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Deriving collinear scaling algorithms as extensions of quasi-Newton methods and the local convergence of DFP- and BFGS-related collinear scaling algorithms

K.A. Ariyawansa

Department of Pure and Applied Mathematics, Washington State University, Pullman, WA 99164-2930, USA

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This paper is concerned with collinear scaling algorithms for unconstrained minimization where the underlying local approximants are forced to interpolate the objective function value and gradient at only the two most recent iterates. By suitably modifying the procedure of Sorensen (1980) for deriving such algorithms, we show that two members of the algorithm class derived related to the DFP and BFGS methods respectively are locally and q-superlinearly convergent. This local analysis as well as the results they yield exhibit the same sort of "duality" exhibited by those of Broyden, Dennis and Moré (1973) and Dennis and Moré (1974) for the DFP and BFGS methods. The results in this paper also imply the local and q-superlinear convergence of collinear scaling algorithms of Sorensen (1982, pp. 154-156) related to the DFP and BFGS methods.

Key words: Quasi-Newton methods, collinear scalings, conic approximations, local and q-superlinear convergence.

1. Introduction

Consider the minimization problem:

$$\text{Given } f: X \to \mathbb{R},\ X \subseteq \mathbb{R}^n,\ f \in C^1(X) \text{ produce a sequence } \{x_k\} \subset X \text{ that converges to a local minimizer of } x_* \in X \text{ of } f. \tag{1.1}$$

In this paper we shall be concerned with the unconstrained case of (1.1) where $X := \mathbb{R}^n$.

The sequence $\{x_k\}$ is usually generated by iterative algorithms starting with a given estimate x_0 of x_*. In most of these algorithms it is possible to interpret the computations in the kth step which produces x_{k+1} as being based on an appropriate local scaling of X and/or an appropriate local approximation of f. We use the word "local" to indicate that these scalings and approximations are defined in terms of quantities known after x_k has been obtained and to indicate that they are intended to be used in appropriate neighborhoods of x_k. The quasi-Newton methods [7], for example, are based on local affine scalings of X and local quadratic approximations of f.

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In [4, 5], Davidon proposed generalizations of local affine scalings (l.a.s.'s) and local quadratic approximations (l.q.a.'s) termed local collinear scalings (l.c.s.'s) and local conic approximations (l.c.a.'s) respectively. We refer the reader to [5] for a detailed discussion of l.c.s.'s and l.c.a.'s. In the rest of the paper an l.c.s. and an l.c.a. shall have the following meaning.

A l.c.s. (with reference point x_k) is a mapping $S_k : w \mapsto x$ of the form

$$x = x_k + J_k w/(1 + h_k^{\mathrm{T}} w), \quad w \in W_k, \tag{1.2}$$

depending on the parameters $J_k \in \mathbb{R}^{n\times n}$ (J_k nonsingular) and $h_k \in \mathbb{R}^n$. In (1.2) $W_k := \{w\colon w \in \mathbb{R}^n, 1 + h_k^{\mathrm{T}} w \neq 0\}$ is the domain of the l.c.s. For use in the rest of the paper we let $W_k^+ := \{w\colon w \in \mathbb{R}^n,\ 1 + h_k^{\mathrm{T}} w > 0\}$. Note that $0 \in W_k^+$ maps to x_k.

A l.c.a. (with reference point x_k) is a function $\Psi_k : X_k \to \mathbb{R}$ of the form

$$\Psi_k(x) := c_k + \frac{g_k^{\mathrm{T}}(x - x_k)}{1 - a_k^{\mathrm{T}}(x - x_k)} + \frac{1}{2}\frac{(x - x_k)^{\mathrm{T}} A_k (x - x_k)}{[1 - a_k^{\mathrm{T}}(x - x_k)]^2}, \quad x \in X_k, \tag{1.3}$$

with value $\Psi_k(x_k) = c_k$ and gradient $\Psi_k'(x_k) = g_k$, depending on the parameters $A_k \in \mathbb{R}^{n\vee n}$ (where $\mathbb{R}^{n\vee n}$ is the subspace of symmetric matrices in $\mathbb{R}^{n\times n}$) and $a_k \in \mathbb{R}$. In (1.3) $X_k := \{x\colon x \in \mathbb{R}^n, 1 - a_k^{\mathrm{T}}(x - x_k) \neq 0\}$. Let $X_k^+ := \{x\colon x \in \mathbb{R}^n, 1 - a_k^{\mathrm{T}}(x - x_k) > 0\}$ and note that $x_k \in X_k^+$. If we decide to approximate f by Ψ_k "near" x_k, then, since $f \in C^1(X)$ and Ψ_k is discontinuous on its *horizon* $X_k^0 := \{x\colon x \in \mathbb{R}^n, 1 - a_k^{\mathrm{T}}(x - x_k) = 0\}$, we may do so on a neighborhood $N_{X_k^+}(x_k) \subseteq X_k^+$ of x_k.

Since (1.2) and (1.3) generalize l.a.s.'s and l.q.a.'s respectively we may expect to be able to develop algorithms extending quasi-Newton methods based on (1.2) and (1.3). Although algorithms based on (1.2) and (1.3) were given by Davidon in [4, 5], it was Sorensen [11] who first derived a class of algorithms using (1.2), *explicitly* indicating the relationships to quasi-Newton methods. He referred to his algorithms as *collinear scaling algorithms* since his derivation uses (1.2) *explicitly* while the underlying l.c.a.'s are implicit. We shall also use the term in the same sense.

The class of collinear scaling algorithms that Sorensen presents [11, Algorithm 3.1] is derived as follows. At x_k ($k \geq 1$), l.c.s. (1.2) is used to scale X and a l.q.a. ψ_k is used to approximate $\varphi := f \circ S_k$:

$$\begin{aligned} &f(x_k + J_k w/(1 + h_k^{\mathrm{T}} w)) \\ &\quad = \varphi_k(w) \approx \psi_k(w) := f(x_k) + [J_k^{\mathrm{T}} f'(x_k)]^{\mathrm{T}} w + \tfrac{1}{2} w^{\mathrm{T}} B_k w \end{aligned} \tag{1.4}$$

where $B_k \in \mathbb{R}^{n\vee n}$. If in (1.4) $w \in N_{W_k^+}(0)$—a neighborhood of $0 \in W_k^+$—then l.q.a. in (1.4) and the l.c.s. (1.2) yield the l.c.a.

$$\begin{aligned} &f(x) \approx \Psi_k(x) := f(x_k) + \frac{[f'(x_k)]^{\mathrm{T}}(x - x_k)}{1 - h_k^{\mathrm{T}} J_k^{-1}(x - x_k)} + \frac{1}{2}\frac{(x - x_k)^{\mathrm{T}} J_k^{-\mathrm{T}} B_k J_k^{-1}(x - x_k)}{[1 - h_k^{\mathrm{T}} J_k^{-1}(x - x_k)]^2}, \\ &x \in N_{X_k^+}(x_k), \end{aligned} \tag{1.5}$$

where $X_k^+ := \{x\colon x \in \mathbb{R}^n, 1 - h_k^{\mathrm{T}} J_k^{-1}(x - x_k) > 0\}$. Sorensen [11] chooses J_k, h_k and B_k by means of appropriate updating formulae so that the l.c.a. in (1.5) interpolates the value and gradient of f at x_k and x_{k-1} and *at several additional past iterates.*

Most of Sorensen's paper [11] however, is concerned with a *specific member* of the above algorithm class. This specific member, stated in [11, Algorithm 6.1], is related to the BFGS algorithm [7] because of the formula Sorensen uses for updating $H_k := B_k^{-1}$. The l.c.a. (1.5) it uses at x_k $(k \geq 1)$ interpolates the value and gradient of f *only at* x_k *and* x_{k-1} and the update formulae used for J_k and h_k [11, equations (4.1a, b)] are (specializations of) those given in [11, Algorithm 3.1]. Sorensen analyzes the direct iterates [11, equations 4.5, 4.6] of his algorithm [11, Algorithm 6.1] and shows that it is locally and q-superlinearly convergent. This analysis very critically depends on the specific formulae used for updating H_k, J_k and h_k. In particular, Sorensen implies [11, p. 95] that the member of his Algorithm 3.1 related to the DFP method in analogy with his Algorithm 6.1 could not be analyzed. This is because it seems impossible to obtain the analogue of [11, Lemma 4.1] to provide a closed-form update formula for $C_k := J_k H_k J_k^{\mathrm{T}}$ in the case of the appropriate DFP-related member of [11, Algorithm 3.1]. This last observation also implies that such a method may not be implemented without having to maintain and update two matrices (J_k and H_k or equivalently $L_k := J_k^{-\mathrm{T}}$ and $B_k := H_k^{-1}$).

The work of Sorensen [11] indicates how collinear scaling algorithms may be derived as very natural generalizations of quasi-Newton methods. It is therefore of interest to ask whether local and global convergence results similar to those known for quasi-Newton methods hold for collinear scaling algorithms. The analysis of Sorensen [11] of his Algorithm 6.1 is a positive step in this direction. The difficulties in using the same methods to analyze the analogous member of his Algorithm 3.1 related to the DFP method seems however to be a stumbling block in attempting to respond to such questions on convergence.

This paper, based on the two earlier reports [1, 2], is an attempt to continue the theme of the work of Sorensen [11]: Collinear scaling algorithms may be derived extending the quasi-Newton methods very naturally so that the relationships between the two classes of algorithms extend to convergence analyses and results as well.

In Section 2 of the paper we derive collinear scaling algorithms whose underlying l.c.a.'s at x_k $(k \geq 1)$ are forced to interpolate the function value and gradient of f at x_k and x_{k-1}. We emphasize that throughout the rest of the paper we are concerned with collinear scaling algorithms whose underlying l.c.a's interpolate function values and gradients at the current and previous points only. The purpose of Section 2 is to modify the derivation of Sorensen [11] so that the "duality" that exists between the local convergence results for the DFP and BFGS methods extends to the resulting collinear scaling algorithms related to these two methods. In particular, we use the l.c.s. (1.2) with $J_k := I$ for all k and replace Sorensen's consistency condition [11, equation (2.7)], $x_{k-1} = S_k(-v_{k-1})$ where v_{k-1} is such that $x_k = S_{k-1}(v_{k-1})$, with the condition $x_{k-1} = S_k(-\tilde{v}_{k-1})$ where $\tilde{v}_{k-1}$ is *chosen* appropriately. Note that since $J_k := I$ for all k we do not need (the analogue of) [11, Lemma 4.1] for local analysis and that the issue of having to maintain and update two matrices in implementations does not arise. Section 2 simply demonstrates that $J_k := I$ for all k can indeed be used and yet have the underlying l.c.a.'s interpolate function values and gradients at the two most recent iterates by relaxing [11, equation (2.7)].

Algorithmic Schema 2.1 in Section 2 is the class of collinear scaling algorithms that results from our derivation. It maintains and updates h_k and B_k or equivalently h_k and H_k. Despite the simple way our derivation differs from that of Sorensen [11], members of Algorithmic Schema 2.1 and the appropriate special cases of [11, Algorithm 3.1] (to enforce interpolation of function values and gradients at the two most recent iterates only) are in general different. The following simple relation exists between a member of our Algorithmic Schema 2.1 related to the BFGS method and [11, Algorithm 6.1]. If in our algorithm we update $\gamma_k^2 H_k$ (where $\gamma_k > 0$ would be available when we are about to update H_k) instead of H_k to get H_{k+1} we get [11, Algorithm 6.1] provided certain conditions are satisfied by the inputs to and the line searches of the two algorithms. However, we have not been able to find similar relations between other appropriate members of the two algorithm classes. In particular, this is true of appropriate DFP-related members of the two algorithm classes.

In [12, pp. 154–156] Sorensen provides another derivation of collinear scaling algorithms in which underlying l.c.a.'s interpolate function values and gradients only at the two most recent iterates. In this derivation he uses the l.c.s. S_k of (1.2) at x_k ($k \geq 1$) to scale X, and the l.q.a. ψ_k of (1.4) *with* $B_k := I$ *for all* k to approximate $\varphi_k := f \circ S_k$. Moreover, in the process of forcing the l.c.a. at x_k to interpolate function values and gradients at x_k and x_{k-1} he does not use the consistency condition [11, equation (2.7)] but rather uses the condition $x_{k-1} = S_k(-\bar{v}_{k-1})$ for an appropriately chosen $\bar{v}_{k-1}$ [12, equation (6.4)]. At the end of Section 2 we show that if the parameter b_k in Algorithmica Schema 2.1 is chosen so that $b_k := f'(x_k)$ for all k (and if certain conditions are satisfied by inputs to algorithms) then this special case of Algorithmic Schema 2.1 and the class of algorithms implicit in [12, pp. 154–156] are equivalent. Indeed this class of algorithms of Sorensen may be treated as a "factored" version of that portion of our Algorithmic Schema 2.1 specified by the choice $b_k := f'(x_k)$ for all k.

As mentioned earlier, since we maintain $J_k := I$ for all k, we may expect that the methods of [11] may be used to show local and q-superlinear convergence of both the (appropriate) DFP- and BFGS-related members of Algorithmic Schema 2.1. Sections 3 and 4 are devoted to verifying that indeed this expectation is true for the DFP- and BFGS-related members of Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k. We hasten to add that *because of the relationship we mentioned above* between this BFGS-related member of Algorithmic Schema 2.1 and [11, Algorithm 6.1] the local and q-superlinear convergence of the former essentially follows from the results of [11] (after some technical estimates to allow for updating H_k rather than $\gamma_k^2 H_k$). However, the local and q-superlinear convergence of the DFP-related members of Algorithmic Schema 2.1 *do not follow* from the results in [11]. Of course due to the (essential) equivalence of collinear scaling algorithms implicit in [12, pp.

154–156] and those of Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k, the results in Sections 3 and 4 readily imply the local and q-superlinear convergence of DFP- and BFGS-related members of algorithms in [12, pp. 154–156].

2. Derivation of the class of algorithms

The main purpose of this section is to demonstrate that by setting $J_k := I$ for all k and relaxing the consistency condition [11, equation (2.7)] in the derivation of Sorensen [11], collinear scaling algorithms in which the underlying l.c.a's interpolate function values and gradients at the two most recent iterates only can be derived to extend quasi-Newton methods very naturally. As we shall see in Sections 3 and 4 the resulting algorithms are related to quasi-Newton methods naturally in the sense that local analyses of certain DFP- and BFGS-related methods exhibit the same sort of "duality" that is well known with respect to the DFP and BFGS methods. In this section we shall also indicate certain relationships between the class of algorithms derived here and those given in [11, 12].

Suppose that the current point is x_k and that we apply the current l.c.s. $S_k : w \mapsto x$ (setting $J_k := I$ in (1.2)) so that

$$x = x_k + w/(1 + h_k^{\mathrm{T}} w), \quad w \in W_k, \; h_k \in \mathbb{R}^n. \tag{2.1}$$

If we now let $\varphi_k := f \circ S_k$ then

$$\varphi_k(w) = f(x_k + w/(1 + h_k^{\mathrm{T}} w)) \tag{2.2a}$$

and

$$\varphi_k'(w) = [1/(1 + h_k^{\mathrm{T}} w)][I - h_k w^{\mathrm{T}}/(1 + h_k^{\mathrm{T}} w)] f'(x_k + w/(1 + h_k^{\mathrm{T}} w)) \tag{2.2b}$$

for $w \in W_k$. We now approximate φ_k by the l.q.a. ψ_k in $N_{W_k^+}(0)$ as follows.

$$\varphi_k(w) \approx \psi_k(w) := \varphi_k(0) + [\varphi_k'(0)]^{\mathrm{T}} w + \tfrac{1}{2} w^{\mathrm{T}} B_k w, \quad w \in N_{W_k^+}(0). \tag{2.3}$$

In (2.3) $B_k \in \mathbb{R}^{n \vee n}$ is supposed to approximate $\varphi_k''(0)$. The aim now is to use the l.q.a. (2.3) and the l.c.s. (2.1) to compute the next point x_{k+1}. Several issues (including those that depend on the updating procedure we are about to describe) need to be considered when computing x_{k+1}. We shall therefore comment on the computation of x_{k+1} while we describe the updating procedure. Suppose then for the moment that we have computed x_{k+1}, and let $s_k = x_{k+1} - x_k$.

We now wish to move to x_{k+1}, update h_k to h_{k+1} and B_k to B_{k+1} so that we have the updated l.c.s. S_{k+1} and the l.q.a. ψ_{k+1} to $\varphi_{k+1} := f \circ S_{k+1}$ as follows.

$$\begin{aligned} & f(x_{k+1} + w/(1 + h_{k+1}^{\mathrm{T}} w)) \\ & = \varphi_{k+1}(w) \approx \psi_{k+1}(w) \\ & := \varphi_{k+1}(0) + [\varphi_{k+1}'(0)]^{\mathrm{T}} w + \tfrac{1}{2} w^{\mathrm{T}} B_{k+1} w, \quad w \in N^+_{W_{k+1}}(0). \end{aligned}$$

We shall then repeat the above procedure at x_{k+1} to get x_{k+2}.

We update B_k and h_k to B_{k+1} and h_{k+1} respectively by requiring

$$\psi_{k+1}(0) = \varphi_{k+1}(0), \tag{2.4a}$$

$$\psi'_{k+1}(0) = \varphi'_{k+1}(0), \tag{2.4b}$$

$$\psi_{k+1}(-\tilde{v}_k) = \varphi_{k+1}(-\tilde{v}_k), \tag{2.4c}$$

$$\psi'_{k+1}(-\tilde{v}_k) = \varphi'_{k+1}(-\tilde{v}_k), \tag{2.4d}$$

where $\tilde{v}_k \in \mathbb{R}^n$ is *chosen* such that $-\tilde{v}_k \in W^+_{k+1}$ and $x_k = S_{k+1}(-\tilde{v}_k)$. Note that (2.4a) through (2.4d) require that Ψ_{k+1}, the underlying l.c.a. at x_{k+1}, interpolates the function value and gradient of f at x_{k+1} and x_k.

It is easy to show that the requirements $x_k = S_{k+1}(-\tilde{v}_k)$ and $-\tilde{v}_k \in W^+_{k+1}$, and (2.4a) through (2.4d) are satisfied by choosing $\gamma_k > 0$, $\tilde{v}_k$, h_{k+1} and B_{k+1} to satisfy

$$h^{\mathrm{T}}_{k+1}\tilde{v}_k = 1 - \gamma_k, \tag{2.5a}$$

$$\tilde{v}_k = \gamma_k s_k, \tag{2.5b}$$

$$B_{k+1}\tilde{v}_k = r_k, \quad r_k := f'(x_{k+1}) - (1/\gamma_k)[I + h_{k+1}s^{\mathrm{T}}_k]f'(x_k), \tag{2.5c}$$

and

$$[\{f'(x_{k+1})\}^{\mathrm{T}}s_k]\gamma_k^2 + 2[f(x_k) - f(x_{k+1})]\gamma_k + \{f'(x_k)\}^{\mathrm{T}}s_k = 0. \tag{2.5d}$$

The discriminant D_k of the quadratic equation in γ_k of (2.5d) is given by $D_k := 4[\{f(x_k) - f(x_{k+1})\}^2 - \{f'(x_{k+1})\}^{\mathrm{T}}s_k\{f'(x_k)\}^{\mathrm{T}}s_k]$. If we compute x_{k+1} so that $D_k > 0$ then it can be shown that the roots $\gamma_k^{\pm}$ of (2.5d) are given by $\gamma_k^{\pm} := -\{f'(x_k)\}^{\mathrm{T}}s_k/[\{f(x_k) - f(x_{k+1})\} \pm \rho_k]$ where $\rho_k := \frac{1}{2}\sqrt{D_k}$. For future reference we also note that $\tilde{v}^{\mathrm{T}}_k B_{k+1}\tilde{v}_k = \tilde{v}^{\mathrm{T}}_k r_k = s^{\mathrm{T}}_k y_k = \pm 2\rho_k$ where $y_k := \gamma_k^{\pm} f'(x_{k+1}) - (1/\gamma_k^{\pm})f'(x_k)$. In order to achieve $\gamma_k > 0$ therefore, we shall require that x_{k+1} be computed so that

$$\{f'(x_k)\}^{\mathrm{T}}s_k < 0, \tag{2.6a}$$

$$D_k > 0, \tag{2.6b}$$

and

$$f(x_k) - f(x_{k+1}) > 0. \tag{2.6c}$$

We can then let

$$\gamma_k := \gamma_k^{+} = -\{f'(x_k)\}^{\mathrm{T}}s_k/[\{f(x_k) - f(x_{k+1})\} + \rho_k] > 0 \tag{2.7a}$$

which leads to

$$\tilde{v}^{\mathrm{T}}_k B_{k+1}\tilde{v}_k = \tilde{v}^{\mathrm{T}}_k r_k = s^{\mathrm{T}}_k y_k = 2\rho_k, \quad y_k := \gamma_k f'(x_{k+1}) - (1/\gamma_k)f'(x_k). \tag{2.7b}$$

We shall now comment on the computation of x_{k+1} based on (2.3) and (2.1). Let us assume that the level set $\{x\colon f(x) \leqslant f(x_0)\}$ is bounded, so that in view of (2.6c) we can without loss of generality assume that $\{x\colon f(x) \leqslant f(x_k)\}$ is bounded. As in [5, 11] we propose to choose B_k positive definite and to compute x_{k+1} based on a linesearch strategy. One possibility that comes to mind is as follows. Compute the minimizer $v_k := -B_k^{-1}\varphi_k'(0)$ of ψ_k, let $\delta_k := h_k^T v_k$ and search $\varphi_k(\alpha v_k)$ over $\alpha \in [0, \infty) \cup (-\infty, -1/\delta_k)$ if $\delta_k > 0$ or over $\alpha \in [0, -1/\delta_k)$ if $\delta_k \leq 0$ until an $\alpha := \alpha_k$ is found so that $x_{k+1} := S_k(\alpha_k v_k)$ with $(s_k := x_{k+1} - x_k)$ satisfies (2.6a, b, c). In view of the assumptions that $\{x: f(x) \leq f(x_k)\}$ is bounded and that B_k is positive definite such an α_k always exists unless $f'(x_k) = 0$. Note however, that if we choose $\alpha_k \in (-\infty, -1/\delta_k)$ (when $\delta_k > 0$) then x_k and x_{k+1}, or if $1 + \delta_k < 0$ then x_k and $S_k(v_k)$, are on opposite sides of the horizon X_k^0 of the underlying l.c.a. Ψ_k. The neighborhood of x_k on which Ψ_k is really used under these conditions therefore includes (part of) the horizon X_k^0. Since Ψ_k is discontinuous on X_k^0 and f is smooth, under these conditions, some readers may question the validity of using Ψ_k to approximate f.

Another possibility (also implicit in [5, p. 279]) is to note that $[f'(x_k)]^T v_k < 0$ (unless $f'(x_k) = 0$) so that v_k *may be treated* as defining a descent direction for f at x_k *in the original variable space* X. We may therefore search $f(x_k + \lambda v_k)$ over $\lambda \in (0, \infty)$ until a $\lambda := \lambda_k$ is found so that $x_{k+1} := x_k + \lambda_k v_k$ (with $s_k := x_{k+1} - x_k$) satisfies (2.6a, b. c). Again under the assumptions that $\{x: f(x) \leq f(x_k)\}$ is bounded and B_k is positive definite such a λ_k always exists unless $f'(x_k) = 0$. One may however question this approach since the l.c.s. (2.1) is not fully utilized in computing x_{k+1}.

In addition to satisfying (2.6a, b, c) it is also desirable that the linesearch yields x_{k+1} to provide a "sufficient decrease" in the sense of Ortega and Rheinboldt [10].

Computing x_{k+1} so that all the above issues are properly addressed is very much an open question. Since we are concerned with local convergence of *direct iterates*, when stating algorithmic schemata in the rest of the paper, we shall assume that we have a line search procedure LSP: $C^1(X) \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ which takes f, x_k, v_k and δ_k as input and produces a point LSP(f, x_k, v_k, δ_k) that satisfies (2.6a, b, c) and other desirable criteria. We can then let $x_{k+1} :=$ LSP(f, x_k, v_k, δ_k). The reader may agree after reading Sections 3 and 4 of the paper that LSP should begin by considering the trial point $S_k(v_k)$ as a candidate for x_{k+1} if $1 + \delta_k > 0$.

Once γ_k is determined by (2.7a), note that

$$h_{k+1} := \frac{(1-\gamma_k) b_k}{\gamma_k (s_k^T b_k)} \tag{2.8a}$$

for any $b_k \in \mathbb{R}^n$ such that $s_k^T b_k \neq 0$ will satisfy (2.5a). In particular, by (2.6a), we can use $b_k := f'(x_k)$ so that

$$h_{k+1} = \frac{(1-\gamma_k) f'(x_k)}{\gamma_k [s_k^T f'(x_k)]}. \tag{2.8b}$$

Note that (2.8a) and (2.5c) readily imply that

$$r_k = y_k + \frac{(1-\gamma_k)}{\gamma_k^2}\left[\gamma_k^2 f'(x_{k+1}) - \frac{s_k^T f'(x_k)}{s_k^T b_k} b_k\right] \tag{2.9a}$$

and if we select $b_k := f'(x_k)$ leading to (2.8b) then

$$r_k = y_k / \gamma_k \tag{2.9b}$$

where y_k is as defined in (2.7b).

The choice for h_{k+1} in (2.8a) is as in [11, 12]. We use it here since our aim is to modify *only* those aspects of the derivation of Sorensen [11] that, in our opinion, prevented him from obtaining local convergence results for DFP-related collinear scaling algorithms.

Let us now consider updating B_k to B_{k+1} to satisfy (2.5c). In view of (2.7b) and the need to have positive definite B_k for all k, we propose using an updating formula $U_k^1: \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^{n \vee n} \to \mathbb{R}^{n \vee n}$ which takes $\tilde{v}_k$, r_k and B_k as input and produces B_{k+1} that satisfies (2.5c) and is positive definite whenever $\tilde{v}_k^{\mathrm{T}} r_k > 0$. We write

$$B_{k+1} := U_k^1(\tilde{v}_k, r_k, B_k).$$

If we started off with an approximation $H_k \in \mathbb{R}^{n \vee n}$ to $[\varphi_k''(0)]^{-1}$ in (2.3) then we would have ended up with

$$H_{k+1} r_k = \tilde{v}_k, \quad r_k := f'(x_{k+1}) - (1/\gamma_k)[I + h_{k+1} s_k^{\mathrm{T}}] f'(x_k), \tag{2.10}$$

instead of (2.5c). So supposing $U_k^2: \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^{n \vee n} \to \mathbb{R}^{n \vee n}$ to be an updating formula which takes r_k, $\tilde{v}_k$ and H_k as input and produces H_{k+1} that satisfies (2.10) and is positive definite whenever $r_k^{\mathrm{T}} \tilde{v}_k > 0$, we have

$$H_{k+1} := U_k^2(r_k, \tilde{v}_k, H_k).$$

In particular, the DFP formula, the BFGS formula and indeed the formulae for the Broyden family of updates indicated in Algorithmic Schema 2.1 below, represent such update formulae U_k^1 and U_k^2.

Our discussion so far leads to the following algorithmic schema.

Algorithmic Schema 2.1.

Step 0 (*Initialization*).

Initialize x_0, h_0, symmetric and positive definite B_0 (or H_0); $k := 0$.

Step 1 (*Search Direction*).

Set

$v_k = -B_k^{-1} f'(x_k)$ (or $v_k = -H_k f'(x_k)$),

$\delta_k = h_k^{\mathrm{T}} v_k$.

Step 2 (*Linesearch*).

Set $x_{k+1} = \mathrm{LSP}(f, x_k, v_k, \delta_k)$.

/*LSP$(\cdot, \cdot, \cdot, \cdot)$ is as described above in Section 2. If $1 + \delta_k > 0$ it begins by attempting the trial point $x_k + v_k/(1 + \delta_k)$ for x_{k+1}. x_{k+1} it generates satisfies (2.6a, b, c) and any other desirable criteria.*/

Step 3 (*Stopping Criterion*).

If stopping criteria are satisfied return with x_{k+1} as an estimate of x_*.

Otherwise go to Step 4.

Step 4 (*Updates*).

Set

$s_k = x_{k+1} - x_k$,

$\rho_k = \sqrt{\{f(x_k) - f(x_{k+1})\}^2 - \{f'(x_{k+1})\}^{\mathrm{T}} s_k \{f'(x_k)\}^{\mathrm{T}} s_k}$,

$\gamma_k = -\{f'(x_k)\}^{\mathrm{T}} s_k / [f(x_k) - f(x_{k+1}) + \rho_k]$,
$y_k = \gamma_k f'(x_{k+1}) - (1/\gamma_k) f'(x_k)$,
$\tilde{v}_k = \gamma_k s_k$,
$r_k = y_k + [(1-\gamma_k)/\gamma_k^2][\gamma_k^2 f'(x_{k+1}) - (s_k^{\mathrm{T}} f'(x_k)/s_k^{\mathrm{T}} b_k) b_k]$.
/*b_k is such that $s_{kb_k}^{\mathrm{T}} \neq 0$. A possible choice is $b_k := f'(x_k)$. Then $r_k = y_k/\gamma_k$.*/
$B_{k+1} = U_k^1(\tilde{v}_k, r_k, B_k)$ (or $H_{k+1} = U_k^2(r_k, \tilde{v}_k, H_k)$).
/*Update formulae U_k^1 and U_k^2 are as described in Section 2. Some possible choices are

$$B_{k+1} = \left(I - \frac{r_k \tilde{v}_k^{\mathrm{T}}}{\tilde{v}_k^{\mathrm{T}} r_k}\right) B_k \left(I - \frac{\tilde{v}_k r_k^{\mathrm{T}}}{\tilde{v}_k^{\mathrm{T}} r_k}\right) + \frac{r_k r_k^{\mathrm{T}}}{\tilde{v}_k^{\mathrm{T}} r_k}$$
$$-(1-\Phi_k)(\tilde{v}_k^{\mathrm{T}} B_k \tilde{v}_k)\left(\frac{r_k}{r_k^{\mathrm{T}}\tilde{v}_k} - \frac{B_k \tilde{v}_k}{\tilde{v}_k^{\mathrm{T}} B_k \tilde{v}_k}\right)\left(\frac{r_k}{r_k^{\mathrm{T}}\tilde{v}_k} - \frac{B_k \tilde{v}_k}{\tilde{v}_k^{\mathrm{T}} B_k \tilde{v}_k}\right)^{\mathrm{T}}$$

where $B_k \tilde{v}_k \neq r_k$ and $\Phi_k > 1/[1 - (r_k^{\mathrm{T}} B_k^{-1} r_k)(\tilde{v}_k^{\mathrm{T}} B_k \tilde{v}_k)/(\tilde{v}_k^{\mathrm{T}} r_k)^2]$ or

$$H_{k+1} = \left(I - \frac{\tilde{v}_k r_k^{\mathrm{T}}}{r_k^{\mathrm{T}} \tilde{v}_k}\right) H_k \left(I - \frac{r_k \tilde{v}_k^{\mathrm{T}}}{r_k^{\mathrm{T}} \tilde{v}_k}\right) + \frac{\tilde{v}_k \tilde{v}_k^{\mathrm{T}}}{r_k^{\mathrm{T}} \tilde{v}_k}$$
$$-(1-\phi_k)(r_k^{\mathrm{T}} H_k r_k)\left(\frac{\tilde{v}_k}{\tilde{v}_k^{\mathrm{T}} r_k} - \frac{H_k r_k}{r_k^{\mathrm{T}} H_k r_k}\right)\left(\frac{\tilde{v}_k}{\tilde{v}_k^{\mathrm{T}} r_k} - \frac{H_k r_k}{r_k^{\mathrm{T}} H_k r_k}\right)^{\mathrm{T}}$$

where $H_k r_k \neq \tilde{v}_k$ and $\phi_k > 1/[1 - (r_k^{\mathrm{T}} H_k r_k)(\tilde{v}_k^{\mathrm{T}} H_k^{-1} \tilde{v}_k)/(\tilde{v}_k^{\mathrm{T}} r_k)^2]$.*/
$h_{k+1} = [(1-\gamma_k)/(\gamma_k s_k^{\mathrm{T}} b_k)] b_k$.
Set $k := k+1$ and return to Step 1.

Note that Algorithmic schema 2.1 has two degrees of freedom in the following sense. The choice of update functions $\{U_k^1\}$ (or $\{U_k^2\}$) and the choice of $\{b_k\}$ would generate different members of the algorithmic schema. In particular, with the choice of update functions indicated in the comment on Step 4, Algorithmic Schema 2.1 represents generalizations of the quasi-Newton methods with the Broyden family [7, pp. 76–77] of updates for the Hessian or inverse Hessian approximants. The cases $\Phi_k := 1$ (or $\phi_k := 0$) and $\Phi_k := 0$ (or $\phi_k := 1$) for all k are of special interest. The former represents algorithms that extend the DFP methods while the latter represents algorithms that extend the BFGS method. With different choices of $\{b_k\}$ we get different *generalizers of the Broyden family*, and in particular, different *DFP generalizers* and *BFGS generalizers*.

We now compare the BFGS generalizer of Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k with Algorithm 6.1 of Sorensen [11]. In order to be specific we use a superscript S on symbols in [11, Algorithm 6.1] whenever the same symbols is used in Algorithmic Schema 2.1. We have:

Lemma 2.2. *Suppose that Algorithm* 6.1 *of* [11] *is modified by removing Step* 1^{S} *and using Step* 2 *of Algorithmic Schema* 2.1 *instead and that Algorithmic Schema* 2.1 *is modified in Step* 4 *so that* $B_{k+1} := U_k^1(\tilde{v}_k, r_k, (1/\gamma_k^2) B_k)$ (*or* $H_{k+1} := U_k^2(r_k, \tilde{v}_k, \gamma_k^2 H_k)$).

Let the inputs to these modified Algorithm 6.1 *of* [11] *and Algorithmic Schema* 2.1 *be such that* $x_0^S = x_0$, $v_0^S = -C_0 f'(x_0^S)$, $\delta_0^S = h_0^T v_0^S$ *and* $C_0 = H_0$ *and suppose that stopping criteria in Step* 2^S *and Step* 3 *are identical. Then, when applied to* (1.1) *satisfying the condition that the set* $\{x\colon f(x) \leq f(x_0)\}$ *is bounded, this modified Algorithm* 6.1 *of Sorensen* [11] *and the BFGS generalizer of this modified Algorithmic Schema* 2.1 *with* $b_k := f'(x_k)$ *for all k generate identical sequences of points so that* $x_k^S = x_k$ *for all k.*

Proof. We have $x_1 = x_1^S$. Therefore note that in view of the formulae specifying the computations in [11, Algorithm 6.1] and Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k, the conclusion follows by an induction argument if we could show that if $x_k = x_k^S$ and $x_{k+1} = x_{k+1}^S$ then $H_{k+1} = C_{k+1}$. It is easy to verify this latter fact since $\tilde{v}_k = \gamma_k s_k$ and when $b_k = f'(x_k)$, by (2.9b), $r_k = y_k/\gamma_k$ where $y_k = \gamma_k f'(x_{k+1}) - (1/\gamma_k) f'(x_k)$. □

We note in passing that Lemma 2.2 depends on [11, Lemma 4.1] since the update formula for C_k in Algorithm 6.1 of [11] depends on the latter. Since we do not have the analogue of [11, Lemma 4.1] for the DFP formula, we do not have a relation like the one in Lemma 2.2 for DFP generalizers of Algorithmic Schema 2.1 and [11, Algorithm 3.1].

In [12, pp. 154–156] Sorensen presented another derivation of collinear scaling algorithms for (1.1). We refer the reader to Section 1 for a brief description of the forms of l.c.s.'s and l.c.a.'s used in that derivation and of course to [12] for details. We shall show that Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k and the algorithmic schema implicit in [12, pp. 154–156] are equivalent (under certain mild conditions). Since we believe that the algorithmic schema implicit in [12, pp. 154–156] is useful in implementing Algorithmic Schema 2.1 (when $b_k := f'(x_k)$ for all k) we record the former in the following format for convenient reference.

Algorithmic Schema 2.3.

Step 0 (*Initialization*).

Initialize x_0, h_0, nonsingular L_0 (or J_0); $k := 0$.

Step 1 (*Search Direction*).

Set

$$v_k = -L_k^{-1} f'(x_k) \text{ (or } v_k = -J_k^T f'(x_k)),$$
$$\delta_k = h_k^T v_k.$$

Step 2 (*Linesearch*).

Set $x_{k+1} = \mathrm{LSP}(f, x_k, L_k^{-T} v_k, \delta_k)$ (or $x_{k+1} = LSP(f, x_k, J_k v_k, \delta_k)$).

/*LSP(·, ·, ·, ·) is as described above in Section 2. If $1 + \delta_k > 0$ it begins by attempting the trial point $x_k + L_k^{-T} v_k/(1+\delta_k)$ (or $x_k + J_k v_k/(1+\delta_k)$) for x_{k+1}. x_{k+1} it generates satisfies (2.6a, b, c) and any other desirable criteria.*/

Step 3 (*Stopping Criterion*).

If stopping criteria are satisfied return with x_{k+1} as an estimate of x_*.

Otherwise go to Step 4.

Step 4 (Updates).

Set

$s_k = x_{k+1} - x_k,$

$\rho_k = \sqrt{\{f(x_k) - f(x_{k+1})\}^2 - \{f'(x_{k+1})\}^{\mathrm{T}} s_k \{f'(x_k)\}^{\mathrm{T}} s_k},$

$\gamma_k = \{f'(x_k)\}^{\mathrm{T}} s_k / [f(x_k) - f(x_{k+1}) + \rho_k],$

$y_k = \gamma_k f'(x_{k+1}) - (1/\gamma_k) f'(x_k),$

$\tilde{v}_k = \gamma_k s_k,$

$r_k = y_k / \gamma_k.$

Choose $\bar{v}_k$ such that $\bar{v}_k^{\mathrm{T}} \bar{v}_k = \tilde{v}_k^{\mathrm{T}} r_k (>0)$.

Choose L_{k+1} (or J_{k+1}) such that $L_{k+1}\bar{v}_k = r_k$ and $L_{k+1}^{\mathrm{T}} \tilde{v}_k = \bar{v}_k$ (or $J_{k+1}\bar{v}_k = \tilde{v}_k$ and $J_{k+1}^{\mathrm{T}} r_k = \bar{v}_k$).

/*A possible choice of $\bar{v}_k$ and L_{k+1} (or $\bar{v}_k$ and J_{k+1}) is: Choose $\bar{v}_k$ such that $\bar{v}_k^{\mathrm{T}}\bar{v}_k = \tilde{v}_k^{\mathrm{T}} r_k$ with $(L_k^{\mathrm{T}}\tilde{v}_k - \bar{v}_k)^{\mathrm{T}}\bar{v}_k \neq 0$ and set $L_{k+1} = L_k + (r_k - L_k\bar{v}_k)(L_k^{\mathrm{T}}\tilde{v}_k - \bar{v}_k)^{\mathrm{T}} / (L_k^{\mathrm{T}}\tilde{v}_k - \bar{v}_k)^{\mathrm{T}}\bar{v}_k$ (or choose $\bar{v}_k$ such that $\bar{v}_k^{\mathrm{T}}\bar{v}_k = \tilde{v}_k^{\mathrm{T}} r_k$ with $(J_k^{\mathrm{T}} r_k - \bar{v}_k)^{\mathrm{T}}\bar{v}_k \neq 0$ and set $J_{k+1} = J_k + (\tilde{v}_k - J_k\bar{v}_k)(J_k^{\mathrm{T}} r_k - \bar{v}_k)^{\mathrm{T}} / (J_k^{\mathrm{T}} r_k - \bar{v}_k)^{\mathrm{T}}\bar{v}_k$).*/

$h_{k+1} = [(1-\gamma_k)/(\gamma_k s_k^{\mathrm{T}} f'(x_k))] L_{k+1}^{-1} f'(x_k)$

(or $h_{k+1} = [(1-\gamma_k)/(\gamma_k s_k^{\mathrm{T}} f'(x_k))] J_{k+1}^{\mathrm{T}} f'(x_k)$).

Set $k := k+1$ and return to Step 1.

We have the following lemma which spells out the relationship between Algorithmic Schemata 2.1 and 2.3. In the statement of the lemma and its proof whenever the same symbol is used in Algorithmic Schemata 2.1 and 2.3 we use the superscript S to denote symbols pertinent to Algorithmic Schema 2.3. We hope that this use and the use of superscript S earlier in relation to Lemma 2.2 would not lead to confusion, since we do not intend to refer to both groups of symbols in the same context.

Lemma 2.4. *Let the inputs to Algorithmic Schemata* 2.1 *and* 2.3 *be such that* $x_0 = x_0^{\mathrm{S}}$, $B_0 = L_0 L_0^{\mathrm{T}}$ (*or* $H_0 = J_0 J_0^{\mathrm{T}}$) *and* $h_0 = L_0 h_0^{\mathrm{S}}$ (*or* $h_0 = J_0^{-\mathrm{T}} h_0^{\mathrm{S}}$) *and suppose that stopping criteria in Step* 3 *and Step* 3^{S} *are the same. Then Algorithmic Schema* 2.1 *with* $b_k := f'(x_k)$ *for all k and Algorithmic Schema* 2.3 *are equivalent in the following sense when applied to* (1.1) *where* $\{x\colon f(x) \leqslant f(x_0)\}$ *is bounded. There is a sequence of update functions* $\{U_k^1\}$ (*or* $\{U_k^2\}$) *of Algorithmic Schema* 2.1 *specifying* $\{B_k\colon k \geqslant 1\}$ (*or* $\{H_k\colon k \geqslant 1\}$) *if and only if there exists a sequence of vectors* $\{\bar{v}_k\}$ *in Algorithmic Schema* 2.3 *specifying a sequence* $\{L_k\colon k \geqslant 1\}$ (*or* $\{J_k\colon k \geqslant 1\}$) *so that* $x_k = x_k^{\mathrm{S}}$ *for all k.*

Proof. We have $x_1 = x_1^{\mathrm{S}}$. Therefore note that in view of the formulae specifying the computations in the two algorithmic schemata, the result follows from an induction argument provided we could show that given $x_k = x_k^{\mathrm{S}}$ and $x_{k+1} = x_{k+1}^{\mathrm{S}}$ there exists symmetric and positive definite B_{k+1} (or H_{k+1}) satisfying $B_{k+1}\tilde{v}_k = r_k$ (or $H_{k+1} r_k = \tilde{v}_k$) where $\tilde{v}_k^{\mathrm{T}} r_k > 0$ if and only if there exists $\bar{v}_k$ and nonsingular L_{k+1} (or J_{k+1}) satisfying $\bar{v}_k^{\mathrm{T}}\bar{v}_k = (\tilde{v}_k^{\mathrm{S}})^{\mathrm{T}} r_k^{\mathrm{S}} > 0$, $L_{k+1}\bar{v}_k = r_k^{\mathrm{S}}$ and $L_{k+1}^{\mathrm{T}}\tilde{v}_k^{\mathrm{S}} = \bar{v}_k$ (or $J_{k+1}\bar{v}_k = \tilde{v}_k^{\mathrm{S}}$ and $J_{k+1}^{\mathrm{T}} r_k^{\mathrm{S}} = \bar{v}_k$). This latter fact follows from [8, Lemma 2.1] since when $x_k = x_k^S$ and $x_{k+1} = x_{k+1}^S$ we have $\tilde{v}_k = \tilde{v}_k^S$ and $r_k = r_k^S$. □

Using arguments similar to those in the proof of Lemma 2.4 and [8, Theorems 2.2, 2.3] it can easily be verified that under the same hypotheses of Lemma 2.4, the BFGS generalizer (or DFP generalizer) of Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k and the member of Algorithmic Schema 2.3 specified by $\bar{v}_k := \sqrt{2\rho_k/(\tilde{v}_k^T L_k L_k^T \tilde{v}_k)}\, L_k^T \tilde{v}_k$ (or $\bar{v}_k := \sqrt{2\rho_k/(r_k J_k J_k^T r_k)}\, J_k^T r_k$) for all k are equivalent.

In view of Lemma 2.4 we may think of Algorithmic Schema 2.3 as a "factored" version of Algorithmic Schema 2.1 with $b_k := f'(x_k)$ for all k. We also remark that readers familiar with quasi-Newton methods may recall that convergence analyses are usually performed using unfactored forms of updates while a popular way of implementing them is based on factored forms of updates (whenever they exist). In view of the results in Sections 3 and 4 and in [2] it seems that the form of updates in Algorithmic Schema 2.1 is more suitable for convergence analyses. On the other hand, we believe that for purposes of implementation of those members of Algorithmic Schema 2.1 with equivalent members in Algorithmic Schema 2.3, the latter form of updates may be more suitable.

3. Local and q-linear convergence of two members of Algorithmic Schema 2.1 that extend the DFP and BFGS methods

The purpose of this section is to analyze locally the two members of Algorithmic Schema 2.1 that extend the DFP and BFGS methods when $b_k := f'(x_k)$ for all k.

We will first specify the two iterations that we wish to analyze. They are Iterations 3.1 and 3.2 below which state the *direct iterations* corresponding to the DFP generalizer and the BFGS generalizer respectively of Algorithmic Schema 2.1 when $b_k := f'(x_k)$ for all k. We refer the readers to [3, pp. 224–225] for motivation for undertaking analyses of direct iterations.

Iteration 3.1.

Initialize x_0, h_0, and symmetric and positive definite B_0.

For $k = 0, 1, \ldots$ **do**

$v_k = -B_k^{-1} f'(x_k)$,

$\lambda_k = 1/(1 + h_k^T v_k)$,

$x_{k+1} = x_k + \lambda_k v_k$,

$s_k = x_{k+1} - x_k$,

$\rho_k = \sqrt{\{f(x_k) - f(x_{k+1})\}^2 - \{f'(x_{k+1})\}^T s_k \{f'(x_k)\}^T s_k}$,

$\gamma_k = -\{f'(x_k)\}^T s_k / [f(x_k) - f(x_{k+1}) + \rho_k]$,

$\tilde{v}_k = \gamma_k s_k$,

$y_k = \gamma_k f'(x_{k+1}) - (1/\gamma_k) f'(x_k)$,

$r_k = y_k / \gamma_k$,

$B_{k+1} = [I - r_k\tilde{v}_k^{\mathrm{T}}/(\tilde{v}_k^{\mathrm{T}} r_k)]B_k[I - \tilde{v}_k r_k^{\mathrm{T}}/(\tilde{v}_k^{\mathrm{T}} r_k)] + r_k r_k^{\mathrm{T}}/(\tilde{v}_k^{\mathrm{T}} r_k)$,
$h_{k+1} = [(1-\gamma_k)/(\gamma_k s_k^{\mathrm{T}} f'(x_k))]f'(x_k)$,
end do.

Iteration 3.2.
Initialize x_0, h_0, and symmetric and positive definite H_0.
For $k = 0, 1, \ldots$ **do**
$v_k = -H_k f'(x_k)$,
$\lambda_k = 1/(1 + h_k^{\mathrm{T}} v_k)$,
$x_{k+1} = x_k + \lambda_k v_k$,
$s_k = x_{k+1} - x_k$,
$\rho_k = \sqrt{\{f(x_k) - f(x_{k+1})\}^2 - \{f'(x_{k+1})\}^{\mathrm{T}} s_k \{f'(x_k)\}^{\mathrm{T}} s_k}$,
$\gamma_k = -\{f'(x_k)\}^{\mathrm{T}} s_k / [f(x_k) - f(x_{k+1}) + \rho_k]$,
$\tilde{v}_k = \gamma_k s_k$,
$y_k = \gamma_k f'(x_{k+1}) - (1/\gamma_k) f'(x_k)$,
$r_k = y_k/\gamma_k$,
$H_{k+1} = [I - \tilde{v}_k r_k^{\mathrm{T}}/(r_k^{\mathrm{T}}\tilde{v}_k)]H_k[I - r_k\tilde{v}_k^{\mathrm{T}}/(r_k^{\mathrm{T}}\tilde{v}_k)] + \tilde{v}_k\tilde{v}_k^{\mathrm{T}}/(r_k^{\mathrm{T}}\tilde{v}_k)$,
$h_{k+1} = [(1-\gamma_k)/(\gamma_k s_k^{\mathrm{T}} f'(x_k))]f'(x_k)$,
end do.

The operations in Iterations 3.1 and 3.2 may not be well-defined in general. However, in the results of this and the next sections we shall refer to them under conditions which will ensure that they are well-defined. In the rest of the paper when we refer to Iterations 3.1 and 3.2 we shall also tacitly assume that they generate infinite sequences of $\{x_k\}$ with $f'(x_k) \neq 0$ for any k. Since in practice we would terminate the iterations if we have $f'(x_k) = 0$ for some k we do not lose generality. Moreover, this assumption facilitates stating our results.

Before proceeding with the analysis we remark that in view of Lemma 2.2 it is possible to establish local and q-superlinear convergence of Iteration 3.2 using appropriate estimates involving γ_k *starting* with the local and q-superlinear convergence of [11, equations (4.5), (4.6)] established by Sorensen [11]. However, it does not seem possible to establish the local and q-superlinear convergence of iteration 3.1 using a scheme paralleling such an approach. The results we state in this and the following sections with respect to Iterations 3.1 and 3.2 on the other hand exhibit the same sort of "duality" that one observes in the local convergence results for the direct iterations of the DFP and BFGS methods. These results, in view of Lemma 2.3 readily imply the local and q-superlinear convergence of both the DFP- and BFGS-related algorithms of Sorensen [12, pp. 154–156].

In our analyses we shall have occasion to use norms on $\mathbb{R}^n$ and $\mathbb{R}^{n\times n}$. $\|\cdot\|$ shall represent the l_2 vector norm on $\mathbb{R}^n$ and the induced operator norm on $\mathbb{R}^{n\times n}$. We shall also have occasion to use the Frobenius norm on $\mathbb{R}^{n\times n}$ which we denote by $\|\cdot\|_{\mathrm{F}}$. In our analyses, as in those of [3, 6] of quasi-Newton methods, it becomes necessary to use a matrix norm $\|\cdot\|_A$ on $\mathbb{R}^{n\times n}$ that is not induced by a norm on $\mathbb{R}^n$.

However, the equivalence of norms on finite-dimensional vector spaces implies that there is $\eta > 0$ such that

$$\|Q\| \leq \eta \|Q\|_A, \quad Q \in \mathbb{R}^{n\times n}. \tag{3.1}$$

We shall have occasion to use (3.1).

As in [11] we shall now state the following definition and assumptions regarding $f : X \to \mathbb{R}$.

Definition 3.3. Given $f : X \to \mathbb{R}, f \in C^2(D)$ where $D \subseteq X$ is an open convex set, a point $x_* \in D$ is said to be a *strong* local minimizer of f if $f'(x_*) = 0$ and $f''(x_*)$ is positive definite.

Assumption 3.4. $f \in C^2(D)$ where $D \subseteq X$ is an open convex set and $x_* \in D$ is a strong local minimizer of f. Furthermore, there is a neighborhood $N \subseteq D$ of x_* and a constant $L > 0$ such that

$$\|f''(x_+) - f''(x)\| \leq L\|x_+ - x\| \tag{3.2a}$$

and

$$\|f'(x_+) - f'(x)\| \leq L\|x_+ - x\| \tag{3.2b}$$

for all $x_+, x \in N$.

Note that by [3, Lemma 3.1], (3.2a, b) are not inconsistent. An immediate consequence of Assumption 3.4 and [3, Lemma 3.1] is that for all $x_+, x \in N$,

$$\begin{aligned} &\|f'(x_+) - f'(x) - f''(x_*)(x_+ - x)\| \\ &\quad \leq L \max\{\|x_+ - x_*\|, \|x - x_*\|\}\|x_+ - x\|. \end{aligned} \tag{3.3}$$

We shall begin by stating the following lemma due to Sorensen [11]. It will ensure that there is a neighborhood of x_* where Iterations 3.1 and 3.2 are well-defined.

Lemma 3.5. *Let $f : X \to \mathbb{R}$ satisfy Assumption 3.4. Then there is a neighborhood N of the strong local minimizer x_* so that $f''(x)$ is positive definite for all $x \in N$; and* (3.2a, b), (3.3) *are satisfied,*

$$(f - f_+)^2 - (f'_+)^{\mathrm{T}} s (f')^{\mathrm{T}} s \geq \tau \|s\|^4, \tag{3.4a}$$

$\gamma = \gamma(x_+, x) := -(f')^{\mathrm{T}} s / (f - f_+ + \rho)$ *satisfies*

$$|1 - \gamma| / \|s\| \leq M \tag{3.4b}$$

and

$$\tfrac{1}{2} \leq \gamma \leq \tfrac{3}{2} \tag{3.4c}$$

for all $x_+, x \in N$, $x_+ \neq x$, where $s := x_+ - x$, $f := f(x)$, $f_+ := f(x_+)$, $f' := f'(x)$, $f'_+ := f'(x_+)$, $\rho := \sqrt{(f - f_+)^2 - (f'_+)^{\mathrm{T}} s (f')^{\mathrm{T}} s}$ and $\tau > 0$ and $M > 0$ are constants.

Proof. See [11, Lemmas 4.2, 4.3 and Corollary 4.4] and their proofs. □

We shall now state a result that plays a role in our analyses similar to the one played by equation (3.2) of Broyden, Dennis and Moré [3] in their analyses of quasi-Newton methods.

Lemma 3.6. *Let $f: X \to \mathbb{R}$ satisfy Assumption 3.4. Suppose that N is the neighborhood of the strong local minimizer x_* indicated in Lemma 3.5. Then there is a positive constant K such that for all $x_+, x \in N$,*

$$\|r - f''(x_*)\tilde{v}\| \leq K\sigma(x_+, x)\|\tilde{v}\| \tag{3.5}$$

where $\tilde{v} := \gamma s$, $r := y/\gamma$, $y := \gamma f'_+ - (1/\gamma)f'$ and $\sigma(x_+, x) := \max\{\|x_+ - x_*\|, \|x - x_*\|\}$.

Proof.

$$\begin{aligned}\|r - f''(x_*)\tilde{v}\| &= \|f'_+ - (1/\gamma)^2 f' - f''(x_*)\gamma s\| \\ &= \|\gamma\{f'_+ - f' - f''(x_*)s\} + (1-\gamma)f'_+ - \{(1-\gamma^3)/\gamma^2\}\|f'\| \\ &\leq |\gamma|\,\|f'_+ - f' - f''(x_*)s\| + |1-\gamma|\,\|f'_+ - f'(x_*)\| \\ &\quad + |1-\gamma|\,|1 + (1+\gamma)/\gamma^2|\,\|f' - f'(x_*)\|.\end{aligned}$$

Now using (3.3), (3.2b), (3.4b) and (3.4c) to estimate terms on the last right-hand side we get

$$\|r - f''(x_*)\tilde{v}\| \leq (\tfrac{3}{2} + 8M)L\sigma(x_+, x)\|s\| \leq 2(\tfrac{3}{2} + 8M)L\sigma(x_+, x)\|\tilde{v}\|$$

so that (3.5) holds with $K := 2(\tfrac{3}{2} + 8M)L$ for all $x_+, x \in N$. □

We shall now focus our attention on Iteration 3.1. A key preliminary result used in the local analysis of quasi-Newton methods is the so called "bounded deterioration condition" for Hessian or inverse Hessian approximations. In the following lemma we give such a result for use in analyzing Iteration 3.1. In order to do that we need to define a weighted Frobenius norm $\|Q\|_A$ for any $Q \in \mathbb{R}^{n\times n}$ and given positive $A \in \mathbb{R}^{n\vee n}$ by

$$\|Q\|_A := \|A^{-1/2}QA^{-1/2}\|_F \tag{3.6}$$

where $A^{-1/2}$ is the symmetric, positive definite square root of A^{-1}. In the rest of the paper, whenever used with respect to Iteration 3.1, $\|\cdot\|_A$ will have the meaning indicated by (3.6).

Lemma 3.7. *Let $f: X \to \mathbb{R}$ satisfy Assumption 3.4 and put $A := f''(x_*)$ and $\xi := \|A^{-1}\|$. Let N be the neighborhood of x_* in Lemma 3.6. Suppose that N is further restricted, if necessary, so that*

$$\sigma(x_+, x) \leq 1/(3\xi K) \tag{3.7}$$

for all $x_+, x \in N$. Let $B \in \mathbb{R}^{n\vee n}$ and define $B_+ := [I - r\tilde{v}^T/(\tilde{v}^T r)]B[I - \tilde{v}r^T/(\tilde{v}^T r)] + rr^T/(\tilde{v}^T r)$ for $x_+, x \in N$ where $x_+ \neq x$. Then there are constants $\alpha_1 > 0$, $\alpha_2 > 0$ and

α ($\frac{3}{8} \leq \alpha \leq 1$) independent of x_+, x such that for all $x_+, x \in N$, $x_+ \neq x$,

$$\|B_+ - A\|_A \leq [\sqrt{1-\alpha\theta^2} + \alpha_1 \sigma(x_+, x)]\|B - A\|_A + \alpha_2 \sigma(x_+, x) \tag{3.8}$$

where $\theta := \|A^{-1/2}(B-A)\tilde{v}\| / (\|B-A\|_A \|A^{1/2}\tilde{v}\|) \leq 1$ if $B \neq A$ and $\theta := 0$ otherwise.

Proof. For $x_+, x \in N$, $x_+ \neq x$ we have $\tilde{v} \neq 0$. Now consider the case where $B \neq A$. Then (3.8) follows from [3, Lemma 5.2] (with y, c, s and M in that lemma substituted by r, r, $\tilde{v}$ and $A^{-1/2}$ respectively) if $\|A^{-1/2}r - A^{1/2}\tilde{v}\| / \|A^{1/2}\tilde{v}\| \leq \frac{1}{3}$, since $\|r - A\tilde{v}\| / \|A^{1/2}\tilde{v}\| \leq \|A^{-1/2}\| \, \|r - A\tilde{v}\| / \|\tilde{v}\| \leq \sqrt{\xi}\, K\sigma(x_+, x)$ by (3.5). But $\|A^{-1/2}r - A^{1/2}\tilde{v}\| / \|A^{1/2}\tilde{v}\| \leq \|A^{-1}\| \, \|r - A\tilde{v}\| / \|\tilde{v}\| \leq \frac{1}{3}$ by (3.5) and (3.7).

Now consider the case $B = A$. By the discussion in [3] preceding Lemma 5.2 it follows that when $B = A$ we can neglect the first term on the right-hand side of (3.8). (See also [6, Lemma 3.1].) Therefore, we can simply let $\theta := 0$ when $B = A$. $\square$

We are now going to present a result which we shall use to measure the closeness of the quantity λ_k of Iteration 3.1 to unity. Our result is very much motivated by Lemma 4.7 of Sorensen [11] for his collinear scaling algorithm related to the BFGS method. However, we obtain it in a form for $\{\lambda_k\}$ of Iteration 3.1 (which is related to the DFP method) so that a similar result could be established for $\{\lambda_k\}$ of Iteration 3.2 (which is related to the BFGS method).

Lemma 3.8. *Let $x \in \mathbb{R}^n$, $h \in \mathbb{R}^n$ and positive definite $B \in \mathbb{R}^{n \times n}$. Put $f := f(x)$ and $f' := f'(x)$ and suppose that $f' \neq 0$ and that $1 - h^T B^{-1} f' \neq 0$. Define $\lambda := 1/(1 - h^T B^{-1} f')$, $x_+ := x - \lambda B^{-1} f'$ and $s := x_+ - x$. Put $f_+ := f(x_+)$, $f'_+ := f'(x_+)$ and suppose that $f - f_+ > 0$ and that $(f - f_+)^2 - (f'_+)^T s (f')^T s > 0$. Let $\gamma := -s^T f' / (f - f_+ + \rho)$ where $\rho := \sqrt{(f-f_+)^2 - (f'_+)^T s (f')^T s}$ and define $h_+ := [(1-\gamma)/(\gamma s^T f')] f'$ and B_+ as in Lemma 3.7. Then whenever $|1-\gamma|\kappa < 1$ where $\kappa := [\{\|B^{-1}\| + \|B_+^{-1}\|\}\|B\| + |\gamma^3\lambda - 1|](1/|\gamma^3\lambda|)$, we have that $1 - h_+^T B_+^{-1} f'_+ > 0$ and that $\lambda_+ := 1/(1 - h_+^T B_+^{-1} f'_+)$ satisfies*

$$|1 - \lambda_+| \leq \frac{|1-\gamma|\kappa}{1 - |1-\gamma|\kappa}. \tag{3.9}$$

Proof. $h_+^T B_+^{-1} f'_+ = (1-\gamma)\beta$ where $\beta := (1/\gamma)[(f')^T B_+^{-1} f'_+]/(s^T f')$. Using the fact that $B_+ \tilde{v} = r$ where $\tilde{v} = \gamma s$ and $r = f'_+ - (1/\gamma^2) f'$ it is easy to verify that β can be expressed as

$$\beta = \frac{1}{\gamma^3 \lambda} \frac{(f')^T (B^{-1} - B_+^{-1}) f'}{(f')^T B^{-1} f'} + \frac{\gamma^3 \lambda - 1}{\gamma^3 \lambda}.$$

Hence

$$\begin{aligned} |\beta| &\leq (1/|\gamma^3\lambda|) \frac{|(f')^T (B^{-1} - B_+^{-1}) f'|}{|(f')^T B^{-1} f'|} + |\gamma^3\lambda - 1| / |\gamma^3\lambda| \\ &\leq [\|B^{-1} - B_+^{-1}\| \, \|B\| + |\gamma^3\lambda - 1|](1/|\gamma^3\lambda|) \\ &\leq [\{\|B^{-1}\| + \|B_+^{-1}\|\} \|B\| + |\gamma^3\lambda - 1|](1/|\gamma^3\lambda|). \end{aligned}$$

The conclusions of the lemma follow. $\square$

In Theorem 3.9 below we establish the local and q-linear convergence of Iteration 3.1. Before proceeding however, we remark that the hypotheses of Lemma 3.8 (which may seem restrictive) and (3.9) are really motivated by the proof of Theorem 3.9.

Theorem 3.9. *Let $f: X \to \mathbb{R}$ satisfy Assumption 3.4 and let x_* be a strong local minimizer of f. Put $A := f''(x_*)$. Suppose that the sequence $\{x_k\}$ is generated by Iteration 3.1 from initial quantities x_0, h_0 and symmetric, positive definite B_0. Then given any $\mu \in (0, 1)$, there are positive constants $\varepsilon = \varepsilon(\mu)$ and $\delta = \delta(\mu)$ such that if*

$$\|x_0 - x_*\| < \varepsilon, \qquad \|B_0 - A\|_A < \delta \quad \text{and} \quad |1 - \lambda_0| < \delta,$$

the sequence $\{x_k\}$ is well-defined and converges to x_*. Furthermore

$$\|x_{k+1} - x_*\| < \mu \|x_k - x_*\|, \quad k = 0, 1, \ldots,$$

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

Proof. Put $\zeta := \|A\|$ and $\xi := \|A^{-1}\|$. Choose any $l \in (0, 1)$ and then choose $\varepsilon, \delta > 0$ such that the following inequalities are satisfied.

$$2\eta\delta\xi \leqslant \mu/(1+\mu), \tag{3.10a}$$

$$\xi(1+\mu)[L(\varepsilon+\delta)+2\eta\delta] \leqslant \mu, \tag{3.10b}$$

$$(2\alpha_1\delta + \alpha_2)\varepsilon/(1-\mu) \leqslant \delta, \tag{3.10c}$$

$$2M\varepsilon[2\xi(1+\mu)(2\eta\delta+\zeta)+\delta(1+2M\varepsilon)^3+2M\varepsilon(3+6M\varepsilon+4M^2\varepsilon^2)],$$
$$\leqslant l\delta[1-\{\delta(1+2M\varepsilon)^3+2M\varepsilon(3+6M\varepsilon+4M^2\varepsilon^2)\}], \tag{3.10d}$$

$$\delta \leqslant (1-l)/l. \tag{3.10e}$$

In (3.10a, b, c, d, e) η, L, α_1, α_2 and M are as in (3.1), (3.2a, b), (3.8), (3.8), and (3.4b) respectively. A moment's reflection would indicate that given ξ, ζ, L, M, α_1, α_2 all positive and μ, $l \in (0, 1)$, selecting ε, $\delta > 0$ to satisfy (3.10a, b, c, d, e) is possible.

Let N be the neighborhood of x_* where the hypotheses of Lemma 3.7 are satisfied for all $x_+, x \in N$. If necessary further restrict ε so that $\|x - x_*\| < \varepsilon$ implies $x \in N$. Suppose that $\|x_0 - x_*\| < \varepsilon$, $\|B_0 - A\|_A < \delta$ and $|1 - \lambda_0| < \delta$.

Now by (3.1), $\|B_0 - A\| \leqslant \eta \|B_0 - A\|_A < \eta\delta < 2\eta\delta$ and the Banach Perturbation Lemma [10, p. 45] and (3.10a) give $\|B_0^{-1}\| \leqslant \xi(1+\mu)$. We have

$$\begin{aligned} x_1 - x_* &= x_0 - x_* - \lambda_0 B_0^{-1} f'(x_0) \\ &= B_0^{-1}[-\{(f'(x_0) - f'(x_*) - A(x_0 - x_*)\} \\ &\qquad + (1-\lambda_0)(f'(x_0) - f'(x_*)) + (B_0 - A)(x_0 - x_*)]. \end{aligned}$$

Therefore

$$\|x_1-x_*\| \leqslant \|B_0^{-1}\|[\|f'(x_0)-f'(x_*)-A(x_0-x_*)\| + |1-\lambda_0|\,\|f'(x_0)-f'(x_*)\| + \|B_0-A\|\,\|x_0-x_*\|]$$

which together with (3.3) implies

$$\begin{aligned}\|x_1-x_*\| &< \xi(1+\mu)[L\|x_0-x_*\|^2+\delta L\|x_0-x_*\|+2\eta\delta\|x_0-x_*\|]\\ &< \xi(1+\mu)[L(\varepsilon+\delta)+2\eta\delta]\|x_0-x_*\|\\ &< \mu\|x_0-x_*\| \quad \text{(by (3.10b))}.\end{aligned}$$

The proof is completed with an induction argument. Suppose that $\|B_k-A\|_A<2\delta$, $\|x_{k+1}-x_*\|<\mu\|x_k-x_*\|$ and $|1-\lambda_k|<\delta$ for $k=0,1,\ldots,m-1$ where $m\geqslant 2$. Let $\sigma_k:=\sigma(x_{k+1},x_k)$. Then Lemma 3.7 implies that $\|B_{k+1}-A\|_A\leqslant [1+\alpha_1\sigma_k]\|B_k-A\|_A+\alpha_2\sigma_k$ for $k=0,1,\ldots,m-1$. Hence for $k=0,1,\ldots,m-1$,

$$\|B_{k+1}-A\|_A-\|B_k-A\|_A<2\alpha_1\varepsilon\mu^k\delta+\alpha_2\varepsilon\mu^k.$$

Summing both sides from $k=0$ to $k=(m-1)$ we have

$$\begin{aligned}\|B_m-A\|_A &< \|B_0-A\|_A+(2\alpha_1\delta+\alpha_2)\varepsilon/(1-\mu)\\ &< \delta+\delta=2\delta \quad \text{(by (3.10c))}.\end{aligned} \tag{3.11}$$

Also

$$\begin{aligned}\|B_k\| &\leqslant \|B_k-A\|+\|A\|\\ &\leqslant \eta\|B_k-A\|_A+\|A\|<2\eta\delta+\zeta, \quad k=0,1,\ldots,m,\end{aligned} \tag{3.12}$$

and by the Banach Perturbation Lemma and (3.10a),

$$\|B_k^{-1}\|\leqslant \xi(1+\mu), \quad k=0,1,\ldots,m. \tag{3.13}$$

Now by Lemma 3.8 we have $|1-\lambda_m|\leqslant(|1-\gamma_{m-1}|\kappa_{m-1})/(1-|1-\gamma_{m-1}|\kappa_{m-1})$ whenever $|1-\gamma_{m-1}|\kappa_{m-1}<1$ where $\kappa_{m-1}:=[\{\|B_{m-1}^{-1}\|+\|B_m^{-1}\|\}\|B_{m-1}\|+|\gamma_{m-1}^3\lambda_{m-1}-1|]\times(1/|\gamma_{m-1}^3\lambda_{m-1}|)$. But $|1-\gamma_{m-1}|\leqslant M\|x_m-x_{m-1}\|\leqslant 2M\|x_{m-1}-x_*\|<2M\varepsilon\mu^{m-1}<2M\varepsilon$ by Lemma 3.5 and the induction hypothesis. Therefore

$$\begin{aligned}|1-\gamma_{m-1}^3\lambda_{m-1}| &\leqslant |(1-\lambda_{m-1})\gamma_{m-1}^3)\gamma_{m-1}^3+(1-\gamma_{m-1}^3)|\\ &\leqslant |1-\lambda_{m-1}|\,|\gamma_{m-1}^3|+|1-\gamma_{m-1}|\,|1+\gamma_{m-1}+\gamma_{m-1}^2|\\ &< \delta(1+2M\varepsilon)^3+2M\varepsilon(3+6M\varepsilon+4M^2\varepsilon^2).\end{aligned}$$

Consequently, $|\gamma_{m-1}^3\lambda_{m-1}|>1-[\delta(1+2M\varepsilon)^3+2M\varepsilon(3+6M\varepsilon+4M^2\varepsilon^2)]>0$ and

$$\kappa_{m-1}<\frac{2\xi(1+\mu)(2\eta\delta+\zeta)+\delta(1+2M\varepsilon)^3+2M\varepsilon(3+6M\varepsilon+4M^2\varepsilon^2)}{1-\{\delta(1+2M\varepsilon)^3+2M\varepsilon(2+6M\varepsilon+4M^2\varepsilon^2)\}}.$$

Hence by (3.10d, e), $|1-\gamma_{m-1}|\kappa_{m-1}<l\delta<1$ which implies

$$|1-\lambda_m|<l\delta/(1-l\delta)<\delta. \tag{3.14}$$

To complete the proof we must show that $\|x_{m+1}-x_*\|<\mu\|x_m-x_*\|$. Since we have established $\|B_m-A\|_A<2\delta$ and $|1-\lambda_m|<\delta$ it follows that

$$\|x_{m+1}-x_*\|<\xi(1+\mu)[L(\varepsilon+\delta)+2\eta\delta]\|x_m-x_*\|<\mu\|x_m-x_*\| \quad (3.15)$$

by (3.10b) as in the case of $k=0$.

With (3.11), (3.12), (3.13), (3.14) and (3.15) established the induction argument is complete and the conclusions of the theorem follow. □

Theorem 3.9 establishes the local and q-linear [10, Chapter 9] convergence of Iteration 3.1. In the rest of this section we shall concentrate on Iteration 3.2. We shall end this section with a theorem for Iteration 3.2 analogous to Theorem 3.9 for Iteration 3.1.

We begin with the following lemma analogous to Lemma 3.7. Here and in the rest of the paper whenever used with respect to Iteration 3.2 $\|\cdot\|_A$ will have the following meaning. Given positive definite $A\in\mathbb{R}^{n\vee n}$, $\|Q\|_A:=\|A^{1/2}QA^{1/2}\|_F$ for any $Q\in\mathbb{R}^{n\times n}$.

Lemma 3.10. *Let $f: X\to\mathbb{R}$ satisfy Assumption 3.4 and put $A:=f''(x_*)$, $\zeta:=\|A\|$ and $\xi:=\|A^{-1}\|$. Let N be the neighborhood of x_* in Lemma 3.6, further restricted if necessary, so that*

$$\sigma(x_+,x)\leqslant 8\sqrt{\tau}/(27K\sqrt{\zeta\xi}) \quad (3.16)$$

for all $x_+, x\in N$ where τ is as in (3.4a) and K is as in Lemma 3.6. Let $H\in\mathbb{R}^{n\vee n}$ and define $H_+:=[I-\tilde{v}r^T/(r^T\tilde{v})]H[I-r\tilde{v}^T/(r^T\tilde{v})]+\tilde{v}\tilde{v}^T/(r^T\tilde{v})$ for x_+, $x\in N$, $x_+\neq x$. Then there exist constants α_1 $(\alpha_1>0)$, α_2 $(\alpha_2>0)$ and α $(\frac{3}{8}\leqslant\alpha\leqslant 1)$ independent of x_+, x such that for all $x_+, x\in N$, $x_+\neq x$,

$$\|H_+-A^{-1}\|_A\leqslant[\sqrt{(1-\alpha\theta^2)}+\alpha_1\sigma(x_+,x)]\|H-A^{-1}\|_A+\alpha_2\sigma(x_+,x) \quad (3.17)$$

where $\theta:=\|A^{1/2}(H-A^{-1})r\|/(\|H-A^{-1}\|_A\|A^{-1/2}r\|)\leqslant 1$ if $H\neq A^{-1}$ and $\theta:=0$ otherwise.

Proof. Note that $\tilde{v}^Tr=2\rho$ by (2.7b). Therefore (3.4a) and Cauchy-Schwarz inequality gives $\|\tilde{v}\|\,\|r\|\geqslant\tilde{v}^Tr\geqslant 2\sqrt{\tau}\|s\|^2$. Since $x_+\neq x$, using (3.4c) we get

$$\|r\|\geqslant 2\sqrt{\tau}\|s\|^2/\|\tilde{v}\|\geqslant\tfrac{8}{9}\sqrt{\tau}\|\tilde{v}\|. \quad (3.18)$$

We therefore have that $\|r\|\neq 0$. The proof now proceeds as the proof of Lemma 3.7 using [3, Lemma 5.2]. Consider the case $H\neq A^{-1}$. We first note that $\|A^{1/2}\tilde{v}-A^{-1/2}r\|/\|A^{-1/2}r\|\leqslant\sqrt{\zeta\xi}\|r-A\tilde{v}\|/\|r\|$. Therefore when (3.16) holds, by (3.18) and Lemma 3.6 we have that $\|A^{1/2}\tilde{v}-A^{-1/2}r\|/\|A^{-1}r\|\leqslant\frac{1}{3}$. (3.17) now follows from [3, Lemma 5.2] with $\tilde{v}$, $\tilde{v}$, r and $A^{1/2}$ in place of y, c, s and M respectively in that lemma, since $\|\tilde{v}-A^{-1}r\|/\|A^{-1/2}r\|\leqslant(3\sqrt{\zeta\xi}\tau K)\sigma(x_+,x)$ by (3.18) and (3.5).

Now consider the case where $H=A^{-1}$. By the discussion in [3] prior to Lemma 5.2 we can neglect the first term on the right-hand side of (3.17) when $H=A^{-1}$. It follows that we can let $\theta:=0$ when $H=A^{-1}$. □

Before we present the result on the local and q-linear convergence of Iteration 3.2 we need the analogue of Lemma 3.8.

Lemma 3.11. *Let $x \in \mathbb{R}^n$, $h \in \mathbb{R}^n$ and positive definite $H \in \mathbb{R}^{n \vee n}$. Put $f := f(x)$ and $f' := f'(x)$ and suppose that $f' \neq 0$ and that $1 - h^T H f' \neq 0$. Define $\lambda := 1/(1 - h^T H f')$, $x_+ := x - \lambda H f'$ and $s := x_+ - x$. Put $f_+ := f(x_+)$, $f'_+ := f'(x_+)$ and suppose that $f - f_+ > 0$ and that $(f - f_+)^2 - (f'_+)^T s (f')^T s > 0$. Let $\gamma := -s^T f'/(f - f_+ + \rho)$ where $\rho := \sqrt{(f - f_+)^2 - (f'_+)^T s (f')^T s}$ and define $h_+ := [(1-\gamma)/(\gamma s^T f')] f'$ and H_+ as in Lemma 3.10. Then whenever $|1-\gamma|\kappa < 1$ where $\kappa := [\{\|H\| + \|H_+\|\}\|H^{-1}\| + |\gamma^3 \lambda - 1|] \times (1/|\gamma^3\lambda|)$, we have that $1 - h_+^T H_+ f'_+ > 0$ and that $\lambda_+ := 1/(1 - h_+^T H_+ f'_+)$ satisfies*

$$|1 - \lambda_+| \leqslant \frac{|1-\gamma|\kappa}{1 - |1-\gamma|\kappa}.$$

Proof. $h_+^T H_+ f'_+ = (1-\gamma)\beta$ where $\beta := (1/\gamma)[(f')^T H_+ f'_+]/(s^T f')$. Using the fact $H_+ r = \tilde{v}$, where $\tilde{v} = \gamma s$ and $r = f'_+ - (1/\gamma)^2 f'$ it is easy to verify that β can be expressed as

$$\beta = \frac{1}{\gamma^3 \lambda} \frac{z^T (H - H_+) z}{z^T H z} + \frac{\gamma^3 \lambda - 1}{\gamma^3 \lambda}$$

where $z := H^{-1} s$. Hence

$$\begin{aligned}|\beta| &\leqslant \frac{1}{|\gamma^3\lambda|} \frac{|z^T(H - H_+)z|}{|z^T H z|} + \frac{|\gamma^3\lambda - 1|}{|\gamma^3\lambda|} \\ &\leqslant [\|H - H_+\| \, \|H^{-1}\| + |\gamma^3\lambda - 1|](1/|\gamma^3\lambda|) \\ &\leqslant [\{\|H\| + \|H_+\|\}\|H^{-1}\| + |\gamma^3\lambda - 1|](1/|\gamma^3\lambda|).\end{aligned}$$

The conclusions of the lemma follow. □

We now state the following theorem on the local and q-linear convergence of Iteration 3.2. Its proof uses Lemmas 3.10 and 3.11 in a manner analogous to the way Lemmas 3.7 and 3.8 were used in the proof of Theorem 3.9. We omit its proof and refer the reader to [2] where a complete proof is given. It should be noted however, that its proof is *independent* of the proof of Theorem 3.9 just as much as the proofs of Theorems 3.2 and 3.4 of [3] are independent of each other.

Theorem 3.12. *Let $f: X \to \mathbb{R}$ satisfy Assumption 3.4 and let x_* be a strong local minimizer of f. Put $A := f''(x_*)$. Suppose that the sequence $\{x_k\}$ is generated by Iteration 3.2 from initial quantities x_0, h_0 and symmetric, positive definite H_0. Then given any $\mu \in (0, 1)$, there are positive constants $\varepsilon = \varepsilon(\mu)$ and $\delta = \delta(\mu)$ such that if*

$$\|x_0 - x_*\| < \varepsilon, \qquad \|H_0 - A^{-1}\|_A < \delta \quad \text{and} \quad |1 - \lambda_0| < \delta,$$

the sequence $\{x_k\}$ *is well-defined and converges to* x_*. *Furthermore*

$$\|x_{k+1}-x_*\|<\mu\|x_k-x_*\|, \quad k=0,1,\ldots,$$

and $\{\|H_k\|\}, \{\|H_k^{-1}\|\}$ *are uniformly bounded.* □

4. Q-superlinear convergence of two members of Algorithmic Schema 2.1 that extend the DFP and BFGS methods

The purpose of this section is to demonstrate that Iterations 3.1 and 3.2 discussed in Section 3 are q-superlinearly convergent. We refer the reader to [10, Chapter 9] for definitions on rates of convergence of convergent sequences. For our purposes here it suffices to note that if $\{x_k\}\subset\mathbb{R}^n$ converges to x_*, and if

$$\lim_{k\to\infty}(\|x_{k+1}-x_*\|/\|x_k-x_*\|)=0$$

then the rate of convergence of the sequence $\{x_k\}$ is q-superlinear.

We can proceed to obtain results on rate of convergence of Iterations 3.1 and 3.2 assuming that "starting quantities" are "close" to given quantities that depend on x_*, as in [3, 9] with respect to quasi-Newton methods. However, following Dennis and Moré [6] with respect to quasi-Newton methods and Sorensen [11] with respect to his collinear scaling algorithm related to the BFGS method we shall demonstrate q-superlinear convergence of Iterations 3.1 and 3.2 assuming that $\{x_k\}$ generated by the iterations converge to x_* satisfying

$$\sum_{k=0}^{\infty}\|x_k-x_*\|<\infty. \tag{4.1}$$

In our analysis, we shall need to show uniform boundedness of $\{\|B_k\|\}$ and $\{\|B_k^{-1}\|\}$ in the case of Iteration 3.1 and of $\{\|H_k\|\}$ and $\{\|H_k^{-1}\|\}$ in the case of Iteration 3.2. We shall need the following two lemmas to do so.

Lemma 4.1. *Let* $\{\phi_k\}$ *and* $\{\delta_k\}$ *be sequences of nonnegative numbers such that*

$$\phi_{k+1}\leqslant(1+\delta_k)\phi_k+\delta_k$$

and that

$$\sum_{k=1}^{\infty}\delta_k<\infty.$$

Then $\{\phi_k\}$ *converges.*

Proof. See [6, pp. 555-556]. □

The following lemma is Lemma 5.5 of Sorensen [11], where we have corrected a few typographical errors in the original statement in [11].

Lemma 4.2. *Let $E \in \mathbb{R}^{n\vee n}$ be positive definite. Let $u, v \in \mathbb{R}^n$ be such that $u, v \neq 0$ and $u^{\mathrm{T}}v \neq 0$. Define*

$$E_+ := E + \frac{vv^{\mathrm{T}}}{u^{\mathrm{T}}v} - \frac{Euu^{\mathrm{T}}E}{u^{\mathrm{T}}Eu}.$$

If $M \in \mathbb{R}^{n\vee n}$ is nonsingular, then

$$\|E_+\|_{M,2} \leqslant \max\{1, \|E\|_{M,2}\} + (1/\omega_M)[\|Mv - M^{-1}u\|/\|M^{-1}u\| + \sqrt{1-\omega_M^2}]$$

where $\omega_M := |u^{\mathrm{T}}v|/(\|Mv\|\,\|M^{-1}u\|)$ and $\|Q\|_{M,2} := \|MQM\|$ for any $Q \in \mathbb{R}^{n\times n}$.

Proof. See [11, pp. 107–108]. □

With these preliminaries out of our way we are now ready to estimate the rates of convergence of Iterations 3.1 and 3.2. We shall first consider Iteration 3.1. The following theorem brings us almost to our objective of establishing the q-superlinear convergence of Iteration 3.1.

Theorem 4.3. *Let $f: X \to \mathbb{R}$ satisfy Assumption 3.4 and put $A := f''(x_*)$. In addition assume that $\{x_k\} \subset X$ is a sequence that satisfies (4.1). Then there is a positive integer k_0 such that for any positive definite $B_{k_0} \in \mathbb{R}^{n\vee n}$ the following statements are true for quantities defined by formulae in Iteration 3.1.*

(i) *ρ_k is real; γ_k, $\tilde{v}_k$, y_k and r_k are well-defined; and B_k is positive definite; for all $k \geqslant k_0$.*

(ii) *$\{\|A^{1/2}B_k^{-1}A^{1/2}\|\}$ is uniformly bounded.*

(iii) *$\lim_{k\to\infty} \|A^{-1/2}B_kA^{-1/2}\|$ exists.*

(iv) *$\lim_{k\to\infty} |1-\gamma_k| = 0$.*

(v) *$\lim_{k\to\infty} |1-\lambda_k| = 0$.*

(vi) *$\lim_{k\to\infty} (\|B_k - f''(x_*)]\tilde{v}_k\|/\|\tilde{v}_k\|) = 0$.*

Proof. (4.1) implies convergence of $\{x_k\}$ to x_*. Hence it is possible to choose a k_0 such that for $k \geqslant k_0$, x_k is in the neighborhood N mentioned in the hypotheses of Lemma 3.7, further restricted if necessary so that

$$\sigma_k := \sigma(x_{k+1}, x_k) \leqslant \min\{1/(3\xi K), 4\sqrt{\tau}/(9\sqrt{\zeta\xi}\,K)\} \tag{4.2}$$

where $\zeta := \|A\|$ and $\xi := \|A^{-1}\|$. Conclusion (i) immediately follows. Furthermore, since then (3.8) holds for $k \geqslant k_0$, Lemma 4.1 immediately leads to conclusion (iii).

To establish conclusion (ii) we need to appeal to Lemma 4.2. We note that when B_{k+1} is as in Iteration 3.1, $B_{k+1}^{-1} = B_k^{-1} + \tilde{v}_k\tilde{v}_k^{\mathrm{T}}/\tilde{v}_k^{\mathrm{T}}r_k - B_k^{-1}r_kr_k^{\mathrm{T}}B_k^{-1}/r_k^{\mathrm{T}}B_k^{-1}r_k$ and apply Lemma 4.2 for $k \geqslant k_0$ with $M := A^{1/2}$, $v := \tilde{v}_k$, $u := r_k$, $E := B_k^{-1}$, $E_+ := B_{k+1}^{-1}$ and $\omega_{A^{1/2}} := \omega_k := \tilde{v}_k^{\mathrm{T}}r_k/(\|A^{1/2}\tilde{v}_k\|\,\|A^{-1/2}r_k\|)$. We get

$$\|B_{k+1}^{-1}\|_{A^{1/2},2} \leqslant \max\{1, \|B_k^{-1}\|_{A^{1/2},2}\} + (1/\omega_k)[\|A^{1/2}\tilde{v}_k - A^{-1/2}r_k\|/\|A^{-1/2}r_k\| + \sqrt{1-\omega_k^2}]. \tag{4.3}$$

To estimate the second term on the right-hand side of (4.3) we apply [7, Lemma 3.2]. To that end we note, by (3.18), that

$$\|A^{-1/2}r_k\| \geq \|r_k\|/\sqrt{\zeta} \geq (8\sqrt{\tau}/(9\sqrt{\zeta}))\|\tilde{v}_k\|.$$

Therefore

$$\begin{aligned}\frac{\|A^{1/2}\tilde{v}_k - A^{-1/2}r_k\|}{\|A^{-1/2}r_k\|} &\leq (9\sqrt{\zeta\xi}/(8\sqrt{\tau}))\frac{\|r_k - A\tilde{v}_k\|}{\|\tilde{v}_k\|} \\ &\leq (9\sqrt{\zeta\xi}/(8\sqrt{\tau}))K\sigma_k \leq \tfrac{1}{2} \end{aligned} \tag{4.4}$$

where the second and third inequalities follow from Lemma 3.6 and (4.2) respectively. When (4.4) holds, [7, Lemma 3.2] gives

$$\|A^{1/2}\tilde{v}_k - A^{-1/2}r_k\|/\|A^{-1/2}r_k\| \leq (9\sqrt{\zeta\xi}/(8\sqrt{\tau}))K\sigma_k$$

and

$$1-\omega_k^2 \leq [9\sqrt{\zeta\xi}/(8\sqrt{\tau})K\sigma_k]^2 \leq \tfrac{1}{4}.$$

With these estimates (4.3) gives

$$\max\{1, \|B_{k+1}^{-1}\|_{A^{1/2},2}\} \leq \max\{1, \|B_k^{-1}\|_{A^{1/2},2}\} + (36K\sqrt{\zeta\xi}/(8\sqrt{3\tau}))\sigma_k.$$

Lemma 4.1 with $\phi_k := \|B_k^{-1}\|_{A^{1/2},2}$ and $\delta_k := (36K\sqrt{\zeta\xi}/(8\sqrt{3\tau}))\sigma_k$ now yields the desired conclusion (ii).

Conclusion (iv) is almost trivial since $|1-\gamma_k| \leq M\|s_k\| \leq 2M\sigma_k$, and σ_k tends to zero since $\{x_k\}$ converges to x_* by (4.1).

To establish conclusion (v) note that

$$\lambda_{k+1} - 1 = [(1-\gamma_k)\beta_k]/[1-(1-\gamma_k)\beta_k]$$

where

$$\beta_k := 1 - (1/\gamma_k^3\lambda_k)[((f'(x_k))^{\mathrm{T}}B_{k+1}^{-1}f'(x_k))/((f'(x_k))^{\mathrm{T}}B_k^{-1}f'(x_k))]$$

as in the proof of Lemma 3.8. Hence $|\beta_k| \leq 1 + (1/|\gamma_k^3\lambda_k|)\|B_{k+1}^{-1}\|\,\|B_k\|$. Now since $s_k = -\lambda_k B_k^{-1}f'(x_k)$ implying that $|\lambda_k| \geq \|s_k\|/(\|B_k^{-1}\|\,\|f'(x_k)\|)$, by (3.4b, c) we get

$$|(1-\gamma_k)\beta_k| \leq M\|s_k\| + 8M\|B_k^{-1}\|\,\|B_k\|\,\|B_{k+1}^{-1}\|\,\|f'(x_k)\| \quad \text{for all } k \geq k_0.$$

(ii), (iii) and the convergence of $\{x_k\}$ to x_* now lead to conclusion (v).

Once we have established part (ii) and (3.8) the proof of (vi) proceeds as the proof of Dennis and Moré [6] of part (ii) of their Theorem 3.4: We observe that if $\{B_k\}$ does not converge to A (otherwise (vi) trivially holds) then $\{\theta_k\}$ converges to 0 (where $\theta_k := \|A^{-1/2}(B_k - A)\tilde{v}_k\|/(\|B_k - A\|_A\|A^{1/2}\tilde{v}_k\|)$) which leads to conclusion (vi) □

We invite the reader to compare Theorem 4.3 above with [6, Theorem 3.4]. As in the latter theorem, $\{x_k\}$ is *any* sequence converging to x_* satisfying (4.1). Suppose now that $\{x_k\}$ converges to x_* satisfying (4.1), say due to criteria in the line search procedure LSP. Theorem 4.3 implies that then operations in Iteration 3.1 eventually become well-defined. Therefore if the direct iterate it specifies does not violate the criteria in LSP that force $\{x_k\}$ to converge to x_*, then the direct iterate may be used as the next point. Theorem 4.4 below implies q-superlinear convergence of $\{x_k\}$ to x_* under these circumstances.

Of course the comments in the previous paragraph apply to the DFP generalizer direct iterates in Iteration 3.1 and to the BFGS generalizer direct iterates in Iteration 3.2 (after we have indicated pertinent results for Iteration 3.2). Nonetheless they form the basis for our comments in Step 2 of Algorithmic Schemata 2.1 and 2.3 on the use of direct iterates as the beginning trial point in LSP.

Theorem 4.4. *Let $f: X \to \mathbb{R}$ satisfy Assumption* 3.4. *Let $\{x_k\}$ be defined by Iteration* 3.1 *and suppose that $\{x_k\}$ converges to x_* satisfying* (4.1). *Then $\{x_k\}$ converges q-superlinearly to x_*.*

Proof. Note that $x_{k+1} = x_k - \lambda_k B_k^{-1} f'(x_k)$, and that by part (vi) of Theorem 4.3, $\lim_{k\to\infty} (\|[B_k - f''(x_*)](x_{k+1} - x_k)\| / \|x_{k+1} - x_k\|) = 0$. Part (v) of Theorem 4.3 and [6, Corollary 2.3] now yield the desired result. □

We shall now concentrate on Iteration 3.2. The proof of q-superlinear convergence proceeds in a very similar manner to that of Iteration 3.1. First Lemma 3.10—the analogue of Lemma 3.7—and Lemmas 4.1 and 4.2 are used to prove the analogue of Theorem 4.3. This theorem provides us with all the results necessary to prove the q-superlinear convergence of Iteration 3.2 leading to a theorem analogous to Theorem 4.4. The proofs of these results are *independent* of the proofs of Theorems 4.3 and 4.4. The methods of proof though are similar to those of Theorems 4.3 and 4.4. In view of this and limitations of space we first state the analogue of Theorem 4.3 for Iteration 3.2 without proof.

Theorem 4.5. *Let $f: X \to \mathbb{R}$ satisfy Assumption* 3.4 *and put $A := f''(x_*)$. In addition assume that $\{x_k\} \subset X$ is a sequence that satisfies* (4.1). *Then there is a positive integer k_0 such that for any positive definite $H_{k_0} \in \mathbb{R}^{n \vee n}$ the following statements are true for quantities defined by formulae in Iteration* 3.2.

(i) *ρ_k is real, γ_k, $\tilde{v}_k$, y_k and r_k are well-defined, and H_k is positive definite, for all $k \geq k_0$.*

(ii) *$\{\|A^{-1/2} H_k^{-1} A^{-1/2}\|\}$ is uniformly bounded.*

(iii) *$\lim_{k\to\infty} \|A^{1/2} H_k A^{1/2}\|$ exists.*

(iv) *$\lim_{k\to\infty} |1 - \gamma_k| = 0$.*

(v) *$\lim_{k\to\infty} |1 - \lambda_k| = 0$.*

(vi) *$\lim_{k\to\infty} (\|[H_k - (f''(x_*))^{-1}] r_k\| / \|r_k\|) = 0$.* □

Once Theorem 4.5 is established the proof of q-superlinear convergence of Iteration 3.2 proceeds in a very similar manner to that of Dennis and Moré

[6, p. 559] of the q-superlinear convergence of the BFGS method and to that of Sorensen [11, pp. 109–110] of his BFGS-related collinear scaling algorithm.

Theorem 4.6. *Let* $f: X \to \mathbb{R}$ *satisfy Assumption* 3.4. *Let* $\{x_k\}$ *be defined by Iteration* 3.2 *and suppose that* $\{x_k\}$ *converges to* x_* *satisfying* (4.1). *Then* $\{x_k\}$ *converges q-superlinearly to* x_*.

Proof. Consider iterates $k \geq k_0$ where k_0 is the positive integer mentioned in the hypotheses of Theorem 4.5. Put $A := f''(x_*)$. Now

$$\begin{aligned}[H_k - A^{-1}]r_k &= H_k f'(x_{k+1}) - (1/\gamma_k^2) H_k f'(x_k) - A^{-1} r_k \\ &= H_k f'(x_{k+1}) - A^{-1}(r_k - A\tilde{v}_k) \\ &\quad + [(\lambda_k + (\gamma_k + 1)/\gamma_k^2)(\gamma_k - 1) + (\lambda_k - 1)] H_k f'(x_k).\end{aligned}$$

Therefore by parts (ii), (iv), (v) and (vi) of Theorem 4.5, (3.4b) and (3.18), it follows that

$$\lim_{k \to \infty} \|f'(x_{k+1})\| / \|s_k\| = 0. \tag{4.5}$$

Dennis and Moré [6, pp. 551–552] show that (4.5) implies q-superlinear convergence of $\{x_k\}$ to x_*. □

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