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Superlinear convergence of Broyden's method and BFGS algorithm using Kantorovich-type assumptions

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ABSTRACT

Broyden's method is a quasi-Newton method which is used to solve a system of nonlinear equations. Almost all convergence theories in the literature assume existence of a root and bounds on the nonlinear function and its derivative in some neighbourhood of the root. All these conditions cannot be checked in practice. The motivation of this work is to derive a local convergence theory where all assumptions can be verified, and the existence of a root and its superlinear rate of convergence are consequences of the theory. The BFGS algorithm is a quasi-Newton method for unconstrained minimization. Also, all known convergence theories assume existence of a solution and bounds of the function in a neighbourhood of the minimizer. The second main result of this paper is a local convergence theory where all assumptions are verifiable and existence of a minimizer and superlinear convergence of the iteration are conclusions. In addition, both theories are simple in the sense that they contain as few constants as possible.

1. Introduction

It is well known that the classical Newton's method to solve a nonlinear system of equations converges quadratically if the initial guess is close enough to a solution. One drawback of this theory is that the solution is unknown a priori. Kantorovich's version of this theory (see, for instance, [1]) only makes assumptions in a region about the initial point and the existence of a solution and the rate of local convergence are consequences of the theory.

Another disadvantage of the classical Newton's method is that the Jacobian matrix must be formed at every iteration. In practice, the matrix may not be available analytically or its formation may be very expensive. Quasi-Newton methods are designed so that it is relatively inexpensive to compute an approximation to the Jacobian matrix at every iteration. The first and most important contribution is due to Broyden [2], where the matrix approximation from one iteration to the next one can be calculated by a rank-one update. Assuming existence of a root, local convergence of the basic method as well as global convergence of a version with line search are known. See, for instance [3] or [4]. In the first part of this paper, we give a local convergence theory of the basic Broyden's method where all assumptions are about the initial point. The existence of a solution and superlinear convergence of the iteration are outcomes of the theory.

There are other approximations to Newton's method, for instance, inexact Newton's methods. See [5–8] and references therein.

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For the problem of unconstrained minimization of a function f, a popular quasi-Newton method is the BFGS (Broyden–Fletcher–Goldfarb–Shanno) algorithm. While the approximate Jacobian of the Broyden's method applied to solve the nonlinear system $\nabla f = 0$ is, in general, non-symmetric, the corresponding approximation of the BFGS algorithm is symmetric positive definite (SPD) if f is uniformly convex. Its update is a rank-2 matrix. Again, local convergence of the basic method and global convergence of a version with line search have been shown. See, for instance [3] or [4]. In the second part of this paper, we show existence of a solution and superlinear convergence of the basic BFGS algorithm assuming only conditions in a neighbourhood of the initial point.

The main thrust of this article is to give superlinear convergence of Broyden's method and BFGS algorithm where all assumptions are made about some region about the initial iterate and hence are verifiable. We shall refer to this as **Kantorovich-type assumptions**. Existence of the root or minimizer and the superlinear convergence are deductions of the theory. Following [1], we try to construct a theory with as few constants as possible.

In the remainder of this introductory section, an outline of the paper is given. We shall give some notations and recall some well known useful results. In section two, as a warmup, we give a simple local convergence theory for the Chord's method for a system of nonlinear equations using Kantorovich-type hypotheses. In section three, superlinear convergence of Broyden's method is given using Kantorovich-type assumptions. This is followed by an analogous theory for the BFGS algorithm. For the latter, we introduce a norm which depends on the iteration number to estimate the difference between inverses of the approximate and exact Jacobians. This idea may be applicable in other situations. In the final section, we summarize and offer some open problems.

Throughout the article, $\|\cdot\|$ denotes the Euclidean vector or matrix norm and $B_r(x)$ denotes the open ball of radius r with center at x. Recall that the Frobenius norm of any $N \times N$ matrix $X = \left(x_{ij}\right)$ is defined as $\|X\|_F^2 = \sum_{i,j} x_{ij}^2$, and $\|X\| \le \|X\|_F \le \sqrt{N}\|X\|$. Assume $\{x_n\} \subseteq \mathbb{R}^N$ converges to x^*. Then the sequence $\{x_n\}$ converges q-superlinearly to x^* if and only if either $x_n = x^*$ for all sufficiently large n or $x_n \neq x^*$ for all large n and

$$\lim_{n\to\infty} \frac{\|x_{n+1} - x^*\|}{\|x_n - x^*\|} = 0.$$

Henceforth, this will be referred to simply as superlinear convergence. We collect together some lemmas which will be used later.

Lemma 1.1. *Let A, B be SPD matrices. Then*

$$\|AB\|^2 \le \|A^2 B^2\|.$$

Proof. Define the inner product $\langle x, y\rangle = x^T A^{-1} y$. It is well known that AB is self adjoint with respect to this inner product and is positive definite. Let $\lambda_{\max}(M)$ be the maximum eigenvalue of matrix M. By the variational characterization of the maximum eigenvalue of a self-adjoint operator,

$$\lambda_{\max}(AB) = \max_{y\neq 0} \frac{\langle ABy, y\rangle}{\langle y, y\rangle} = \max_{y\neq 0} \frac{y^T By}{y^T A^{-1} y}.$$

Since $\lambda_{\max}(A^2B^2) \le \|A^2B^2\|$, it follows that

$$\begin{aligned}\|AB\|^2 &= \|AB(AB)^T\| = \|AB^2A\| \\ &= \max_{x\neq 0} \frac{x^T AB^2 A\, x}{x^T x} = \max_{y\neq 0} \frac{y^T B^2\, y}{y^T A^{-2} y} = \lambda_{\max}(A^2B^2) \le \|A^2B^2\|. \quad \square\end{aligned}$$

The next three lemmas are well known. They can be found, for instance, in [9].

Lemma 1.2. *Let A be a square matrix and $\|I - A\| < 1$. Then A is invertible and*

$$\|A^{-1}\| \le \frac{1}{1 - \|I - A\|}.$$

Lemma 1.3. *Let u, v be vectors so that $u^T v \neq 0$. Then*

$$\left\| I - \frac{uv^T}{u^T v} \right\| = \frac{\|u\|\,\|v\|}{|u^T v|}.$$

Lemma 1.4. *Let u, v be non-zero vectors so that $\|u - v\| \le \lambda\|u\|$ for some $\lambda \in (0, 1)$. Then*

$$1 - \left(\frac{u^T v}{\|u\|\,\|v\|}\right)^2 \le \lambda^2.$$

Lemma 1.5 (*See [3], Lemma 4.1.12*). *Let Ω be an open set in $\mathbb{R}^N$ and $F : \Omega \to \mathbb{R}^N$ be $C^1(\Omega)$. Suppose there is some positive constant L such that*

$$\|F'(u) - F'(v)\| \le L\|u - v\|, \qquad u, v \in \Omega.$$

Then

$$\|F(u) - F(v) - F'(v)(u - v)\| \le \frac{L}{2}\|u - v\|^2, \qquad u, v \in \Omega.$$

2. Chord's method

The Chord's method to solve the nonlinear system $F(x) = 0$ is given by the iteration

$$x_{n+1} = x_n - A^{-1}F(x_n), \qquad n \ge 0,$$

where x_0 is an initial guess and the Jacobian $A = F'(x_0)$ is invertible. The Chord's method is Newton's iteration except that the Jacobian is fixed at A for all n. This is an alternative to Newton's method because the Jacobian is formed only once in the beginning. The drawback is that the convergence is only linear. Below is a local convergence theory using Kantorovich-type assumptions.

Theorem 2.1. *Let Ω be an open set in $\mathbb{R}^N$ and $F : \Omega \to \mathbb{R}^N$ be continuously differentiable on Ω. Given $x_0 \in \Omega$. Suppose $A = F'(x_0)$ is non-singular. Assume for some $r \in (0, 1)$ that $\overline{B_r(x_0)} \subset \Omega$, $\|A^{-1}F(x_0)\| \le (1 - r)r$ and*

$$\|A^{-1}(F'(v) - F'(w))\| \le \|v - w\|, \qquad v, w \in B_r(x_0).$$

Let $\{x_n\}$ be the iterates of the Chord's method. Then $x_n \to x^* \in \overline{B_r(x_0)}$, where $F(x^*) = 0$. Let $e_n = x_n - x^*$. Then $\|e_n\| \le r^{n+1}$, $n \ge 0$. Furthermore, x^* is the unique zero of F in $\overline{B_r(x_0)}$.

Proof. Let $s_n = x_{n+1} - x_n$. We claim by induction that $x_{n+1} \in B_r(x_0)$ and $\|s_n\| \le (1 - r)r^{n+1}$, $\forall n \ge 0$.

The base case $n = 0$ holds trivially since $s_0 = -A^{-1}F(x_0)$ and so by hypothesis, $\|s_0\| \le (1 - r)r < r$. This also shows that $x_1 \in B_r(x_0)$. Assume that the claims hold for $n - 1$. We show that they also hold for n.

By Taylor's Theorem, there is some ξ along the line joining x_n and x_{n-1} so that $F(x_n) - F(x_{n-1}) = F'(\xi)s_{n-1}$. By the induction hypothesis,

$$\begin{aligned}
\|s_n\| &= \|A^{-1}F(x_n)\| = \|A^{-1}\big(F(x_n) - F(x_{n-1})\big) - s_{n-1}\| \\
&\le \|\big(A^{-1}F'(\xi) - I\big)s_{n-1}\| = \|A^{-1}\big(F'(\xi) - F'(x_0)\big)s_{n-1}\| \\
&\le \|\xi - x_0\|\,(1 - r)r^n \le (1 - r)r^{n+1}.
\end{aligned}$$

Since $x_{n+1} - x_0 = \sum_{j=0}^{n} s_j$, it follows that $\|x_{n+1} - x_0\| \le \sum_{j=0}^{n}(1 - r)r^{j+1} < r$, or $x_{n+1} \in B_r(x_0)$. For any non-negative p, we have $x_{n+p+1} - x_n = \sum_{j=n}^{n+p} s_j$, and so

$$\|x_{n+p+1} - x_n\| \le (1 - r)\sum_{j=n}^{n+p} r^{j+1} \le r^{n+1}.$$

This implies that $\{x_n\}$ is a Cauchy sequence and so it must converge to some $x^* \in \overline{B_r(x_0)}$. Also, taking $p \to \infty$,

$$\|e_n\| \le r^{n+1}.$$

Consequently, $A^{-1}F(x_n) = -s_n \to 0$. This shows that $F(x^*) = 0$.

Let $\hat{x}$ be any zero of F in $\overline{B_r(x_0)}$. Define $\hat{e}_n = x_n - \hat{x}$. We show $\|\hat{e}_n\| \le r^{n+1}$ by induction. The base case is trivial. Suppose the claim is true for n. There is some ξ in between x_n and $\hat{x}$ so that $F(x_n) - F(\hat{x}) = F'(\xi)(x_n - \hat{x})$. Then

$$\hat{e}_{n+1} = x_{n+1} - \hat{x} = x_n - A^{-1}F(x_n) + A^{-1}F(\hat{x}) - \hat{x} = \hat{e}_n - A^{-1}F'(\xi)\hat{e}_n.$$

Therefore

$$\begin{aligned}
\|\hat{e}_{n+1}\| &\le \|A^{-1}\big(F'(x_0) - F'(\xi)\big)\|\ \|\hat{e}_n\| \\
&\le \|x_0 - \xi\|\ r^{n+1} \le r^{n+2}.
\end{aligned}$$

As a result,

$$\|x^* - \hat{x}\| \le \|x^* - x_n\| + \|x_n - \hat{x}\| \le 2r^{n+1} \to 0.$$

Hence $x^* = \hat{x}$. $\square$

3. Broyden's method

Let Ω be an open set in $\mathbb{R}^N$. Given a smooth $F : \Omega \to \mathbb{R}^N$, the problem is to find $x^* \in \Omega$ so that $F(x^*) = 0$. A classical method to solve this problem is Newton's method: $x_{n+1} = x_n - F'(x_n)^{-1}F(x_n)$, $n \geq 0$ for a given x_0. The formation of the Jacobian $F'(x_n)$ may be computationally intensive, or it may not be available analytically. Broyden [2] devised an approximate Jacobian which can be calculated from the approximate Jacobian of the previous iteration by a rank-one update. Given $x_0 \in \Omega$ and an invertible initial approximate Jacobian A_0, Broyden's method is

$$x_{n+1} = x_n + s_n, \qquad s_n = -A_n^{-1}F(x_n), \qquad n \geq 0,$$
$$A_{n+1} = A_n + \frac{F(x_{n+1})s_n^T}{\|s_n\|^2} .$$

Using classical assumptions (existence of a solution x^* and bounds on F and F' in a neighbourhood of x^*), superlinear convergence and global convergence of the method with line search are known. See, for instance, [3] or [4].

Since x^* is not known a priori, the assumptions cannot be checked in practice. The purpose of this section is to give a superlinear convergence of Broyden's method using Kantorovich-type assumptions.

We are now ready to show local convergence of the basic Broyden's method (without line search), which will be followed by a proof of superlinear convergence. Our technique of proof combines the elegant Newton–Kantorovich theory with only one constant (Theorem 7.7-5 in [1]) and the local convergence of Broyden's method of [3]. Our theory will also contain only one constant (r). Note that [10] has shown a local Kantorovich-type convergence result, but without superlinear convergence. Following the proof of the theorem, we justify via an example the strength of the assumptions.

Theorem 3.1. *Let Ω be open in $\mathbb{R}^N$, $F : \Omega \to \mathbb{R}^N$, $F \in C^1(\Omega)$, $x_0 \in \Omega$ and A_0 be invertible. For some $0 < r \leq 1/2$ assume $\overline{B_r(x_0)} \subset \Omega$ and*

$$\|F'(x_0)^{-1}F(x_0)\| \leq \xi r^2, \tag{3.1}$$
$$\|F'(x_0)^{-1}(F'(u) - F'(v))\| \leq \frac{\eta\|u - v\|}{r}, \qquad \forall u, v \in B_r(x_0)$$
$$\|I - F'(x_0)^{-1}A_0\| \leq dr, \tag{3.2}$$

where ξ, η and d are positive constants dependent on r (to be defined later). Then the Broyden's iteration $\{x_n\}$ is well defined and exactly one of the following cases holds,
(i) $F(x_n) = 0$ for some $n \geq 0$.
(ii) Broyden's iteration converges to a unique zero of F in $\overline{B_r(x_0)}$.

Proof. Define $G(y) = F'(x_0)^{-1}F(y)$. By this definition, $F(x^*) = 0$ if and only if $G(x^*) = 0$, zeros of F are zeros of G and also $G'(y) = F'(x_0)^{-1}F'(y)$, G is differentiable as F is. Define

$$B_0 = F'(x_0)^{-1}A_0, \quad y_0 = x_0,$$
$$y_{n+1} = y_n + t_n, \qquad t_n = -B_n^{-1}G(y_n), \qquad n \geq 0,$$
$$B_{n+1} = B_n + \frac{G(y_{n+1})t_n^T}{\|t_n\|^2} .$$

Assume $F(x_n) \neq 0$ for all $n \geq 0$. First we show by induction that $y_n = x_n$ and $B_n = F'(x_0)^{-1}A_n$ for all $n \geq 0$. The basic step is true obviously, $y_0 = x_0$ and $B_0 = F'(x_0)^{-1}A_0$ by using definition. Let $x_n = y_n$ and $B_n = F'(x_0)^{-1}A_n$ for some positive integer n, then we need to show $x_{n+1} = y_{n+1}$ and $B_{n+1} = F'(x_0)^{-1}A_{n+1}$. Notice that:

$$t_n = -B_n^{-1}G(x_n) = -(F'(x_0)^{-1}A_n)^{-1}F'(x_0)^{-1}F(x_n) = -A_n^{-1}F(x_n) = s_n,$$

and also $y_{n+1} = y_n + t_n = x_n + s_n = x_{n+1}$. By definition of B_{n+1} we get:

$$B_{n+1} = B_n + \frac{G(x_{n+1})t_n^T}{\|t_n\|^2} = F'(x_0)^{-1}A_n + \frac{F'(x_0)^{-1}F(x_{n+1})s_n^T}{\|s_n\|^2}$$
$$= F'(x_0)^{-1}(A_n + \frac{F(x_{n+1})s_n^T}{\|s_n\|^2}) = F'(x_0)^{-1}A_{n+1}.$$

Furthermore, by using assumptions of the theorem, it is easy to show that $\|G(x_0)\| \leq \xi r^2$ and

$$\|G'(u) - G'(v)\| \leq \frac{\eta\|u - v\|}{r}, \qquad u, v \in B_r(x_0).$$

We have $G'(x_0) = F'(x_0)^{-1}F'(x_0) = I$ and for $u \in B_r(x_0)$,

$$\|I - G'(u)\| = \|G'(x_0) - G'(u)\| \leq \frac{\eta\|x_0 - u\|}{r} < \eta .$$

If we assume $\eta < 1$, then by using Lemma 1.2, $G'(u)$ is invertible and

$$\|G'(u)^{-1}\| \le \frac{1}{1-\|I-G'(u)\|} \le \frac{1}{1-\dfrac{\eta\|x_0-u\|}{r}}\ . \tag{3.3}$$

(*Note that all additional assumptions on constants such as $\eta < 1$ are summarized at the beginning of Section* 3.1)

Also, from Lemma 1.5,

$$\|G(u)-G(v)-G'(v)(u-v)\| \le \frac{\eta\|u-v\|^2}{2r}, \qquad u, v \in B_r(x_0). \tag{3.4}$$

Claim 1. *There are some positive constants α, μ and β dependent on r (to be defined later), such that for $n \ge 0$,*

(i) $\|x_n - x_0\| \le r(1-r^n)$;
(ii) $\|G(x_n)\| \le \xi\ r^{n+2}$;
(iii) $\|G'(x_n) - B_n\| \le \alpha r$;
(iv) $G'(x_n)$ *is invertible and* $\|G'(x_n)^{-1}\| \le \mu$;
(v) B_n *is invertible and* $\|B_n^{-1}\| \le \beta$;
(vi) $\|s_n\| \le r^{n+2}$.

The proof of this claim is by mathematical induction. The basic step for Claim 1(i) and (ii) is trivial. By definition of B_0, it is invertible thus s_0 is well defined and x_1 exists. Also $\|G'(x_0) - B_0\| = \|I - F'(x_0)^{-1}A_0\| \le dr \le \alpha r$, if we choose α such that $d \le \alpha$. By assumption $G'(x_0) = I$, therefore $\|G'(x_0)^{-1}\| \le \mu$ if $\mu \ge 1$. In addition $\|I - B_0\| = \|I - F'(x_0)^{-1}A_0\| \le dr$. If we assume $dr < 1$, then $\|I - B_0\| < 1$ and by using Lemma 1.2

$$\|B_0^{-1}\| \le \frac{1}{1-\|I-B_0\|} \le \frac{1}{1-dr}.$$

So by assuming $\beta \ge \dfrac{1}{1-dr}$, we have $\|B_0^{-1}\| \le \beta$. Also

$$\|s_0\| = \|-B_0^{-1}G(x_0)\| \le \|B_0^{-1}\|\|G(x_0)\| \le \beta\xi r^2 \le\ r^2,$$

by assuming $\beta\xi \le 1$. Next we assume all of the statements are true for some integer $n \ge 1$, we will show they hold for $n+1$.

For proving the induction step for Claim 1(i), since B_n is invertible by hypothesis of induction, x_{n+1} exists and

$$\begin{aligned}\|x_{n+1} - x_0\| &\le \|x_{n+1} - x_n\| + \|x_n - x_0\| \\ &\le\ r^{n+2} +\ r(1-r^n) = r(1-r^n(1-r)) \le r(1-r^{n+1}),\end{aligned}$$

since $r \le 1/2$. Thus $\|x_{n+1} - x_0\| \le r(1-r^{n+1}) < r$, which establishes Claim 1(i).

For proving the induction step for Claim 1(ii), since $G(x_n) = -B_n s_n$, use (3.4) and induction hypothesis to obtain

$$\begin{aligned}\|G(x_{n+1})\| &= \|G(x_{n+1}) - G(x_n) - G'(x_n)s_n + (G'(x_n) - B_n)s_n\| \\ &\le \|G(x_{n+1}) - G(x_n) - G'(x_n)s_n\| + \|(G'(x_n) - B_n)s_n\| \\ &\le \frac{\eta\|s_n\|^2}{2r} + \alpha r\|s_n\| = \|s_n\|(\frac{\eta\|s_n\|}{2r} + \alpha r) \\ &\le r^{n+2}\ (\frac{\eta r^{n+2}}{2r} + \alpha r) \le r^{n+3}\ (\eta+\alpha) \le \xi r^{n+3},\end{aligned} \tag{3.5}$$

if we assume $\eta + \alpha \le \xi$. Then $\|G(x_{n+1})\| \le \xi\ r^{n+3}$, as we need for Claim 1(ii).

To prove Claim 1(iii), observe that

$$\begin{aligned}\|G'(x_{n+1}) - B_{n+1}\| &= \left\|G'(x_{n+1}) + G'(x_n) - G'(x_n) - B_n - \frac{G(x_{n+1})s_n^T}{\|s_n\|^2}\right\| \\ &\le \|G'(x_{n+1}) - G'(x_n)\| + \left\|G'(x_n) - B_n - \frac{G(x_{n+1})s_n^T}{\|s_n\|^2}\right\|.\end{aligned} \tag{3.6}$$

Consider the second term of this inequality:

$$\begin{aligned}G'(x_n) - B_n - \frac{G(x_{n+1})s_n^T}{\|s_n\|^2} &= G'(x_n) - B_n - \frac{\big(G(x_{n+1}) - G(x_n) + G(x_n)\big)s_n^T}{\|s_n\|^2} \\ &= G'(x_n) - B_n - \frac{\big(G(x_{n+1}) - G(x_n)\big)s_n^T}{\|s_n\|^2} + \frac{B_n s_n s_n^T}{\|s_n\|^2}\end{aligned}$$

$$
\begin{aligned}
&= G'(x_n) - B_n - \int_0^1 G'(\,(1-t)x_n + tx_{n+1}\,)\frac{s_n s_n^T}{\|s_n\|^2}\,dt + \frac{B_n s_n s_n^T}{\|s_n\|^2} \\
&= G'(x_n) - B_n + \int_0^1 \Big(G'(x_n) - G'(\,(1-t)x_n + tx_{n+1}\,)\Big)\frac{s_n s_n^T}{\|s_n\|^2}\,dt \\
&\qquad - \int_0^1 G'(x_n)\frac{s_n s_n^T}{\|s_n\|^2}\,dt + \frac{B_n s_n s_n^T}{\|s_n\|^2} \\
&= (G'(x_n) - B_n)(I - \frac{s_n s_n^T}{\|s_n\|^2}) + \int_0^1 [G'(x_n) - G'((1-t)x_n + tx_{n+1})]\frac{s_n s_n^T}{\|s_n\|^2}\,dt.
\end{aligned}
$$

Therefore:

$$
\begin{aligned}
\left\| G'(x_n) - B_n - \frac{G(x_{n+1})s_n^T}{\|s_n\|^2} \right\| &\le \|G'(x_n) - B_n\| \left\| I - \frac{s_n s_n^T}{\|s_n\|^2} \right\| + \int_0^1 \|G'(x_n) - G'(\,(1-t)x_n + tx_{n+1}\,)\| \frac{\|s_n\|\,\|s_n^T\|}{\|s_n\|^2}\,dt \\
&\le \|G'(x_n) - B_n\| + \int_0^1 \frac{\eta\|x_n - [(1-t)x_n + tx_{n+1}]\|}{r}\,dt \\
&\le \|G'(x_n) - B_n\| + \int_0^1 \frac{t\eta\|s_n\|}{r}\,dt \le \|G'(x_n) - B_n\| + \frac{\eta\|s_n\|}{2r}\ .
\end{aligned}
$$

Substitute this in inequality (3.6) we get:

$$
\begin{aligned}
\|G'(x_{n+1}) - B_{n+1}\| &\le \|G'(x_{n+1}) - G'(x_n)\| + \|G'(x_n) - B_n\| + \frac{\eta\|s_n\|}{2r} \\
&\le \frac{\eta\|s_n\|}{r} + \|G'(x_n) - B_n\| + \frac{\eta\|s_n\|}{2r} \\
&\le \frac{3\eta}{2r}(\|s_n\| + \|s_{n-1}\| + \cdots + \|s_0\|\,) + \|G'(x_0) - B_0\| \\
&\le \frac{3\eta}{2r}\big(\,r^{n+2} + r^{n+1} + \cdots + r^2\big) + dr \\
&\le \frac{3\eta r}{2}\Big(\frac{1 - r^{n+1}}{1 - r}\Big) + dr \le 3\eta r + dr \le \alpha r,
\end{aligned}
$$

if we choose α such that $\alpha \ge 3\eta + d$. This establishes Claim 1(iii).

For proving the induction step for Claim 1(iv), by using Claim 1(i), $\|x_{n+1} - x_0\| \le\ r(1 - r^{n+1}) < r$, and so $x_{n+1} \in B_r(x_0)$. From (3.3), $G'(x_{n+1})$ is invertible and

$$
\|G'(x_{n+1})^{-1}\| \le \frac{1}{1 - \dfrac{\eta\|x_{n+1} - x_0\|}{r}} \le \frac{1}{1-\eta}\ .
$$

Define $\mu = \dfrac{1}{1-\eta} > 1$. Then $\|G'(x_{n+1})^{-1}\| \le \mu$, as we need for Claim 1(iv).

To prove Claim 1(v), notice that:

$$
G'(x_{n+1})^{-1}B_{n+1} = I + G'(x_{n+1})^{-1}\big(B_{n+1} - G'(x_{n+1})\,\big), \tag{3.7}
$$

and

$$
\|G'(x_{n+1})^{-1}(B_{n+1} - G'(x_{n+1}))\| \le\ \|G'(x_{n+1})^{-1}\|\ \|B_{n+1} - G'(x_{n+1})\|\ \le \mu\alpha r.
$$

Assume $\mu\alpha r < 1$, then by Lemma 1.2, $G'(x_{n+1})^{-1}B_{n+1}$ is invertible which means B_{n+1} is invertible and

$$
\begin{aligned}
\left\| \Big(I + G'(x_{n+1})^{-1}\,(B_{n+1} - G'(x_{n+1})\,)\Big)^{-1} \right\| &\le \frac{1}{1 - \|G'(x_{n+1})^{-1}\big(B_{n+1} - G'(x_{n+1})\,\big)\|} \\
&\le \frac{1}{1 - \mu\alpha r}\ .
\end{aligned}
$$

From (3.7), $B_{n+1}^{-1} = \Big(\ I + G'(x_{n+1})^{-1}\,(B_{n+1} - G'(x_{n+1}))\Big)^{-1}\ G'(x_{n+1})^{-1}$,

$$
\|B_{n+1}^{-1}\| \le \left\| \Big(\ I + G'(x_{n+1})^{-1}\ \big(B_{n+1} - G'(x_{n+1})\,\big)\ \Big)^{-1} \right\|\ \big\|G'(x_{n+1})^{-1}\big\| \le \frac{\mu}{1 - \mu\alpha r}\ .
$$

Let $\beta = \max\left\{\dfrac{1}{1-dr}, \dfrac{\mu}{1-\mu\alpha r}\right\}$, then $\|B_{n+1}^{-1}\| \le \beta$, establishing Claim 1(v). Notice that $\beta > 1$, since

$$\frac{\mu}{1-\mu\alpha r} = \frac{1}{1-\eta-\alpha r} = 1 + \frac{\eta+\alpha r}{1-\eta-\alpha r} > 1.$$

To prove the induction step of Claim 1(vi), since B_{n+1} is invertible, s_{n+1} is well defined. Also $\beta\xi \le 1$ by assumption, therefore,

$$\|s_{n+1}\| = \| - B_{n+1}^{-1} G(x_{n+1})\| \le \|B_{n+1}^{-1}\| \|G(x_{n+1})\| \le \beta\xi r^{n+3} \le r^{n+3},$$

which is Claim 1(vi).

Therefore by using mathematical induction we have the results. By using Claim 1(vi) we could say $\{x_n\}$ is a Cauchy sequence lying in $B_r(x_0)$. Given $p, q \ge 0$,

$$\|x_p - x_{p+q}\| \le \sum_{k=p}^{p+q-1} \|x_{k+1} - x_k\| \le \sum_{k=p}^{p+q-1} r^{k+2} < r^2 \sum_{k=p}^{\infty} r^k = \frac{r^{p+2}}{1-r} \le r^{p+1},$$

since $r \le \dfrac{1}{2} \Rightarrow \dfrac{1}{1-r} \le \dfrac{1}{r}$. Therefore $\{x_n\}$ converges to a point $x^* \in \overline{B_r(x_0)}$. By using the fact that G is a continuous function and $\|G(x_n)\| \le \xi r^{n+2}$, it follows that $G(x^*) = 0$, which implies $F(x^*) = 0$. By taking $q \to \infty$ and $p = n$ in the above calculation we get $\|e_n\| \le r^{n+1}$, where $e_n = x_n - x^*$.

Now for proof of uniqueness, let $\hat{x}$ be any zero of F in $\overline{B_r(x_0)}$. Below, we show that $\|\hat{e}_{n+1}\| \le \|\hat{e}_n\|/2$ for all $n \ge 0$, where $\hat{e}_n = x_n - \hat{x}$. Notice that:

$$\begin{aligned}
\hat{e}_{n+1} &= x_{n+1} - \hat{x} = x_n + s_n - \hat{x} = x_n - B_n^{-1} G(x_n) - \hat{x} \\
&= B_n^{-1} B_n\, \hat{e}_n + B_n^{-1}\big(-G(x_n) + G(\hat{x})\,\big) \\
&= B_n^{-1}\big(B_n - G'(x_n)\,\big)\, \hat{e}_n + B_n^{-1}\, \big(-G(x_n) + G(\hat{x}) + G'(x_n)\hat{e}_n\big).
\end{aligned}$$

By (3.4),

$$\begin{aligned}
\|\hat{e}_{n+1}\| &= \left\| B_n^{-1}\left(-G(x_n) + G(\hat{x}) + G'(x_n)\,\hat{e}_n + (B_n - G'(x_n))\,\hat{e}_n\right)\right\| \\
&\le \|B_n^{-1}\|\ \|\hat{e}_n\|\ \big(\frac{\eta\|\hat{e}_n\|}{2r} + \|B_n - G'(x_n)\ \|\big).
\end{aligned}$$

Since $\hat{x}\,,\ x_n \in \overline{B_r(x_0)}$ then $\|\hat{e}_n\| \le 2r$. The above inequality becomes

$$\|\hat{e}_{n+1}\| \le \beta\ \|\hat{e}_n\|\ \big(\frac{\eta\|\hat{e}_n\|}{2r} + \alpha r\big) \le \beta(\eta+\alpha)\|\hat{e}_n\| \le \frac{1}{2}\|\hat{e}_n\|,$$

if we assume $\beta(\eta+\alpha) \le \dfrac{1}{2}$. So $\|\hat{e}_n\| \le \dfrac{1}{2^n}$. Therefore,

$$\|\hat{x} - x^*\| \le \|\hat{x} - x_n\| + \|x_n - x^*\| \le \frac{1}{2^n} + r^{n+1}.$$

Let $n \to \infty$ to obtain the uniqueness result.

Take $\eta = \dfrac{1}{6(2+r)}$. The constants in the proof of this claim could be chosen as:

$$\begin{aligned}
&d = \frac{1+3r}{6(2+r)^2}, \qquad \xi = \frac{11+7r}{6(2+r)^2}, \qquad \beta = \frac{3(2+r)^2}{11+7r}, \\
&\mu = \frac{12+6r}{12+11r}, \qquad \alpha = \frac{3+2r}{2(2+r)^2},
\end{aligned} \tag{3.8}$$

so that all inequalities in the proof are satisfied. The calculations for finding the constants are given in Section 3.1. This completes the proof of the theorem. □

Example 3.1. We now consider an example which illustrates that the constants in the above theorem cannot be arbitrary. Consider $N = 1$ with $\Omega = (0.1, 1)$ and $F(x) = x$. Clearly this trivial example has no solution in Ω. Take, for instance, $x_0 = 0.2$. Then for any $r < 0.1$, $\overline{B_r(x_0)} \subset \Omega$, assumption (3.1) of the theorem reads $\|x_0\| \le \xi r^2$, which cannot be satisfied for $\xi = (11+7r)(2+r)^{-2}/6$. It is not claimed that this value of ξ is optimal, but at least one assumption of the theorem must be violated because there is no solution in Ω.

Next, consider another 1D example with $\Omega = (-1, 1)$ and $F(x) = x(x+2)$. There is a unique root at zero in Ω. We check the hypotheses of the above theorem for this simple example. Consider $r = 0.05$. Using (3.8), the inequality (3.1) is equivalent to $x_0 \in [-0.0011, 0.0012]$, while the inequality (3.2) becomes $x_0 \ge -0.3850$, which is less stringent than (3.1). Finally, (3.2) is equivalent to $1.5439(x_0+1) \le A_0 \le 2.0046(x_0+1)$. Note that the lower bound is positive and, in conjunction with (3.1), guarantees convergence of the iteration to the root 0. The bounds on x_0 and A_0, which are sufficient but not necessary, ensure that the iteration is well defined in Ω and converges to zero. A poor choice of x_0 and/or A_0 may lead to x_1 landing outside of Ω. As a concrete example, consider $x_0 = -0.9$ and $A_0 = F'(x_0) = 0.2$. Then $x_1 = x_0 - F(x_0)/A_0 = 4.05 \notin \Omega$. Here x_1 lies outside of Ω due to a wrong choice of x_0 violating (3.1), while A_0 is acceptable since it satisfies (3.2).

Next we show superlinear convergence of Broyden's method. The proof follows closely that of Theorem 8.2.2 in [3].

Theorem 3.2. *Assume the hypotheses of Theorem 3.1. Then the Broyden's iteration converges superlinearly to a unique zero of F in $\overline{B_r(x_0)}$.*

Proof. By Theorem 3.1, the iterates $\{x_n\}$ defined by Broyden's method converge to x^*, unique zero of G in $\overline{B_r(x_0)}$, where $G(y) = F'(x_0)^{-1}F(y)$. Consequently x^* is the unique zero of F in $\overline{B_r(x_0)}$. Assume that $G(x_n) \neq 0$ for all $n \ge 0$, we have:

$$\|e_n\| \le r^{n+1}, \qquad \|E_n\| \le \alpha r, \qquad \|G'(x_n)^{-1}\| \le \mu,$$
$$\|G(x_n)\| \le \xi r^{n+2}, \qquad \|B_n^{-1}\| \le \beta,$$

where $e_n = x_n - x^*$, $E_n = B_n - G'(x_n)$, and the positive constants are given by (3.8).

Claim 2. $\forall n \ge 0$,

(i). $\|e_{n+1}\| \le \dfrac{\|e_n\|}{2}$;

(ii). $\|E_{n+1}\| \le \|E_n\| + \dfrac{3\eta}{r}\|e_n\|$.

The proof of Claim 2(i) is identical to the proof of $\|\hat{e}_{n+1}\| \le \|\hat{e}_n\|/2$ in Theorem 3.1 and is therefore omitted. To prove Claim 2(ii), for any $n \ge 0$,

$$\begin{aligned}
E_{n+1} &= B_{n+1} - G'(x_{n+1}) = B_n + \frac{G(x_{n+1})s_n^T}{\|s_n\|^2} - G'(x_{n+1}) \\
&= B_n - G'(x_n) + \frac{G(x_{n+1})s_n^T}{\|s_n\|^2} + G'(x_n) - G'(x_{n+1}) \\
&= E_n(I - \frac{s_n s_n^T}{\|s_n\|^2}) + \frac{(G(x_{n+1}) - G(x_n)\ )s_n^T}{\|s_n\|^2} + \frac{E_n s_n s_n^T}{\|s_n\|^2} + \frac{G(x_n)s_n^T}{\|s_n\|^2} + G'(x_n) - G'(x_{n+1}),
\end{aligned}$$

but $G(x_n) = -B_n s_n$, so

$$E_{n+1} = E_n(I - \frac{s_n s_n^T}{\|s_n\|^2}) + \frac{(G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ )s_n^T}{\|s_n\|^2} + G'(x_n) - G'(x_{n+1}). \tag{3.9}$$

Consider the second term on the right-hand side of this equality. By (3.4),

$$\begin{aligned}
\|\ G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ \| &\le \frac{\eta\|s_n\|}{2r}\ \|s_n\| \\
&= \frac{\eta\|s_n\|}{2r}\big(\|x_{n+1} - x^*\| + \|x_n - x^*\|\big) \\
&\le \frac{\eta\|s_n\|}{2r}\ \big(\|e_{n+1}\| + \|e_n\|\big).
\end{aligned}$$

Therefore, by Claim 2(i),

$$\|\ G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ \| \le \frac{\eta\|s_n\|}{r}\|e_n\|, \tag{3.10}$$

and

$$\begin{aligned}
\|E_{n+1}\| &\le \|E_n\| + \frac{\|\ G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ \|\ \|s_n^T\|}{\|s_n\|^2} + \|G'(x_n) - G'(x_{n+1})\| \\
&\le \|E_n\| + \frac{\|\ G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ \|}{\|s_n\|} + \eta\frac{\|x_{n+1} - x_n\|}{r} \\
&\le \|E_n\| + \frac{\eta}{r}\|e_n\| + \frac{\eta}{r}\ \big(\|e_{n+1}\| + \|e_n\|\big) \le \|E_n\| + \frac{3\eta}{r}\|e_n\|,
\end{aligned}$$

which establishes Claim 2(ii).

Claim 3.

(i) There is some positive integer m so that for all $n \ge m$,

$$\|G(x_n)\| \ge \frac{\|e_n\|}{4\|G'(x_n)^{-1}\|};$$

(ii) $\left\| E_n\big(I - \dfrac{s_n s_n^T}{\|s_n\|^2}\big)\right\|_F \le \|E_n\|_F - \dfrac{1}{2\|E_n\|_F}\dfrac{\|E_n s_n\|^2}{\|s_n\|^2}$ *for all $n \ge 0$;*

(iii) $\dfrac{\|E_n s_n\|}{\|s_n\|} \to 0$ *as $n \to \infty$.*

To prove Claim 3(i), recall from (3.5),

$$\|G(x_{n+1})\| \le \frac{\eta\|s_n\|^2}{2r} + \alpha r\|s_n\|,$$

and also

$$G(x_{n+1}) - G(x_n) = G'(x_n)s_n + \int_0^1 \Big(G'(t\, x_{n+1} + (1-t)x_n) - G'(x_n) \Big) s_n dt.$$

Then,

$$\begin{aligned}
\|G(x_n)\| &\ge \|G'(x_n)s_n\| - \|G(x_{n+1})\| - \frac{\eta}{r}\int_0^1 t\|s_n\|^2 dt \\
&\ge \frac{\|s_n\|}{\|G'(x_n)^{-1}\|} - \|G(x_{n+1})\| - \frac{\eta}{2r}\|s_n\|^2 \\
&\ge \frac{\|s_n\|}{\|G'(x_n)^{-1}\|} - \frac{\eta\|s_n\|^2}{r} - \alpha r\|s_n\| \\
&= \|s_n\| \left(\frac{1}{\|G'(x_n)^{-1}\|} - \frac{\eta\|s_n\|}{r} - \alpha r \right).
\end{aligned}$$

Notice that $\|e_{n+1}\| \le \|e_n\|/2$, and so

$$\frac{\|e_n\|}{2} \le \|e_n\| - \|e_{n+1}\| \le \|s_n\| \le \|e_{n+1}\| + \|e_n\| \le 2\|e_n\|,$$

leading to,

$$\|G(x_n)\| \ge \frac{\|e_n\|}{2}\Big(\frac{1}{\|G'(x_n)^{-1}\|} - \frac{2\eta\|e_n\|}{r} - \alpha r \Big). \tag{3.11}$$

Since $\|e_n\| \to 0$, there is some m so that for all $n \ge m$,

$$\|e_n\| \le \frac{r}{4\eta\|G'(x_n)^{-1}\|} - \frac{\alpha r^2}{2\eta}.$$

Note that by (3.8), the right-hand side of the above inequality is positive. Then

$$\frac{2\eta\|e_n\|}{r} + \alpha r \le \frac{1}{2\|G'(x_n)^{-1}\|},$$

and on substituting this into inequality (3.11),

$$\|G(x_n)\| \ge \frac{\|e_n\|}{4\|G'(x_n)^{-1}\|}.$$

This concludes the proof of Claim 3(i).

Claim 3(ii) is Lemma 8.2.5 in [3]. We include its proof for the convenience of the reader. For any matrix E and vectors u and v, we have $\|E + uv^T\|_F^2 = \|E\|_F^2 + 2v^T E^T u + \|u\|^2\|v\|^2$. Apply this with $u = -E_n s_n$ and $v = s_n/\|s_n\|^2$ for any $n \ge 0$ to obtain

$$\left\| E_n - \frac{E_n s_n s_n^T}{\|s_n\|^2} \right\|_F^2 = \|E_n\|_F^2 - \frac{\|E_n s_n\|^2}{\|s_n\|^2}.$$

Consequently

$$\left\| E_n\left(I - \frac{s_n s_n^T}{\|s_n\|^2}\right)\right\|_F = \left(\|E_n\|_F^2 - \frac{\|E_n s_n\|^2}{\|s_n\|^2} \right)^{1/2} \le \|E_n\|_F - \frac{1}{2\|E_n\|_F}\frac{\|E_n s_n\|^2}{\|s_n\|^2},$$

using the inequality $(a^2 + b^2)^{1/2} \le a - b^2/(2a)$ for any $a \ge b > 0$. This concludes the proof of Claim 3(ii).

To prove Claim 3(iii), use (3.9), (3.10) and (3.11),

$$\begin{aligned}\|E_{n+1}\|_F &= \left\| E_n\left(I - \frac{s_n s_n^T}{\|s_n\|^2}\right)\right\|_F + \left\| \frac{(G(x_{n+1}) - G(x_n) - G'(x_n)s_n\ )s_n^T}{\|s_n\|^2}\right\|_F + \|G'(x_n) - G'(x_{n+1})\|_F \\ &\le \|E_n\|_F - \frac{1}{2\|E_n\|_F}\frac{\|E_n s_n\|^2}{\|s_n\|^2} + \frac{3\eta}{r}\sqrt{N}\|e_n\|,\end{aligned}$$

leading to

$$\begin{aligned}\frac{\|E_n s_n\|^2}{\|s_n\|^2} &\le 2\|E_n\|_F(\ \|E_n\|_F - \|E_{n+1}\|_F + \frac{3\eta}{r}\ \sqrt{N}\|e_n\|) \\ &\le 2\sqrt{N}\alpha r(\ \|E_n\|_F - \|E_{n+1}\|_F + \frac{3\eta}{r}\ \sqrt{N}\|e_n\|).\end{aligned}$$

Summing over n from 0 to m for any m, we obtain

$$\begin{aligned}\sum_{n=0}^{m}\frac{\|E_n s_n\|^2}{\|s_n\|^2} &\le 2\sqrt{N}\alpha r\left(\ \|E_0\|_F - \|E_{m+1}\|_F + \frac{3\eta}{r}\ \sqrt{N}\|e_0\|\ \sum_{n=0}^{m}\frac{1}{2^n}\right) \\ &\le 2\sqrt{N}\alpha r(\ \|E_0\|_F + \frac{3\eta}{r}\ \sqrt{N}\|e_0\|\ ).\end{aligned}$$

Since $\|E_0\|_F \le \sqrt{N}dr$ and $\|e_0\| \le r$,

$$\sum_{n=0}^{m}\frac{\|E_n s_n\|^2}{\|s_n\|^2} \le 2N(dr + 3\eta)\alpha r.$$

Take $m \to \infty$ to conclude that

$$\lim_{n\to\infty}\frac{\|E_n s_n\|^2}{\|s_n\|^2} = 0.$$

This completes the proof of Claim 3(iii).

We are now in a position to conclude the proof of Theorem 3.2. From the Broyden's iteration, for any $n \ge 0$,

$$0 = B_n s_n + G(x_n) = E_n s_n + G'(x_n)s_n + G(x_n).$$

Therefore,

$$-G(x_{n+1}) = E_n s_n + G'(x_n)s_n - G(x_{n+1}) + G(x_n),$$

leading to

$$\frac{\|G(x_{n+1})\|}{\|s_n\|} \le \frac{\|E_n s_n\|}{\|s_n\|} + \frac{\|G'(x_n)s_n - G(x_{n+1}) + G(x_n)\|}{\|s_n\|} \le \frac{\|E_n s_n\|}{\|s_n\|} + \frac{\eta}{r}\|e_n\|,$$

by (3.10). By using Claim 3(iii), we have

$$\lim_{n\to\infty}\frac{\|G(x_{n+1})\|}{\|s_n\|} \le \lim_{n\to\infty}\frac{\|E_n s_n\|}{\|s_n\|} + \frac{\eta}{r}\lim_{n\to\infty}\|e_n\| = 0.$$

By Claim 3(i), for n big enough,

$$\frac{\|G(x_{n+1})\|}{\|s_n\|} \ge \frac{1}{4\|G'(x_{n+1})^{-1}\|}\frac{\|e_{n+1}\|}{\|s_n\|} \ge \frac{1}{4\mu}\ \frac{\|e_{n+1}\|}{\|e_n\| + \|e_{n+1}\|}.$$

Let $c_n = \|e_{n+1}\|/\|e_n\|$. Therefore,

$$0 = \lim_{n\to\infty}\frac{\|G(x_{n+1})\|}{\|s_n\|} \ge \frac{1}{4\mu}\lim_{n\to\infty}\frac{\|e_{n+1}\|}{\|e_n\| + \|e_{n+1}\|} = \frac{1}{4\mu}\lim_{n\to\infty}\frac{\|c_{n+1}\|}{1 + \|c_{n+1}\|}.$$

This implies that $\lim_{n\to\infty} c_{n+1} = 0$, which is superlinear convergence. □

3.1. Appendix

This appendix provides the calculations for finding the constants in the proof of Theorem 3.1 so that the following relations among the constants are satisfied:

1. $\eta < 1$ and $dr < 1$,
2. $\xi \geq \eta + \alpha$,
3. $\alpha \geq 3\eta + d$,
4. $\mu = \dfrac{1}{1-\eta}$,
5. $\mu\alpha r < 1$,
6. $\beta = \max\left\{\dfrac{1}{1-dr}, \dfrac{1}{1-\eta-\alpha r}\right\}$,
7. $\beta\xi \leq 1$,
8. $\beta(\eta+\alpha) \leq \dfrac{1}{2}$.

By using Condition 3. we have $\alpha > d$ and so

$$\beta = \max\left\{\frac{1}{1-dr}, \frac{1}{1-\eta-\alpha r}\right\} = \frac{1}{1-\eta-\alpha r}.$$

Let $\xi = \eta + \alpha$ and $\beta\xi = \dfrac{1}{2}$ so that $\beta = \dfrac{1}{2\xi} = \dfrac{1}{2(\eta+\alpha)}$. Thus

$$\frac{1}{1-\eta-\alpha r} = \frac{1}{2(\eta+\alpha)} \quad \Rightarrow \quad \alpha = \frac{1-3\eta}{2+r}, \quad \xi = \frac{\eta r - \eta + 1}{2+r}, \quad \beta = \frac{2+r}{2(\eta r - \eta + 1)}.$$

Note that $\eta r - \eta + 1 > 0$, if $\eta < \dfrac{1}{1-r}$. Define

$$d = \alpha - 3\eta - \frac{2\eta}{2+r} = \frac{1 - 11\eta - 3\eta r}{2+r}.$$

We need to be sure that $d > 0$. It is sufficient to consider

$$0 < \eta < \min\left\{\frac{1}{11+3r}, \frac{1}{1-r}\right\} = \frac{1}{11+3r}.$$

Notice that by the expression of ξ, α, β and d we have, $\mu\alpha r < 1$ if and only if $\eta < \dfrac{1}{1-r}$, which is true. Also $1 - dr = \dfrac{2 + 11\eta r + 3\eta r^2}{2+r} > 0$ lead to $dr < 1$. Furthermore $\beta(\eta+\alpha) = \beta\xi = \dfrac{1}{2}$.

In summary, with $r \leq \dfrac{1}{2}$, we choose $\eta = \dfrac{1}{6(2+r)}$, and

$$d = \frac{1+3r}{6(2+r)^2}, \qquad \xi = \frac{11+7r}{6(2+r)^2}, \qquad \beta = \frac{3(2+r)^2}{11+7r},$$
$$\mu = \frac{12+6r}{12+11r}, \qquad \alpha = \frac{3+2r}{2(2+r)^2}.$$

4. BFGS algorithm

Let Ω be an open set in $\mathbb{R}^N$ and $f : \Omega \to \mathbb{R}$ be smooth. The problem is to find a local minimum of f in Ω. Of course, one can simply apply Broyden's method to the nonlinear system $F := \nabla f = 0$. However, in general, the approximate Jacobian in Broyden's method is not symmetric, clearly not an ideal situation since the exact Jacobian is symmetric. There are many ways to obtain a quasi-Newton method where the approximate Jacobian is symmetric. The most popular is the BFGS algorithm. Given $x_0 \in \Omega$ and SPD initial approximate Jacobian A_0, the iteration is:

$$s_n = -A_n^{-1}F(x_n),$$
$$x_{n+1} = x_n + s_n,$$
$$y_n = F(x_{n+1}) - F(x_n),$$
$$A_{n+1} = A_n + \frac{y_n y_n^T}{y_n^T s_n} - \frac{A_n s_n s_n^T A_n}{s_n^T A_n s_n},$$

for any $n \geq 0$. Notice that consecutive approximate Jacobians differ by a rank-two matrix. Superlinear convergence and global convergence for BFGS algorithm with line search with classical assumptions are known. See, for instance, [3] or [4].

We now show local convergence of the BFGS algorithm using Kantorovich-type assumptions. Except for bounds on the extreme eigenvalues of the Hessian, only one constant appears in the theory.

Theorem 4.1. *Let Ω be an open set in $\mathbb{R}^N$, $f : \Omega \to \mathbb{R}$ and $f \in C^2(\Omega)$. Let $F(x) = \nabla f(x)$ and $F'(x) = D^2 f(x)$. Assume $x_0 \in \Omega$ and $\overline{B_r(x_0)} \subset \Omega$ for some $0 < r \leq 1/2$. Suppose there are positive constants $m \leq 1$ and M such that for any $z \in \mathbb{R}^N$ and $x \in \overline{B_r(x_0)}$,*

$$m\|z\|^2 \leq z^T D^2 f(x) z \leq M\|z\|^2.$$

Also

$$\|F'(x_0)^{-\frac{1}{2}}F(x_0)\| \le ar^2, \tag{4.1}$$

$$\|F'(x_0)^{-\frac{1}{2}}\big(F'(u)-F'(v)\big)F'(x_0)^{-\frac{1}{2}}\| \le \frac{\eta\|u-v\|}{\sqrt{r}}, \qquad \forall u, v \in \overline{B_r(x_0)}, \tag{4.2}$$

where a and η are positive constants dependent on r (to be defined later). If r is sufficiently small (satisfies (4.20)), then the BFGS iteration $\{x_n\}$ with $A_0 = F'(x_0)$ is well defined and exactly one of the following cases holds,
(i) $F(x_n) = 0$ for some $n \ge 0$.
(ii) $\{x_n\}$ converges to a unique zero of F in $\overline{B_r(x_0)}$.

Proof. First notice that by given assumptions of the theorem, $m \le \|F'(x)\|$ for all $x \in \overline{B_r(x_0)}$, especially $\|F'(x_0)^{-1}\| \le 1/m$. Let $G(\xi) = F'(x_0)^{-\frac{1}{2}}F(F'(x_0)^{-\frac{1}{2}}\xi)$. Observe that $G(\xi^*) = 0$ if and only if $F(x^*) = 0$, where $x^* = F'(x_0)^{-\frac{1}{2}}\xi^*$. Since $F'(x_0)^{\frac{1}{2}}$ is invertible,

$$G(\xi^*) = F'(x_0)^{-\frac{1}{2}}F(F'(x_0)^{-\frac{1}{2}}\xi^*) = 0 \;\Leftrightarrow\; F(x^*) = 0.$$

Also we have:

$$G'(\xi) = F'(x_0)^{-\frac{1}{2}}F'_x(F'(x_0)^{-\frac{1}{2}}\xi)F'(x_0)^{-\frac{1}{2}}.$$

We apply BFGS algorithm for $G(\xi)$ with $B_0 = G'(\xi_0) = I$ and $\xi_0 = F'(x_0)^{\frac{1}{2}}x_0$. For $n \ge 0$,

$$\begin{aligned}
t_n &= -B_n^{-1}G(\xi_n),\\
\xi_{n+1} &= \xi_n + t_n,\\
z_n &= G(\xi_{n+1}) - G(\xi_n),\\
B_{n+1} &= B_n + \frac{z_n z_n^T}{z_n^T t_n} - \frac{B_n t_n t_n^T B_n}{t_n^T B_n t_n}\ .
\end{aligned}$$

Assume $F(x_n) \neq 0$ for all $n \ge 0$. We apply mathematical induction for proving $\xi_n = F'(x_0)^{\frac{1}{2}}x_n$ and also $B_n = F'(x_0)^{-\frac{1}{2}}A_nF'(x_0)^{-\frac{1}{2}}$ for all $n \ge 0$. The basic step holds trivially. Assume these statements are true for some positive integer n, then

$$\xi_{n+1} = \xi_n + t_n = F'(x_0)^{\frac{1}{2}}x_n + F'(x_0)^{\frac{1}{2}}s_n = F'(x_0)^{\frac{1}{2}}x_{n+1}.$$

Notice that by using induction hypothesis,

$$\begin{aligned}
t_n &= -B_n^{-1}G(\xi_n) = -\big(F'(x_0)^{-\frac{1}{2}}A_nF'(x_0)^{-\frac{1}{2}}\big)^{-1}\ F'(x_0)^{-\frac{1}{2}}F(F'(x_0)^{-\frac{1}{2}}\xi_n)\\
&= -F'(x_0)^{\frac{1}{2}}A_n^{-1}F(x_n) = F'(x_0)^{\frac{1}{2}}s_n.
\end{aligned}$$

Furthermore,

$$z_n = G(\xi_{n+1}) - G(\xi_n) = F'(x_0)^{-\frac{1}{2}}(F(x_{n+1}) - F(x_n)) = F'(x_0)^{-\frac{1}{2}}y_n,$$

then by using definition for B_{n+1}, we obtain

$$\begin{aligned}
B_{n+1} &= F'(x_0)^{-\frac{1}{2}}A_nF'(x_0)^{-\frac{1}{2}} + F'(x_0)^{-\frac{1}{2}}\frac{y_ny_n^T}{y_n^Ts_n}F'(x_0)^{-\frac{1}{2}} - F'(x_0)^{-\frac{1}{2}}\ \frac{A_ns_ns_n^TA_n}{s_nA_ns_n}\ F'(x_0)^{-\frac{1}{2}}\\
&= F'(x_0)^{-\frac{1}{2}}\ \Big(A_n + \frac{y_ny_n^T}{y_n^Ts_n} - \frac{A_ns_ns_n^TA_n}{s_n^TA_ns_n}\Big)\ F'(x_0)^{-\frac{1}{2}}\\
&= F'(x_0)^{-\frac{1}{2}}A_{n+1}F'(x_0)^{-\frac{1}{2}}.
\end{aligned}$$

By using assumptions of the theorem,

$$\|G(\xi_0)\| = \|F'(x_0)^{-\frac{1}{2}}F(F'(x_0)^{-\frac{1}{2}}\xi_0)\| = \|F'(x_0)^{-\frac{1}{2}}F(x_0)\| \le ar^2.$$

Let $\rho = mr$. Notice that for any $\omega, \tau \in \overline{B_\rho(\xi_0)}$,

$$\begin{aligned}
\|G'(\omega) - G'(\tau)\| &= \|F'(x_0)^{-\frac{1}{2}}F'(F'(x_0)^{-\frac{1}{2}}\omega)F'(x_0)^{-\frac{1}{2}} - F'(x_0)^{-\frac{1}{2}}F'(F'(x_0)^{-\frac{1}{2}}\tau)F'(x_0)^{-\frac{1}{2}}\|\\
&= \|F'(x_0)^{-\frac{1}{2}}\big(F'(u) - F'(v)\big)F'(x_0)^{-\frac{1}{2}}\|\\
&\le \frac{\eta}{\sqrt{r}}\|u - v\| \le \frac{\eta}{\sqrt{r}}\|F'(x_0)^{-\frac{1}{2}}\|\|\omega - \tau\|\\
&\le \frac{\eta}{\sqrt{mr}}\|\omega - \tau\| \le \frac{\eta}{\sqrt{\rho}}\|\omega - \tau\|,
\end{aligned} \tag{4.3}$$

since $\|F'(x_0)^{-\frac{1}{2}}\| \leq \frac{1}{\sqrt{m}}$. Then by Lemma 1.5,

$$\|G(\omega) - G(\tau) - G'(\tau)(\omega - \tau)\| \leq \frac{\eta}{2\sqrt{\rho}}\|\omega - \tau\|^2, \qquad \omega, \tau \in \overline{B_\rho(\xi_0)}. \tag{4.4}$$

Below, we state and prove Claim 4, which is central to this proof.

Claim 4. *There are some positive constants ζ, μ, γ and β dependent on ρ (to be defined later), such that for $n \geq 0$,*

(i) $\|\xi_n - \xi_0\| \leq \rho(1 - \rho^n)$;
(ii) $\|G(\xi_n)\| \leq \zeta\rho^{n+2}$;
(iii) $G'(\xi_n)$ *is invertible and* $\|G'(\xi_n)^{-1}\| \leq \mu$;
(iv) B_n *is invertible and* $\|G'(\xi_n)^{-1} - B_n^{-1}\| \leq \gamma\rho(1 - \rho^n)$;
(v) $\|B_n^{-1}\| \leq \beta$;
(vi) $\|t_n\| \leq \rho^{n+2}$.

Notice that if $\|\xi_n - \xi_0\| \leq \rho(1 - \rho^n)$, then $\|x_n - x_0\| \leq mr(1 - m^n r^n) < r$ since $m \leq 1$. Thus $x_n \in B_r(x_0)$ and $\xi_n \in B_\rho(\xi_0)$. Also $\|t_n\| \leq \rho^{n+2}$ results in $\|s_n\| \leq r^{n+2}$.

Now we prove Claim 4(i)–(vi) by using induction. The base case for Claim 4(i) is trivial. Since $\|G(\xi_0)\| \leq ar^2$, assume $\zeta \geq a/m^2$, then $\|G(\xi_0)\| \leq \zeta\rho^2$. (*Note that all additional assumptions on constants in this proof are summarized at the beginning of Section* 4.1.) Also $\|G'(\xi_0)^{-1}\| = \|I\| = 1$. Let $\mu \geq 1$, then $\|G'(\xi_0)^{-1}\| \leq \mu$. By assumption $B_0 = I$, so it is invertible and by choosing $\beta \geq 1$, the base cases for Claims 4(iv) and (v) are satisfied. Also $\|t_0\| = \| - B_0^{-1}G(\xi_0)\| = \|G(\xi_0)\| \leq \zeta\rho^2 \leq \rho^2$, if we require $\zeta \leq 1$. Next, assume all of the statements are true for some integer $n \geq 1$, we will show they hold for $n + 1$.

To prove the induction step of Claim 4(i), observe that B_n is invertible by the hypothesis of induction, ξ_{n+1} exists and

$$\begin{aligned}\|\xi_{n+1} - \xi_0\| &\leq \|\xi_{n+1} - \xi_n\| + \|\xi_n - \xi_0\| \\ &\leq \rho^{n+2} + \rho(1 - \rho^n) = \rho(1 - \rho^n(1 - \rho)) \leq \rho(1 - \rho^{n+1}),\end{aligned}$$

since $\rho \leq \dfrac{1}{2}$. This completes the proof of Claim 4(i). Moreover $\|\xi_{n+1} - \xi_0\| < \rho$, so $\xi_{n+1} \in B_\rho(\xi_0)$.

To prove Claim 4(ii), we first show that there is a constant α such that

$$\|G'(\xi_n) - B_n\| \leq \alpha\rho.$$

By the induction hypothesis,

$$\begin{aligned}\|I - B_n^{-1}\| &\leq \|I - G'(\xi_n)^{-1}\| + \|G'(\xi_n)^{-1} - B_n^{-1}\| \\ &\leq \|G'(\xi_n)^{-1}\|\,\|G'(\xi_0) - G'(\xi_n)\| + \|G'(\xi_n)^{-1} - B_n^{-1}\| \\ &\leq \mu\eta\sqrt{\rho}(1 - \rho^n) + \gamma\rho(1 - \rho^n).\end{aligned}$$

By assuming $\hat{\gamma} = \mu\eta + \gamma\sqrt{\rho}$, we get $\|I - B_n^{-1}\| \leq \hat{\gamma}\sqrt{\rho}$. Let $\lambda_j,\ 1 \leq j \leq N$ be eigenvalues of B_n^{-1}. Therefore $|1 - \lambda_j| \leq \hat{\gamma}\sqrt{\rho}$ for all $1 \leq j \leq N$. Also $\|B_n\| = \max_{1\leq j\leq N}\left|\dfrac{1}{\lambda_j}\right| \leq \dfrac{1}{1 - \hat{\gamma}\sqrt{\rho}}$, assuming $\hat{\gamma}\sqrt{\rho} < 1$. Then

$$\begin{aligned}\|G'(\xi_n) - B_n\| &= \|G'(\xi_n)(G'(\xi_n)^{-1} - B_n^{-1})B_n\| \\ &\leq \|G'(\xi_n)\|\,\|G'(\xi_n)^{-1} - B_n^{-1}\|\,\|B_n\| \leq \frac{\mu\gamma}{1 - \hat{\gamma}\sqrt{\rho}}\rho \leq \alpha\rho,\end{aligned}$$

by assuming $\dfrac{\mu\gamma}{1 - \hat{\gamma}\sqrt{\rho}} \leq \alpha$.

We proceed to show the induction step for Claim 4(ii). By definition, $t_n = -B_n^{-1}G(\xi_n)$. Use (4.4) to get

$$\begin{aligned}\|G(\xi_{n+1})\| &= \|G(\xi_{n+1}) - G(\xi_n) - G'(\xi_n)t_n + G'(\xi_n)t_n - B_n t_n\| \\ &\leq \|G(\xi_{n+1}) - G(\xi_n) - G'(\xi_n)t_n\| + \|(G'(\xi_n) - B_n)t_n\| \\ &\leq \frac{\eta\|t_n\|^2}{2\sqrt{\rho}} + \alpha\rho\|t_n\| = \|t_n\|\Big(\frac{\eta\|t_n\|}{2\sqrt{\rho}} + \alpha\rho\Big) \\ &\leq \rho^{n+2}\Big(\frac{\eta\rho^{n+2}}{2\sqrt{\rho}} + \alpha\rho\Big) \leq \rho^{n+3}\,(\eta\sqrt{\rho} + \alpha).\end{aligned}$$

If we assume $\eta\sqrt{\rho} + \alpha \leq \zeta$, then $\|G(\xi_{n+1})\| \leq \zeta\rho^{n+3}$, as we need for Claim 4(ii).

Now we show the induction step for Claim 4(iii). By (4.3),

$$\|I - G'(\xi_{n+1})\| = \|G'(\xi_0) - G'(\xi_{n+1})\| \leq \frac{\eta}{\sqrt{\rho}}\|\xi_{n+1} - \xi_0\| \leq \eta\sqrt{\rho}.$$

Assume $\eta\sqrt{\rho} < 1$, then by using Lemma 1.2, $G'(\xi_{n+1})$ is invertible and

$$\|G'(\xi_{n+1})^{-1}\| \le \frac{1}{1-\eta\sqrt{\rho}}.$$

Define

$$\mu = \frac{1}{1-\eta\sqrt{\rho}}, \tag{4.5}$$

then $\|G'(\xi_{n+1})^{-1}\| \le \mu$, which establishes Claim 4(iii).

To prove Claim 4(iv), notice that there is some $\tilde{\xi}$ between ξ_n and ξ_{n+1} so that

$$t_n^T z_n = t_n^T(G(\xi_{n+1}) - G(\xi_n)) = t_n^T G'(\tilde{\xi}) t_n > 0,$$

since $D^2 f$ and hence G' is SPD in a neighbourhood of the initial point. Hence B_{n+1} is invertible and, in fact, SPD. Take any k satisfying $0 \le k \le n$. By using Sherman–Morrison-Woodbury formula,

$$B_{k+1}^{-1} = B_k^{-1} + \frac{t_k t_k^T}{z_k^T t_k}\left(1 + \frac{z_k^T B_k^{-1} z_k}{z_k^T t_k}\right) - \frac{B_k^{-1} z_k t_k^T + t_k z_k^T B_k^{-1}}{z_k^T t_k}.$$

Define

$$P_k = I - \frac{t_k z_k^T}{t_k^T z_k},$$

then,

$$B_{k+1}^{-1} = P_k B_k^{-1} P_k^T + \frac{t_k t_k^T}{t_k^T z_k}.$$

For brevity let $B = G'(\xi_k)$. After some calculations,

$$\begin{aligned} B^{-1} - B_{k+1}^{-1} &= B^{-1} - P_k B_k^{-1} P_k^T - \frac{t_k t_k^T}{t_k^T z_k} \\ &= P_k(B^{-1} - B_k^{-1})P_k^T - \frac{(t_k - B^{-1}z_k)t_k^T + t_k(t_k - B^{-1}z_k)^T P_k^T}{t_k^T z_k}. \end{aligned}$$

Define the following norm which depends on the iteration number $k \ge 0$:

$$\|X\|_k = \|G'(\xi_k)^{1/2}\, X\, G'(\xi_k)^{1/2}\|_F,$$

for any arbitrary matrix $X \in \mathbb{R}^{N\times N}$. Observe that

$$\|B^{-1} - B_{k+1}^{-1}\|_k \le \|P_k(B^{-1} - B_k^{-1})P_k^T\|_k + \frac{\|(t_k - B^{-1}z_k)t_k^T\|_k}{t_k^T z_k} + \frac{\|t_k(t_k - B^{-1}z_k)^T P_k^T\|_k}{t_k^T z_k}. \tag{4.6}$$

Below we will find estimations for each term of this inequality. For the first term,

$$\begin{aligned} \|P_k(B^{-1} - B_k^{-1})P_k^T\|_k &= \|B^{\frac12} P_k B^{-\frac12} B^{\frac12}(B^{-1} - B_k^{-1})B^{\frac12} B^{-\frac12} P_k^T B^{\frac12}\|_F \\ &\le \|B^{\frac12} P_k B^{-\frac12}\|^2\ \|B^{-1} - B_k^{-1}\|_k \\ &= \|B^{\frac12}(I - \frac{t_k z_k^T}{t_k^T z_k})B^{-\frac12}\|^2\ \|B^{-1} - B_k^{-1}\|_k \\ &= \left\| I - \frac{(B^{\frac12}t_k)(B^{-\frac12}z_k)^T}{(B^{\frac12}t_k)^T(B^{-\frac12}z_k)} \right\|^2 \|B^{-1} - B_k^{-1}\|_k \\ &= \left(\frac{\|B^{\frac12}t_k\|\ \|B^{-\frac12}z_k\|}{(B^{\frac12}t_k)^T(B^{-\frac12}z_k)} \right)^2 \|B^{-1} - B_k^{-1}\|_k. \end{aligned}$$

For the last line we used Lemma 1.3. Define

$$w = \frac{(B^{\frac12}t_k)^T(B^{-\frac12}z_k)}{\|B^{\frac12}t_k\|\ \|B^{-\frac12}z_k\|} \le 1,$$

to obtain

$$\|P_k(B^{-1} - B_k^{-1})P_k^T\|_k \le \frac{1}{w^2}\|B^{-1} - B_k^{-1}\|_k. \tag{4.7}$$

Consider the second term of the inequality (4.6),

$$\begin{aligned}\frac{\|(t_k - B^{-1}z_k)t_k^T\|_k}{t_k^T z_k} &= \frac{\|B^{\frac{1}{2}}(t_k - B^{-1}z_k)t_k^T B^{\frac{1}{2}}\|_F}{t_k^T z_k}\\ &= \frac{\|B^{\frac{1}{2}}(t_k - B^{-1}z_k)\|\|B^{\frac{1}{2}}t_k\|}{t_k^T z_k}\\ &= \frac{1}{w}\frac{\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\|}{\|B^{-\frac{1}{2}}z_k\|}.\end{aligned} \tag{4.8}$$

Similarly for the last term of (4.6),

$$\begin{aligned}\frac{\|t_k(t_k - B^{-1}z_k)^T P_k^T\|_k}{t_k^T z_k} &= \frac{\|B^{\frac{1}{2}}t_k(t_k - B^{-1}z_k)^T P_k^T B^{\frac{1}{2}}\|_F}{t_k^T z_k}\\ &= \frac{\|B^{\frac{1}{2}}t_k\big(B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\big)^T B^{-\frac{1}{2}}P_k^T B^{\frac{1}{2}}\|_F}{t_k^T z_k}\\ &\le \frac{\|B^{\frac{1}{2}}t_k\|\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\|\|B^{-\frac{1}{2}}P_k^T B^{\frac{1}{2}}\|}{t_k^T z_k}\\ &= \frac{1}{w^2}\frac{\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\|}{\|B^{-\frac{1}{2}}z_k\|}.\end{aligned} \tag{4.9}$$

For finding an estimation for the right-hand side of this inequality, notice that $B = G'(\xi_k)$,

$$\begin{aligned}t_k - B^{-1}z_k &= t_k - B^{-1}\big(G(\xi_{k+1}) - G(\xi_k)\big)\\ &= t_k - G'(\xi_n)^{-1}\big(G(\xi_{k+1}) - G(\xi_k) - G'(\xi_k)t_k\big) - t_k\\ &= -B^{-1}\int_0^1 \big(G'(\xi_k + \tau t_k) - G'(\xi_k)\big)t_k d\tau.\end{aligned}$$

Therefore by (4.3),

$$\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\| \le \frac{\eta}{2\sqrt{\rho}}\|B^{-\frac{1}{2}}\|\|t_k\|^2. \tag{4.10}$$

Since $z_k = G(\xi_{k+1}) - G(\xi_k) = G'(\tilde{\xi})t_k$ for some $\tilde{\xi}$ between ξ_{k+1} and ξ_k, it follows that $t_k = G'(\tilde{\xi})^{-1}z_k$ and

$$\begin{aligned}&\|t_k\| = \|G'(\tilde{\xi})^{-1}\|\|z_k\| \le \frac{M}{m}\|z_k\| \Rightarrow \frac{1}{\|z_k\|} \le \frac{M}{m\|t_k\|},\\ &\|z_k\| = \|B^{\frac{1}{2}}B^{-\frac{1}{2}}z_k\| \le \|B^{\frac{1}{2}}\|\|B^{-\frac{1}{2}}z_k\|,\\ &\frac{1}{\|B^{-\frac{1}{2}}z_k\|} \le \frac{\|B^{\frac{1}{2}}\|}{\|z_k\|} \le \frac{M\,\|B^{\frac{1}{2}}\|}{m\|t_k\|}.\end{aligned} \tag{4.11}$$

(4.10) and (4.11) together imply:

$$\frac{\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\|}{\|B^{-\frac{1}{2}}z_k\|} \le \frac{M\eta}{2m\sqrt{\rho}}\|B^{-\frac{1}{2}}\|\|B^{\frac{1}{2}}\|\|t_k\|. \tag{4.12}$$

By using the assumptions of the theorem, $\frac{m}{M} \le \|G'(\xi)\| \le \frac{M}{m}$ for any $\xi \in B_\rho(\xi_0)$. This implies $\|B\|\|B^{-1}\| = \|G'(\xi_k)\|\|G'(\xi_k)^{-1}\| \le (\frac{M}{m})^2$. Now choose η such that $\frac{\eta M^2}{m^2} \le \sqrt{2}$, and define

$$\Lambda = \frac{\eta M^2}{\sqrt{2}\,m^2} \le 1. \tag{4.13}$$

Then

$$\frac{\eta M}{2m\sqrt{\rho}}\|B^{-\frac{1}{2}}\|\|B^{\frac{1}{2}}\|\|t_k\| \le \frac{\eta M^2}{2m^2\sqrt{\rho}}\|t_k\| = \frac{\Lambda}{\sqrt{2\rho}}\|t_k\| \le \frac{\rho^{3/2}}{\sqrt{2}} \le \frac{1}{\sqrt{2}}. \tag{4.14}$$

From Lemma 1.4,

$$1 - w^2 \le \left(\frac{\eta M}{2m\sqrt{\rho}}\|B^{-\frac{1}{2}}\|\|B^{\frac{1}{2}}\|\|t_k\|\right)^2 \le \frac{\Lambda^2\|t_k\|^2}{2\rho} \le \frac{1}{2},$$

so $w^2 \geq \dfrac{1}{2}$ and

$$\begin{aligned}\frac{1}{w^2} = 1 + \frac{1-w^2}{w^2} &\leq 1 + 2\left(\frac{\eta M}{2m\sqrt{\rho}}\|B^{-\frac{1}{2}}\|\,\|B^{\frac{1}{2}}\|\,\|t_k\|\right)^2 \\ &\leq 1 + 2\frac{\rho^{3/2}}{\sqrt{2}}\frac{\Lambda}{\sqrt{2\rho}}\|t_k\| = 1 + \Lambda\rho\|t_k\|. \end{aligned} \tag{4.15}$$

Combining all estimates (4.7), (4.8) and (4.9), followed by an application of (4.14), (4.15) and (4.12), inequality (4.6) becomes

$$\begin{aligned}\|B^{-1} - B_{k+1}^{-1}\|_k &\leq \frac{1}{w^2}\|B^{-1} - B_k^{-1}\|_k + \frac{2}{w^2}\frac{\|B^{\frac{1}{2}}t_k - B^{-\frac{1}{2}}z_k\|}{\|B^{-\frac{1}{2}}z_k\|} \\ &\leq (1+\Lambda\rho\|t_k\|)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}(1+\Lambda\rho\|t_k\|)\frac{\Lambda}{\sqrt{\rho}}\|t_k\|. \end{aligned} \tag{4.16}$$

Notice that for any arbitrary matrix $X \in \mathbb{R}^{N\times N}$,

$$\begin{aligned}\|X\|_{k+1} &= \|G'(\xi_{k+1})^{\frac{1}{2}}\, X\, G'(\xi_{k+1})^{\frac{1}{2}}\|_F \\ &= \|G'(\xi_{k+1})^{\frac{1}{2}} G'(\xi_k)^{-\frac{1}{2}}\ G'(\xi_k)^{\frac{1}{2}}\, X\, G'(\xi_k)^{\frac{1}{2}}\ G'(\xi_k)^{-\frac{1}{2}} G'(\xi_{k+1})^{\frac{1}{2}}\|_F \\ &\leq \|G'(\xi_{k+1})G'(\xi_k)^{-1}\|\,\|X\|_k. \end{aligned}$$

In last line we have used Lemma 1.1. Observe that,

$$\begin{aligned}G'(\xi_{k+1})G'(\xi_k)^{-1} &= (G'(\xi_{k+1}) - G'(\xi_k) + G'(\xi_k))G'(\xi_k)^{-1} \\ &= (G'(\xi_{k+1}) - G'(\xi_k))G'(\xi_k)^{-1} + I, \end{aligned}$$

therefore by (4.3),

$$\|G'(\xi_{k+1})G'(\xi_k)^{-1}\| \leq 1 + \|G'(\xi_{k+1}) - G'(\xi_k)\|\,\|G'(\xi_k)^{-1}\| \leq 1 + \frac{\eta\mu}{\sqrt{\rho}}\|t_k\|, \tag{4.17}$$

so we obtain

$$\|X\|_{k+1} \leq (1 + \frac{\eta\mu}{\sqrt{\rho}}\|t_k\|)\,\|X\|_k,$$

Define $\kappa = 1 + \dfrac{\eta\mu}{\sqrt{\rho}}\|t_k\|$. Therefore $\|X\|_{k+1} \leq \kappa\|X\|_k$. Notice that by using induction hypothesis and (4.5)

$$\kappa = 1 + \frac{\eta\mu}{\sqrt{\rho}}\|t_k\| \leq 1 + \eta\mu\rho^{k+3/2} \leq 1 + \frac{\eta\sqrt{\rho}}{1-\eta\sqrt{\rho}} = \mu.$$

From the inequality (4.16),

$$\|B^{-1} - B_{k+1}^{-1}\|_{k+1} \leq \kappa(1+\Lambda\rho\|t_k\|)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda\rho\|t_k\|)\,\|t_k\|,$$

so

$$\begin{aligned}\|B^{-1} - B_{k+1}^{-1}\|_{k+1} - \|B^{-1} - B_k^{-1}\|_k &\leq (\kappa - 1 + \kappa\Lambda\rho\|t_k\|)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\|t_k\| \\ &\leq (\frac{\eta\mu}{\sqrt{\rho}}\|t_k\| + \kappa\Lambda\rho\|t_k\|)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\|t_k\| \\ &\leq \left((\frac{\eta\mu}{\sqrt{\rho}} + \kappa\Lambda\rho)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\right)\|t_k\|. \end{aligned}$$

Notice that $B = G'(\xi_k)$, by adding and subtracting $G'(\xi_{k+1})$,

$$\begin{aligned}&\|G'(\xi_{k+1})^{-1} - B_{k+1}^{-1}\|_{k+1} - \|G'(\xi_k)^{-1} - B_k^{-1}\|_k \\ &\leq \|G'(\xi_{k+1})^{-1} - G'(\xi_k)^{-1}\|_{k+1} + \left((\frac{\eta\mu}{\sqrt{\rho}} + \kappa\Lambda\rho)\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\right)\|t_k\|. \end{aligned} \tag{4.18}$$

Also by Lemma 1.1 and inequality (4.17)

$$\begin{aligned}
\|G'(\xi_{k+1})^{-1} - G'(\xi_k)^{-1}\|_{k+1} &= \|G'(\xi_{k+1})^{-1}G'(\xi_k)G'(\xi_k)^{-1} - G'(\xi_{k+1})^{-1}G'(\xi_{k+1})G'(\xi_k)^{-1}\|_{k+1} \\
&= \|G'(\xi_{k+1})^{-1}\,(G'(\xi_k) - G'(\xi_{k+1}))\,G'(\xi_k)^{-1}\|_{k+1} \\
&= \|G'(\xi_{k+1})^{\frac{1}{2}}G'(\xi_{k+1})^{-1}\,(G'(\xi_k) - G'(\xi_{k+1}))\,G'(\xi_k)^{-1}G'(\xi_{k+1})^{\frac{1}{2}}\|_F \\
&\le \|G'(\xi_{k+1})^{-\frac{1}{2}}\|\|G'(\xi_k)^{-1}G'(\xi_{k+1})^{\frac{1}{2}}\|\frac{\sqrt{N}\eta}{\sqrt{\rho}}\|\xi_{k+1} - \xi_k\| \\
&\le \|G'(\xi_{k+1})^{-\frac{1}{2}}\|\|G'(\xi_k)^{-\frac{1}{2}}\|\sqrt{\|G'(\xi_k)^{-1}G'(\xi_{k+1})\|}\frac{\sqrt{N}\eta}{\sqrt{\rho}}\|\xi_{k+1} - \xi_k\| \\
&\le \frac{\sqrt{\kappa N}\eta\mu}{\sqrt{\rho}}\|t_k\|.
\end{aligned}$$

Then by substituting this in (4.18)

$$\begin{aligned}
&\|G'(\xi_{k+1})^{-1} - B_{k+1}^{-1}\|_{k+1} - \|G'(\xi_k)^{-1} - B_k^{-1}\|_k \\
&\le \left(\frac{\sqrt{\kappa N}\eta\mu}{\sqrt{\rho}} + (\frac{\eta\mu}{\sqrt{\rho}} + \kappa\Lambda\rho)\,\|B^{-1} - B_k^{-1}\|_k + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\right)\|t_k\|.
\end{aligned}$$

From the induction hypothesis, $\|B^{-1} - B_k^{-1}\|_k \le \gamma\rho(1-\rho^k) \le \gamma\rho$. Take the sum from $k = 0$ to $k = n$ and using the induction hypothesis of Claim 4(vi) to obtain

$$\begin{aligned}
&\|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\|_{n+1} - \|G'(\xi_0)^{-1} - B_0^{-1}\|_0 \\
&\le \left(\frac{\sqrt{\kappa N}\eta\mu}{\sqrt{\rho}} + (\frac{\eta\mu}{\sqrt{\rho}} + \kappa\Lambda\rho)\gamma\rho + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\right)\rho^2\sum_{k=0}^{n}\rho^k.
\end{aligned} \tag{4.19}$$

Notice that $G'(\xi_0) = B_0 = I$, so $\|G'(\xi_0)^{-1} - B_0^{-1}\|_0 = 0$.

$$\begin{aligned}
\|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\| &\le \|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\|_F \\
&= \|G'(\xi_{n+1})^{-\frac{1}{2}}G'(\xi_{n+1})^{\frac{1}{2}}\,(G'(\xi_{n+1})^{-1} - B_{n+1}^{-1})\,G'(\xi_{n+1})^{\frac{1}{2}}G'(\xi_{n+1})^{-\frac{1}{2}}\|_F \\
&\le \|G'(\xi_{n+1})^{-1}\|\|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\|_{n+1}.
\end{aligned}$$

Use inequality (4.19) to obtain,

$$\begin{aligned}
\|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\| &\le \|G'(\xi_{n+1})^{-1}\|\left[\frac{\sqrt{\kappa N}\eta\mu}{\sqrt{\rho}} + (\frac{\eta\mu}{\sqrt{\rho}} + \kappa\Lambda\rho)\gamma\rho + \sqrt{2}\kappa\frac{\Lambda}{\sqrt{\rho}}(1+\Lambda)\right]\rho^2\sum_{k=0}^{n}\rho^k \\
&\le \mu\left[\sqrt{\kappa N}\eta\mu + (\eta\mu + \kappa\Lambda\rho^{3/2})\gamma\rho + \sqrt{2}\kappa\Lambda(1+\Lambda)\right]\rho^{3/2}\sum_{k=0}^{n}\rho^k \\
&\le \mu^2(\sqrt{2\mu N}\eta + (\eta + \rho^{3/2})\gamma\rho + 2\sqrt{2})\rho^{3/2}\sum_{k=0}^{n}\rho^k,
\end{aligned}$$

since $\Lambda \le 1$, $\kappa \le \mu$ and $\eta \le \sqrt{2}$ due to (4.13). Notice that $\rho \le \frac{1}{2}$, then

$$\sum_{k=0}^{n}\rho^k = \frac{1-\rho^{n+1}}{1-\rho} \le 2(1-\rho^{n+1}).$$

Therefore by assuming ρ such that $4\mu^2(\sqrt{\mu N} + \gamma\rho + \sqrt{2})\sqrt{\rho} \le \gamma$,

$$\|G'(\xi_{n+1})^{-1} - B_{n+1}^{-1}\| \le 4\mu^2(\sqrt{\mu N} + \gamma\rho + \sqrt{2})\rho^{3/2}(1-\rho^{n+1}) \le \gamma\rho(1-\rho^{n+1}).$$

This concludes the proof of Claim 4(iv).

Now we prove the induction step for Claim 4(v).

$$\|B_{n+1}^{-1}\| \le \gamma\rho + \|G'(\xi_{n+1})^{-1}\| \le \gamma\rho + \mu.$$

Define $\beta \ge \gamma\rho + \mu$, then $\|B_{n+1}^{-1}\| \le \beta$, which is Claim 4(v).

Finally, we prove Claim 4(vi). By using definition,

$$\|t_{n+1}\| = \|-B_{n+1}^{-1}G(\xi_{n+1})\| \le \|B_{n+1}^{-1}\|\|G(\xi_{n+1})\| \le \beta\zeta\ \rho^{n+3},$$

assume $\beta\zeta \le 1$, then $\|t_{n+1}\| \le \rho^{n+3}$, establishing Claim 4(vi).

Therefore by using mathematical induction we have the results. A consequence of Claim 4(vi) is that $\{\xi_n\}$ is a Cauchy sequence lying in $B_\rho(\xi_0)$. Given $p, q \ge 0$,

$$\|\xi_p - \xi_{p+q}\| \le \sum_{k=p}^{p+q-1} \|\xi_{k+1} - \xi_k\| \le \sum_{k=p}^{p+q-1} \rho^{k+2} < \rho^2 \sum_{k=p}^{\infty} \rho^k = \frac{\rho^{p+2}}{1-\rho} \le \rho^{p+1}.$$

Therefore $\{\xi_n\}$ converges to a point $\xi^* \in \overline{B_\rho(\xi_0)}$. By using the fact that G is a continuous function and $\|G(\xi_n)\| \le \zeta\rho^{n+2}$, it follows that $G(\xi^*) = 0$, which implies $F(x^*) = 0$, where $x^* = F'(x_0)^{-\frac{1}{2}}\xi^*$. By taking $q \to \infty$ and $p = n$ in the above calculation, $\|\xi_n - \xi^*\| \le \rho^{n+1}$. Let $e_n = x_n - x^*$ and $\sigma_n = \xi_n - \xi^*$, then

$$\|\sigma_n\| \le \rho^{n+1}, \qquad \|e_n\| \le r^{n+1}.$$

Notice that $\xi^* \in \overline{B_\rho(\xi_0)}$ and $x^* \in \overline{B_r(x_0)}$.

For proof of uniqueness, let $\hat{\xi}$ be any zero of G in $\overline{B_\rho(\xi_0)}$ corresponding to a root $\hat{x}$ of F in $\overline{B_r(x_0)}$. Below we show that $\|\hat{\sigma}_{n+1}\| \le \|\hat{\sigma}_n\|/2$ for $n \ge 0$, where $\hat{\sigma}_n = \xi_n - \hat{\xi}$. Notice that:

$$\begin{aligned}
\hat{\sigma}_{n+1} &= \xi_{n+1} - \hat{\xi} = \xi_n + t_n - \hat{\xi} = \xi_n - B_n^{-1}G(\xi_n) - \hat{\xi} \\
&= B_n^{-1}B_n\,\hat{\sigma}_n + B_n^{-1}\big(-G(\xi_n) + G(\hat{\xi})\,\big) \\
&= B_n^{-1}\big(B_n - G'(\xi_n)\,\big)\,\hat{\sigma}_n + B_n^{-1}\,\big(-G(\xi_n) + G(\hat{\xi}) + G'(\xi_n)\hat{\sigma}_n\big).
\end{aligned}$$

By (4.4),

$$\begin{aligned}
\|\hat{\sigma}_{n+1}\| &= \Big\| B_n^{-1}\,\Big(-G(\xi_n) + G(\hat{\xi}) + G'(\xi_n)\hat{\sigma}_n + (B_n - G'(\xi_n))\hat{\sigma}_n\Big)\Big\| \\
&\le \|B_n^{-1}\|\;\|\hat{\sigma}_n\|\;\Big(\frac{\eta\|\hat{\sigma}_n\|}{2\sqrt{\rho}} + \|B_n - G'(\xi_n)\|\Big).
\end{aligned}$$

Since $\hat{\xi}$, $\xi_n \in \overline{B_\rho(\xi_0)}$ then $\|\hat{\sigma}_n\| \le 2\rho$, then by using above inequality, we have

$$\|\hat{\sigma}_{n+1}\| \le \beta\;\|\hat{\sigma}_n\|\;\Big(\frac{\eta\|\hat{\sigma}_n\|}{2\sqrt{\rho}} + \alpha\rho\Big) \le \beta\;(\eta\sqrt{\rho} + \alpha\rho)\;\|\hat{\sigma}_n\| \le \beta(\eta + \alpha\sqrt{\rho})\|\,\hat{\sigma}_n\| \le \frac{1}{2}\|\,\hat{\sigma}_n\|,$$

if we assume $\beta(\eta + \alpha\sqrt{\rho}) \le \frac{1}{2}$. Therefore $\|\xi_n - \hat{\xi}\| \le \frac{1}{2^n}$ and

$$\|\hat{\xi} - \xi^*\| \le \|\hat{\xi} - \xi_n\| + \|\xi_n - \xi^*\| \le \frac{1}{2^n} + \rho^{n+1}.$$

Let $n \to \infty$ to obtain the uniqueness result. Let

$$\sqrt{\rho} < \frac{\eta}{96\sqrt{2}(\sqrt{N}+1)}, \qquad \eta < \min\left\{\frac{\sqrt{2}\,m^2}{M^2}, \frac{1}{6}\right\}.$$

with the former inequality equivalent to

$$r < \frac{\eta^2}{18432(\sqrt{N}+1)^2 m}. \tag{4.20}$$

Finally, it is enough to define the constants as

$$\mu = \frac{1}{1 - \eta\sqrt{\rho}}, \tag{4.21}$$

$$\gamma = 24\sqrt{2}(\sqrt{N}+1)\sqrt{\rho}, \tag{4.22}$$

$$\beta = \gamma\rho + \mu = 24\sqrt{2}(\sqrt{N}+1)\rho\sqrt{\rho} + \mu, \tag{4.23}$$

$$\zeta = \frac{1}{2\beta} = \frac{1}{2(\gamma\rho + \mu)}, \tag{4.24}$$

$$\alpha = 4\gamma = 96\sqrt{2}(\sqrt{N}+1)\sqrt{\rho}, \tag{4.25}$$

$$a = \frac{m^2}{2(\gamma\rho + \mu)}. \tag{4.26}$$

The calculations for finding the constants are given in Section 4.1. This completes proof of the theorem. □

In classical proofs of global convergence of this method, the minimum is assumed to exist and a fixed, so-called, BFGS norm can be used to estimate the difference between the approximate and exact Jacobians for all iterates. In our setting, in the proof of Claim 4(iv), the minimum is not known a priori, hence requiring a norm which changes with each iteration. We believe that this technique is applicable in more general contexts.

Example 4.1. While Theorem 4.1 assumes uniform convexity of f, it does not follow that the iterates converge to a minimum x^* where $F(x^*) = 0$ without further assumptions. Consider the simple example $N = 1$, $\Omega = (0.1, 1)$ and $f(x) = x^2/2$. Clearly f has no critical point in Ω. Take, for instance, $x_0 = 0.2$. Then for any $r < 0.1$, (4.1) becomes $0.2 < ar^2$, which cannot be satisfied for a defined by (4.26). Again, we do not claim that this value of a is optimal. In this example, at least one assumption of the theorem is violated because the minimum is not attained in Ω.

Next, consider the uniformly convex function $f(x) = x^2/2 - x^4/12$ defined on $\Omega = (-.94, .94)$ with minimum $x^* = 0$. For any $x_0 \in \Omega$, $A_0 = 1 - x_0^2$ and we can take $m = 0.1$, $M = 1$, $\rho = 0.1r$ and $\eta = 0.01$, leading to

$$\mu = \frac{1}{1 - 0.01\sqrt{0.1r}}, \qquad \gamma = 48\sqrt{0.2r}, \qquad a = \frac{0.01}{2(0.1\gamma r + \mu)}.$$

Inequality (4.1) becomes

$$\left| \frac{x_0 - x_0^3/3}{\sqrt{1 - x_0^2}} \right| \le ar^2,$$

which restricts x_0 to be close to the exact solution. Provided (4.1) and (4.2) hold, the latter being not restrictive in light of (4.1), the theorem correctly states that the BFGS iterates converge to the unique minimum superlinearly. Note that without (4.1), an iterate may venture outside of Ω. For instance, take $x_0 = 0.9$, then A_0 is close to zero causing the next iterate to be outside of the domain:

$$x_1 = x_0 - \frac{F(x_0)}{A_0} = 0.9 - \frac{0.9 - 0.9^3/3}{1 - 0.9^2} = -2.5579\ldots \notin \Omega.$$

We remark that in assumption (4.2), we assumed $r^{-1/2}$ dependence on the right-hand side. Initially, we assumed r^{-1} dependence as in the theorem for Broyden's method, but were unable assign values to constants (similar to (4.21) to (4.26)) so that all required inequalities are satisfied.

Below is a result on the superlinear convergence of the BFGS algorithm with Kantorovich-type assumptions.

Theorem 4.2. *Assume the hypotheses of Theorem 4.1. Then the BFGS iteration converges superlinearly to a unique zero of F in $\overline{B_r(x_0)}$.*

Proof. By Theorem 4.1, the iterates $\{\xi_n\}$ defined by BFGS method for $G(\xi) = F'(x_0)^{-\frac{1}{2}} F(F'(x_0)^{-\frac{1}{2}}\xi)$ converge to ξ^*, unique zero of G in $\overline{B_\rho(\xi_0)}$, where $\rho = mr$. Consequently $\{x_n\}$ converges to $x^* = F'(x_0)^{-\frac{1}{2}}\xi^*$, the unique zero of F in $\overline{B_r(x_0)}$. Assume that $G(\xi_n) \neq 0$ for all $n \geq 0$. So $\xi_n \neq \xi^*$. Also we have:

$$\begin{aligned}
&\|G'(\xi_n) - B_n\| \le \alpha\rho, \quad \|G'(\xi_n)^{-1} - B_n^{-1}\| \le \gamma\rho(1-\rho^n), \quad \|G'(\xi_n)^{-1}\| \le \mu, \\
&\|B_n^{-1}\| \le \beta, \qquad\qquad\quad \|G(\xi_n)\| \le \zeta\rho^{n+2}, \qquad \|t_n\| \le \rho^{n+2}, \qquad \|\sigma_n\| \le \rho^{n+1}.
\end{aligned}$$

where $\sigma_n = \xi_n - \xi^*$, and the positive constants $\alpha, \beta, \gamma, \mu$ and ζ are given by Eqs. (4.21) to (4.26). Using exactly the same technique as in the previous theorem to show $\|\hat{\sigma}_{n+1}\| \le \|\hat{\sigma}_n\|/2$, we could prove that $\|\sigma_{n+1}\| \le \|\sigma_n\|/2$. The rest of the proof follows almost exactly as in [4] and is omitted here, but can be found in [11]. □

4.1. Appendix

This appendix provides some of the elementary calculations for finding the constants in the proof of Theorem 4.1, omitting all the details which can be found in [11]. The required relations among the constants could be summarized as:

1. $\rho = mr \le \frac{1}{2}$ and $m \le 1$,
2. $\eta < \min\left\{\frac{\sqrt{2}m^2}{M^2}, \frac{1}{6}\right\}$,
3. $a \le m^2\zeta$,
4. $\mu = \frac{1}{1 - \eta\sqrt{\rho}}$,
5. $4\mu^2(\sqrt{\mu N} + \gamma\rho + \sqrt{2})\sqrt{\rho} \le \gamma$,
6. $\hat{\gamma} = \mu\eta + \gamma\sqrt{\rho}$ and $\hat{\gamma}\sqrt{\rho} < 1$,
7. $\frac{\mu\gamma}{1 - \hat{\gamma}\sqrt{\rho}} \le \alpha$,
8. $\beta \ge \max\{\gamma\rho + \mu, 1\}$,
9. $\beta\zeta \le 1$,
10. $\eta + \alpha \le \zeta \le 1$,
11. $\beta(\eta + \alpha) \le \frac{1}{2}$.

By assuming the value of the constants $\mu, \gamma, \beta, \zeta, \alpha$ and a as defined in (4.21) to (4.26), we need to show that Conditions 1 to 11 could be fulfilled if

$$\sqrt{\rho} < \frac{\eta}{96\sqrt{2}\,(\sqrt{N}+1)}, \quad \text{and} \quad \eta < \min\left\{\frac{\sqrt{2}\,m^2}{M^2}, \frac{1}{6}\right\} < \min\left\{\frac{\sqrt{2}\,m^2}{M^2}, \frac{1}{5+\sqrt{\rho}}\right\}.$$

Notice that by the last assumption,

$$\eta < \frac{1}{5+\sqrt{\rho}} < 1, \tag{4.27}$$

and also

$$\sqrt{\rho} < \frac{\eta}{96\sqrt{2}\,(\sqrt{N}+1)} < \frac{1}{8} < \frac{1-\sqrt{2/3}}{\eta}. \tag{4.28}$$

Therefore

$$(1-\eta\sqrt{\rho})^2 - 4\rho\sqrt{\rho} > (1-\eta\sqrt{\rho})^2 - \frac{1}{2} > \frac{2}{3} - \frac{1}{2} = \frac{1}{6}.$$

Use this and definition of γ given by (4.22).

$$\gamma = 24\sqrt{2}\,(\sqrt{N}+1)\sqrt{\rho} \geq 24(\sqrt{\mu N}+\sqrt{2})\sqrt{\rho} \geq \frac{4(\sqrt{\mu N}+\sqrt{2})\sqrt{\rho}}{(1-\eta\sqrt{\rho})^2 - 4\rho\sqrt{\rho}},$$

since by assumption (4.28), we have $\mu \leq 2$. Thus Condition 5 is satisfied. By definition of β and ζ given by (4.23) and (4.24), Conditions 8 and 9 are satisfied trivially. Observe that (4.28) implies that

$$\gamma = 24\sqrt{2}\,(\sqrt{N}+1)\sqrt{\rho} < \frac{\eta}{4}. \tag{4.29}$$

Moreover,

$$\begin{aligned}
\gamma\rho < \frac{\eta\rho}{4} < \frac{\eta\sqrt{\rho}}{4} \leq \frac{\sqrt{\rho}}{20} &= \eta\sqrt{\rho}\,\frac{1}{20\,\eta} \\
&\leq \eta\sqrt{\rho}\,\Big(\frac{1}{4\eta} - \frac{1}{1-\eta\sqrt{\rho}}\Big) \qquad (4.30)\\
&\leq \frac{1}{2} - \frac{\eta\sqrt{\rho}}{1-\eta\sqrt{\rho}}. \qquad (4.31)
\end{aligned}$$

In last two lines we applied (4.27) and (4.28). Since $\eta\sqrt{\rho} \leq 1$, from (4.30),

$$\gamma\rho < \frac{1}{4\eta} - \frac{1}{1-\eta\sqrt{\rho}},$$

which results in $\zeta - \eta > \eta$ and therefore by using (4.29)

$$\alpha = 4\gamma < \eta < \zeta - \eta.$$

So Conditions 10 and 11 are satisfied. Also from (4.31)

$$\gamma\rho < \frac{1}{2} - \frac{\eta\sqrt{\rho}}{1-\eta\sqrt{\rho}},$$

which results in $1 - \hat{\gamma}\sqrt{\rho} > \frac{1}{2}$, and

$$\frac{\mu\gamma}{1-\hat{\gamma}\sqrt{\rho}} < 2\mu\gamma \leq 4\gamma = \alpha.$$

Thus Conditions 6 and 7 hold. Finally by using relations between constants and definition of a in (4.26), Condition 3 is satisfied.

5. Conclusion

In the first part of this paper, we gave a superlinear convergence theory for the solution of a system of nonlinear equations by the basic Broyden's method assuming Kantorovich-type assumptions, i.e., all assumptions are about the initial iterate and its neighbourhood. The main point is that the assumptions can be verified in practice, and the existence of a root and the convergence rate are consequences of the theory. In the second part, we gave a superlinear convergence theory for the minimizer of a uniformly convex function by the basic BFGS algorithm employing Kantorovich-type assumptions. Both our theories are simple in the sense that they contain as few constants as possible.

Our theory is a local theory. Extension to a global theory is possible if line search is incorporated into the algorithms. This is certainly a worthy future work.

As a continuation of this paper, [12] has shown superlinear convergence of a class of nonlinear conjugate gradient methods and a class of scaled memoryless BFGS algorithms using Kantorovich-type assumptions. There are many other directions for further research. For instance, the Jacobian matrix for a nonlinear system or the Hessian in the case of unconstrained minimization may be sparse or may have a special structure. [13] has a convergence theory for quasi-Newton methods which maintains the sparsity or special structure. A similar result using Kantorovich-type assumptions would be desirable. Another possible future work is to relax the condition that the Jacobian matrix about the initial point is non-singular, or the condition that the Hessian of the objective function is positive definite. See [14] for some early work in this direction. Next, two convergence theories for functions which are not smooth can be found in [15] and [16]. It would be desirable to extend these results for the case of Kantorovich-type assumptions. Smale gives an amazing convergence of Newton's iteration where all assumptions are at the initial iterate—no assumption is necessary in a neighbourhood about the initial iterate. See Chapter 8 in [17]. This theory has been extended to a secant method in [18]. It appears to be an open problem whether this theory carries over to Broyden's method and BFGS algorithm.

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