty constant cancels out in all parts of the algorithm except in the scale of the secant update.

In fact, the SQP augmented scale secant method is an SQP (standard) Lagrangian secant method with a modified (or augmented) scale. It is this change of scale which takes care of the lack of positive definiteness in the Hessian of the Lagrangian and allows us to use positive definite secant updates, like the ones from the convex class, for constraint optimization problem (4.14) without assuming that $\nabla_x^2 l(x_*,\lambda_*)$ is positive definite.

Clearly, since $y^T s$ is not necessarily positive, the augmented scale secant updates in (4.18) do not have the hereditary positive definiteness property. However, they do possess this property on $N(x_+)$ where

$$N(x) = \{ z \in \mathbb{R}^n : \nabla g(x)^T z = 0 \} \tag{4.23}$$

(Proposition 4.4 in Tapia [1984]).

4.2.2 Standard Assumptions.

The following are standard assumptions in the theory of quasi-Newton methods for problem (4.14).

A1: Problem (4.14) has a solution x_* with associated multiplier λ_*.

A2: The functions f and g_i, $i = 1, \ldots, m$ have second derivatives which are locally Lipschitz continuous at x_*, i.e., there exist L, L_i, $i = 1, \ldots, m$ and ϵ such that

$$\| \nabla^2 f(x) - \nabla^2 f(x_*) \| \leq L \, \| x - x_* \| \tag{4.24a}$$

and

$$\| \nabla^2 g_i(x) - \nabla^2 g_i(x_*) \| \leq L_i \, \| x - x_* \| \qquad i = 1, \ldots, m \tag{4.24b}$$

for $x \in D = \{ x : \| x - x_* \| < \epsilon \}$.

A3: The matrix $\nabla^2 l(x_*,\lambda_*) = \begin{pmatrix} \nabla_x^2 l(x_*,\lambda_*) & \nabla g(x_*) \\ \nabla g(x_*)^T & 0 \end{pmatrix}$ is nonsingular.

In the next section, we will use the following well-known results:

RESULT 4.3. *Suppose Assumption* A1 *holds. Then Assumption* A3 *is equivalent to the following two statements:*

A3'a: *The matrix* $\nabla g(x_*)$ *has full rank.*

A3'b: *The matrix* $\nabla_x^2 l(x_*,\lambda_*)$ *is positive definite on the subspace* $N(x_*)$, *where* $N(x)$ *is given by (4.23).*

RESULT 4.4. *Suppose that the standard assumptions for problem (4.14) hold. Then there exists* ρ_* *such that* $\nabla_x^2 L(x_*,\lambda_*;\, \rho)$ *is positive definite for any* $\rho > \rho_*$ (See Corollary 12.9 and Theorem 12.10 of Avriel [1976]).

4.2.3. Local Convergence Theory.

Tapia [1984] used the Fontecilla-Steihaug-Tapia [1987] and Broyden-Dennis-Moré [1973] theories to prove that, under the standard assumptions, the SQP augmented scale BFGS and DFP secant methods were locally and q-superlinearly convergent to x_*. In this section, we will use a similar approach to generalize this result to any SQP augmented scale secant method from the convex class. The main difference in our approach is the unified way in which we obtain the bounded deterioration inequality for all the augmented scale secant updates from the convex class. Indeed, this inequality follows from Theorem 2.5 and the following lemma.

LEMMA 4.5. *Suppose that the standard assumptions for problem (4.14) hold. Then there exists a positive constant* K *such that*

$$\| y - \nabla_x^2 l(x_*,\lambda_*)s \| \leq K\sigma(x, x_+) \| s \| \tag{4.25}$$

where y *is given by (4.20),* $x, x_+ \in D$, *and* $s = x_+ - x$.

Proof. Observe that by adding and subtracting the appropriate term we have

$$
\begin{aligned}
y - \nabla_x^2 l(x_*,\lambda_*)s &= \nabla_x l(x_+,\lambda_+) - \nabla_x l(x,\lambda_+) - \nabla_x^2 l(x_*,\lambda_*)s \\
&= \nabla f(x_+) + \nabla g(x_+)\lambda_+ - \nabla f(x) - \nabla g(x)\lambda_+ - \\
&\quad - \nabla^2 f(x_*)s - \sum_{i=1}^{m} \lambda_*^i \nabla^2 g_i(x_*)s \\
&= \nabla f(x_+) - \nabla f(x) - \nabla^2 f(x_*)s + \\
&\quad + \sum_{i=1}^{m} [\ \nabla g_i(x_+) - \nabla g_i(x) - \nabla^2 g_i(x_*)s\ ]\ \lambda_*^i + \\
&\quad + \sum_{i=1}^{m} [\ \nabla g_i(x_+) - \nabla g_i(x) - \nabla^2 g_i(x_*)s\ ]\ [\ \lambda_+^i - \lambda_*^i\ ] + \\
&\quad + \sum_{i=1}^{m} [\ \lambda_+^i - \lambda_*^i\ ]\ \nabla^2 g_i(x_*)s
\end{aligned}
\tag{4.26}
$$

where λ_+^i and λ_*^i are the i^{th} component of λ_+ and λ_* respectively.

From (4.24) and Lemma 4.1.15 in Dennis and Schnabel [1983] we have

$$\|\nabla f(x_+) - \nabla f(x) - \nabla^2 f(x_*)s\| \le L\,\sigma(x, x_+)\,\|s\| \tag{4.27a}$$

and

$$\|\nabla g_i(x_+) - \nabla g_i(x) - \nabla^2 g_i(x_*)s\| \le L_i\,\sigma(x, x_+)\,\|s\| \quad i=1, \ldots, m \tag{4.27b}$$

Therefore, using (4.26), (4.27) and the Cauchy-Schwarz inequality

$$\| y - \nabla_x^2 l(x_*,\lambda_*)s \| \le L \ \sigma(x,x_+) \| s \| + \sum_{i=1}^m L_i \ |\lambda_*^i| \sigma(x,x_+) \| s \| +$$

$$+ \sum_{i=1}^m L_i \ |\lambda_+^i - \lambda_*^i| \sigma(x,x_+) \| s \| + \sum_{i=1}^m \bar{L}_i \ |\lambda_+^i - \lambda_*^i| \ \| s \|$$

$$\le [\ L + \sum_{i=1}^m L_i \ |\lambda_*^i| \ ] \sigma(x,x_+) \| s \| + \tag{4.28}$$

$$+ [(\sum_{i=1}^m L_i^2)^{1/2} \ \epsilon + (\sum_{i=1}^m \bar{L}_i^2)^{1/2} \ ] \ \| \lambda_+ - \lambda_* \| \ \| s \|$$

where $\bar{L}_i = \| \nabla^2 g_i(x_*) \|$.

From Proposition (4.2) in Fontecilla, Steihaug and Tapia [1987] we have that there exists a positive constant γ such that

$$\| \lambda_+ - \lambda_* \| \le \gamma \ \| x - x_* \| \tag{4.29}$$

for all x close enough to x_*.

Therefore, using (4.28) and (4.29), we establish (4.25) with

$$K = L + \sum_{i=1}^m L_i \ |\lambda_*^i| + \gamma \ [\ (\sum_{i=1}^m L_i^2)^{1/2} \ \epsilon + (\sum_{i=1}^m \bar{L}_i^2)^{1/2} \ ] \ . \tag{4.30}$$

●

THEOREM 4.6. *Suppose that the standard assumptions for problem (4.14) hold and* $\rho \ge 0$ *has been chosen so that* $\nabla_x^2 L(x_*,\lambda_*;\rho)$ *is positive definite (see Result 4.4). Then, there exist positive constants* ϵ, δ *such that, for* $x_0 \in \mathbb{R}^n$ *and symmetric* $B_0 \in \mathbb{R}^n$ *satisfying* $\| x_0 - x_* \| < \epsilon$ *and* $\| B_0 - \nabla_x^2 l(x_*,\lambda_*) \| < \delta$, *the iteration sequence* $\{x_k\}$ *generated by any SQP augmented scale secant method from the convex class is q-superlinearly convergent to* x_*.

Proof. This proof is similar to the one given by Tapia [1984] for the SQP augmented scale DFP secant method. The following can be seen as a generalization of that result.

First of all, let us remember that the quadratic problem (4.19) would have the same solution if we use B_L and $\nabla_x L(x, \lambda; \rho)$ instead of B and $\nabla_x l(x,\lambda)$ respectively (Proposition 3.1 in Tapia [1984]). Now, the bounded deterioration inequality for B_L, the structured secant approximation to $\nabla_x^2 L(x_*,\lambda_*; \rho)$ follows from Lemma 4.5 and Theorem 2.5 for any augmented scale secant update from the convex class. In turn, this bounded deterioration inequality allows us to use Theorem 3.1 in Fontecilla, Steihaug and Tapia [1987] to establish the existence of the constants ϵ, δ and the q-linear convergence of the sequence $\{x_k\}$. Then, using an argument identical to the one used by Broyden, Dennis and Moré [1973], we can prove

$$\lim_k \frac{\| [B_L^k - \nabla_x^2 L(x_*,\lambda_*; \rho)] \, s_k \|}{\|s_k\|} = 0 . \tag{4.31}$$

Finally, the q-superlinear convergence follows from Corollary 5.4 in Fontecilla, Steihaug and Tapia [1987].

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