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PII: S0377-0427(18)30053-0
DOI: https://doi.org/10.1016/j.cam.2018.01.024
Reference: CAM 11496

To appear in: *Journal of Computational and Applied Mathematics*

Received date : 28 September 2017
Revised date : 16 January 2018

Please cite this article as: I.K. Argyros, J.A. Ezquerro, M.A. Hernández-Verón, Á.A. Magreñán, Extending the domain of starting points for Newton's method under conditions on the second derivative, *Journal of Computational and Applied Mathematics* (2018), https://doi.org/10.1016/j.cam.2018.01.024

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Extending the domain of starting points for Newton's method under conditions on the second derivative

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Abstract

In this paper, we propose a center Lipschitz condition for the second Fréchet derivative together with the use of restricted domains in order to improve the domain of starting points for Newton's method. In addition, we compare the new result with an older one and see that the former improves the latter.

Keywords: Newton's method, restricted domain, majorizing sequence, semilocal convergence, error estimates, integral equation.
2000 Mathematics Subject Classification: 47H99, 65H10, 65J15.

This work has been partially supported by the project MTM2014-52016-C2-1-P of Spanish Ministry of Economy and Competitiveness and the International University of La Rioja, under the Plan Propio de Investigación, Desarrollo e Innovación (2015–2017, research group: Modelación matemática aplicada a la ingeniería (MOMAIN) and the grant SENECA 19374/PI/14.

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1 Introduction

In this paper, we are concerned with finding a solution of a nonlinear equation $F(x) = 0$, where F is a nonlinear operator defined on a nonempty open convex subset Ω of a Banach space X with values in a Banach space Y. The solutions of this kind of equations are rarely found in closed form. That is why most solutions of these equations are approximated by iterative methods. Between these, Newton's method,

$$x_0 \in \Omega, \qquad x_{n+1} = x_n - [F'(x_n)]^{-1}F(x_n), \quad n \geq 0, \tag{1}$$

is the most well-known, used and studied iterative method in order to approximate solutions of the nonlinear equation $F(x) = 0$.

In this paper, we study the semilocal convergence of this method. The first semilocal convergence result for Newton's method in Banach spaces was given by Kantorovich [8] under the following conditions:

(A1) There exists $\Gamma_0 = [F'(x_0)]^{-1} \in \mathcal{L}(Y, X)$, for some $x_0 \in \Omega$, with $\|\Gamma_0\| \leq \beta$ and $\|\Gamma_0 F(x_0)\| \leq \eta$, where $\mathcal{L}(Y, X)$ is the set of bounded linear operators from Y to X.

(A2) $\|F''(x)\| \leq M$ for $x \in \Omega$.

(A3) $h = M\beta\eta \leq \frac{1}{2}$.

Theorem 1. *(The Newton-Kantorovich theorem, [8]) Let $F : \Omega \subseteq X \longrightarrow Y$ be a twice continuously Fréchet differentiable operator defined on a non-empty open convex domain Ω of a Banach space X with values in a Banach space Y. Suppose that conditions (A1)–(A3) are satisfied. If $B(x_0, s^*) \subset \Omega$, where $s^* = \frac{1-\sqrt{1-2h}}{h}\eta$, then Newton's sequence, given by (1) and starting at x_0, converges to a solution x^* of the equation $F(x) = 0$ and $x_n, x^* \in \overline{B(x_0, s^*)}$, for all $n \in \mathbb{N}$.*

As you can see in Theorem 1, the Newton-Kantorovich theorem, we use information around the initial point x_0, (A1), a condition on the operator involved F, (A2), and a condition for the parameters introduced in the previous two conditions to give criteria ensuring the convergence, (A3). A very important problem in the study of iterative methods is to locate starting points x_0 such that the sequence $\{x_n\}$ is convergent. The set of this starting points is that we call the convergence domain, which is small in general, so that it is important to enlarge the convergence domain without additional hypotheses. Notice that the convergence domain of the method is connected with the domain of parameters associated with the semilocal convergence conditions required to obtain the convergence of the method. In this case, for each value of M that is fixed by condition (A2), the condition required to the operator F in the domain of definition Ω, the domain of parameters associated with conditions (A1)–(A3) is:

$$D_K(M) = \left\{ x_0 \in \Omega : M\beta\eta \leq \frac{1}{2} \right\}. \tag{2}$$

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On the other hand, Huang proposes in [6] an alternative to condition (A2) that does not consist of relaxing the condition on the operator F and imposes a condition on F that leads to a modification, not a restriction, of the the convergence domain. In particular, Huang proposes that F'' is Lipschitz continuous in Ω and proves the semilocal convergence of Newton's method can be proved under the following conditions:

(B1) There exists $\Gamma_0 = [F'(x_0)]^{-1} \in \mathcal{L}(Y, X)$, for some $x_0 \in \Omega$, with $\|\Gamma_0\| \leq \beta$ and $\|\Gamma_0 F(x_0)\| \leq \eta$; moreover, $\|F''(x_0)\| \leq M_0$.

(B2) $\|F''(x) - F''(y)\| \leq L\|x - y\|$ for $x, y \in \Omega$.

(B3) $3\beta^2\eta L^2 + 3\beta^2 M_0 L + \beta^3 M_0^3 \leq (\beta^2 M_0^2 + 2\beta L)^{\frac{3}{2}}$.

In this case, for each value of L that is fixed by condition (B2), the domain of parameters associated with conditions (B1)–(B3) is:

$$D_H(L) = \left\{x_0 \in \Omega : 3\beta^2\eta L^2 + 3\beta^2 M_0 L + \beta^3 M_0^3 \leq \left(\beta^2 M_0^2 + 2\beta L\right)^{\frac{3}{2}}\right\} \tag{3}$$

But, if we pay attention to the proof of Huang in [6], we see that it is not necessary that $F''(x)$ is Lipschitz continuous in the entire domain Ω, since it is enough that $F''(x)$ is Lipschitz continuous only at x_0. This observation was made by Gutiérrez in [5], where (B2) is replaced by

$$\|F''(x) - F''(x_0)\| \leq L_0\|x - x_0\| \quad \text{for} \quad x \in \Omega,$$

which is a center condition at the starting point x_0. Taking into account this, Gutiérrez obtains a semilocal convergence result for Newton's method under the following conditions:

(B1) There exists $\Gamma_0 = [F'(x_0)]^{-1} \in \mathcal{L}(Y, X)$, for some $x_0 \in \Omega$, with $\|\Gamma_0\| \leq \beta$ and $\|\Gamma_0 F(x_0)\| \leq \eta$; moreover, $\|F''(x_0)\| \leq M_0$.

(C2) $\|F''(x) - F''(x_0)\| \leq L_0\|x - x_0\|$ for $x \in \Omega$.

(C3) $3\beta^2\eta L_0^2 + 3\beta^2 M_0 L_0 + \beta^3 M_0^3 \leq (\beta^2 M_0^2 + 2\beta L_0)^{\frac{3}{2}}$.

Notice that $L_0 \leq L$, so that Huang's result is relaxed by Gutiérrez in [5] by using condition (C2) instead of (B2). In this case, for each value of L_0 that is fixed by condition (C2), the domain of parameters associated with conditions (B1), (C2) and (C3) is:

$$D_G(L_0) = \left\{x_0 \in \Omega : 3\beta^2\eta L_0^2 + 3\beta^2 M_0 L_0 + \beta^3 M_0^3 \leq \left(\beta^2 M_0^2 + 2\beta L_0\right)^{\frac{3}{2}}\right\} \tag{4}$$

Notice that, in this situation, from condition (C2), the convergence domain for Newton's method consists of a single point, x_0, or it is an empty set, and Newton's method is then never convergent. Observe that condition (C3) is (B3) with L_0 instead of L.

To avoid this problem that presents the last condition, we use in this paper a center condition for the second Fréchet derivative of the operator F involved on an auxiliary point $\widetilde{x}$ in the following way:

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(D2) $\|F''(x) - F''(\widetilde{x})\| \leq \widetilde{L}\|x - \widetilde{x}\|$ for $x \in \Omega$,

once the point $\widetilde{x} \in \Omega$ is fixed. So, we obtain a convergence domain which is not reduced to a point or to the empty set, since a nonempty set of possible starting points can be found.

In this work, following the idea of extending the domain of starting points, we try to reduce the value of parameter $\widetilde{L}$ to obtain then a bigger convergence domain. For this, our idea is to restrict the domain Ω by means of considering condition (D2) for $x \in \Omega_0$ with $\Omega_0 \subset \Omega$. Moreover, as condition on the starting point x_0, we keep a condition centered at x_0, which allows us to sharpen the bounds to do and relax then condition (B3).

The paper is organized as follows. In Section 2, we establish the semilocal convergence of Newton's method using condition (D2) and the method of majorizing sequences of Kantorovich. In addition, we see that the result obtained improves that given in [4], which is the base of the new result. In Section 3, we give some a priori error bounds that lead to the quadratic convergence of Newton's method under the semilocal convergence conditions proposed in this work.

Throughout the paper, we denote $\overline{B(x,\varrho)} = \{y \in X; \|y - x\| \leq \varrho\}$ and $B(x,\varrho) = \{y \in X; \|y - x\| < \varrho\}$.

2 Semilocal convergence result

To prove the semilocal convergence of Newton's method, we follow Kantorovich's technique and use the concept of majorizing sequence. A scalar sequence $\{t_n\}$ is a majorizing sequence of $\{x_n\}$ if $\|x_n - x_{n-1}\| \leq t_n - t_{n-1}$, for all $n \in \mathbb{N}$. From the last inequality, it follows the sequence $\{t_n\}$ is nondecreasing. Moreover, it is easy to check that if $\{t_n\}$ converges to $t^* < +\infty$, there exists $x^* \in X$ such that $x^* = \lim_n x_n$ and $\|x^* - x_n\| \leq t^* - t_n$, for $n = 0, 1, 2, \ldots$ Then, the interest of the majorizing sequence is that the convergence of the sequence $\{x_n\}$ in the Banach space X is deduced from the convergence of the scalar sequence $\{t_n\}$. From the concept of majorizing sequence, Kantorovich proves the Newton-Kantorovich theorem given in Theorem 1.

For the last, a majorizing sequence is constructed from conditions (A1)–(A2) of the Newton-Kantorovich theorem, by applying Newton's method,

$$s_0 = 0, \qquad s_{n+1} = N_p(s_n) = s_n - \frac{p(s_n)}{p'(s_n)}, \quad n \geq 0,$$

to Kantorovich's polynomial

$$p(s) = \frac{M}{2}s^2 - \frac{s}{\beta} + \frac{\eta}{\beta}. \tag{5}$$

Note that (5) has two positive solutions $s^* = \frac{1-\sqrt{1-2h}}{h}\eta$ and $s^{**} = \frac{1+\sqrt{1-2h}}{h}\eta$ such that $s^* \leq s^{**}$ if $h = M\beta\eta \leq \frac{1}{2}$. Moreover, we consider $p(s)$ in some interval $[0, s']$ taking into account that $s^* \leq s^{**} < s'$.

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2.1 Main result

Now, we present a semilocal convergence result for Newton's method under a center condition of type (D2) with restricted domain by using the technique of majorizing sequences, such as it appears in [1]. For this, we suppose the following conditions:

(E1) There exists $\widetilde{x} \in \Omega$ such that $\|x_0 - \widetilde{x}\| = \gamma$, where $x_0 \in \Omega$, and $\|F''(\widetilde{x})\| \leq \delta$. There exists the operator $\Gamma_0 = [F'(x_0)]^{-1} \in \mathcal{L}(Y, X)$, with $\|\Gamma_0\| \leq \beta$ and $\|\Gamma_0 F(x_0)\| \leq \eta$. Moreover, there exists $K_0 \geqslant 0$, such that $\|F'(x) - F'(x_0)\| \leq K_0\|x - x_0\|$ for $x \in \Omega$.

(E2) $\|F''(x) - F''(\widetilde{x})\| \leq \widetilde{L}_1\|x - \widetilde{x}\|$ for $x \in \Omega_0 := \Omega \cap B\left(x_0, \frac{1}{\beta K_0}\right)$.

(E3) Define the scalar function ψ_1 by

$$\psi_1(t) = \frac{\widetilde{L}_1}{6}t^3 + \frac{\delta_0}{2}t^2 - \frac{t}{\beta} + \frac{\eta}{\beta}, \tag{6}$$

where $\delta_0 = \max\{\delta + \gamma\widetilde{L}_1, K_0\}$. There exists α_1, unique positive root of $\psi_1'(t) = 0$ with $\psi_1(\alpha_1) \leq 0$.

Next, we construct a majorizing sequence from conditions (E1)–(E3) by applying Newton's method

$$t_0 = 0, \qquad t_{n+1} = N_{\psi_1}(t_n) = t_n - \frac{\psi_1(t_n)}{\psi_1'(t_n)}, \quad n \geq 0, \tag{7}$$

Note that (6) has two positive zeros t^* and t^{**} such that $t^* \leq t^{**}$ if $\psi_1(\alpha_1) \leq 0$, where α_1 is the unique positive root of $\psi_1'(t) = 0$. Moreover, we consider $\psi_1(t)$ in some interval $[0, t']$ taking into account that $t^* \leq t^{**} < t'$.

Theorem 2. *Let $F : \Omega \subseteq X \longrightarrow Y$ be a twice continuously Fréchet differentiable operator defined on a nonempty open convex domain Ω of a Banach space X with values in a Banach space Y. Suppose that conditions (E1)–(E3) are satisfied and $B(x_0, t^*) \subset \Omega$, where t^* is the smallest positive zero of polynomial (6). Then, Newton's sequence, defined in (1) and starting at x_0, converges to a solution x^* of the equation $F(x) = 0$ and $x_n, x^* \in \overline{B(x_0, t^*)}$, for all $n \in \mathbb{N}$. In addition, $\|x^* - x_n\| \leq t^* - t_n$ for $n \geq 0$, where $\{t_n\}$ is defined in (7). Moreover, the solution x^* is unique in $B(x_0, t^{**}) \cap \Omega$ if $t^* < t^{**}$ or in $\overline{B(x_0, t^*)}$ if $t^{**} = t^*$.*

Proof. From $2\delta_0 < \delta_0 + \sqrt{\delta_0 + \dfrac{2\widetilde{L}_1}{\beta}}$, it follows $2K_0 < \delta_0 + \sqrt{\delta_0 + \dfrac{2\widetilde{L}_1}{\beta}}$ and

$$\alpha_1 = \frac{2}{\beta\left(\delta_0 + \sqrt{\delta_0 + \frac{2\widetilde{L}_1}{\beta}}\right)} < \frac{1}{\beta K_0}.$$

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So, $B(x_0, t^*) \subseteq B\left(x_0, \frac{1}{\beta K_0}\right)$, since $t^* \leq \alpha_1$.

The point x_1 is well-defined, since the operator $\Gamma_0 = [F'(x_0)]^{-1}$ exists by condition (E1). Moreover, taking into account $t_0 = 0$ and (E1), we also have

$$\|x_1 - x_0\| = \|\Gamma_0 F(x_0)\| \leq \eta = -\frac{\psi_1(0)}{\psi_1'(0)} = -\frac{\psi_1(t_0)}{\psi_1'(t_0)} = t_1 - t_0 < t^*$$

and $x_1 \in B(x_0, t^*) \subseteq B\left(x_0, \frac{1}{\beta K_0}\right)$, so that $x_1 \in \Omega_0$.

Let $x \in \Omega$ satisfy $\|x - x_0\| \leq t \leq t^*$. It follows from (E1), (E2), (6) and the definition of δ_0 that

$$\begin{aligned}
\|I - \Gamma_0 F'(x)\| &\leq \|\Gamma_0\| \|F'(x) - F'(x_0)\| \\
&\leq \beta K_0 \|x - x_0\| \\
&\leq \beta K_0 t \\
&\leq \beta \delta_0 t + \frac{\beta \widetilde{L}_1}{2} t^2 \\
&= -\frac{1}{\psi_1'(t_0)} (\psi_1'(t) - \psi_1'(t_0)) \\
&= 1 - \frac{\psi_1'(t)}{\psi_1'(t_0)} \\
&< 1,
\end{aligned}$$

By the Banach lemma on invertible operators, the operator $[F'(x)]^{-1}$ exists and

$$\|[F'(x)]^{-1}\| \leq -\frac{1}{\psi_1'(t)}. \tag{8}$$

In particular, $\Gamma_1 = [F'(x_1)]^{-1}$ exists and therefore x_2 is well-defined.

Besides, from

$$\begin{aligned}
F(x_1) &= F(x_0) + F'(x_0)(x_1 - x_0) + \int_{x_0}^{x_1} F''(z)(x_1 - z)\, dz \\
&= \int_0^1 \left(F''(x_0 + \tau(x_1 - x_0)) - F''(\widetilde{x})\right)(x_1 - x_0)^2 (1 - \tau)\, d\tau \\
&\quad + \frac{1}{2} F''(\widetilde{x})(x_1 - x_0)^2,
\end{aligned}$$

(E1), (E3), (6) and $\|x_1 - x_0\| \leq t_1 - t_0$, it follows

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$$
\begin{aligned}
\|F(x_1)\| &\leq \int_0^1 \|F''(x_0+\tau(x_1-x_0)) - F''(\widetilde{x})\| \,(1-\tau)\, d\tau \|x_1-x_0\|^2 \\
&\quad + \frac{1}{2}\|F''(\widetilde{x})\| \, \|x_1-x_0\|^2 \\
&\leq \int_0^1 \psi_1''(t_0+\tau(t_1-t_0))(t_1-t_0)^2(1-\tau)\, d\tau \\
&= \int_{t_0}^{t_1} \psi_1''(\xi)(t_1-\xi)\, d\xi \\
&= \psi_1(t_1).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\|x_2-x_1\| = \|\Gamma_1 F(x_1)\| \leq \|\Gamma_1\|\|F(x_1)\| \leq -\frac{\psi_1(t_1)}{\psi_1'(t_1)} = t_2-t_1, \\
&\|x_2-x_0\| \leq \|x_2-x_1\| + \|x_1-x_0\| \leq (t_2-t_1)+(t_1-t_0) = t_2-t_0 < t^*
\end{aligned}
$$

and $x_2 \in B(x_0,t^*) \subseteq B(x_0, \frac{1}{\beta K_0})$, so that $x_2 \in \Omega_0$.

As with the previous estimate for inverse operator (8), for $x = x_2$, and again by the Banach lemma on invertible operators, the operator $\Gamma_2 = [F'(x_2)]^{-1}$ exists and is such that

$$
\|\Gamma_2\| \leq -\frac{1}{\psi_1'(t_2)}.
$$

If we now assume

$$
x_n \in \Omega_0, \tag{9}
$$

$$
\|\Gamma_n\| \leq -\frac{1}{\psi_1'(t_n)}, \tag{10}
$$

$$
\|F(x_n)\| \leq \psi_1(t_n), \tag{11}
$$

$$
\|x_{n+1}-x_n\| \leq -\frac{\psi_1(t_n)}{\psi_1'(t_n)} = t_{n+1}-t_n, \tag{12}
$$

$$
\|x_{n+1}-x_0\| \leq t_{n+1}-t_0 < t^*, \tag{13}
$$

where the operator $\Gamma_n = [F'(x_n)]^{-1}$ exists, it follows in the same way that the operator $\Gamma_{n+1} = [F'(x_{n+1})]^{-1}$ exists and

$$
\begin{aligned}
x_{n+1} &\in \Omega_0, \\
\|\Gamma_{n+1}\| &\leq -\frac{1}{\psi_1'(t_{n+1})}, \\
\|F(x_{n+1})\| &\leq \psi_1(t_{n+1}), \\
\|x_{n+2}-x_{n+1}\| &\leq -\frac{\psi_1(t_{n+1})}{\psi_1'(t_{n+1})} = t_{n+2}-t_{n+1}, \\
\|x_{n+2}-x_0\| &\leq \|x_{n+2}-x_{n+1}\| + \|x_{n+1}-x_0\| \leq t_{n+2}-t_0 < t^*,
\end{aligned}
$$

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so that (9), (10), (11), (12) and (13) are true for all positive integers n by mathematical induction. As a consequence, the sequence $\{x_n\}$ is well-defined and $x_n \in B(x_0, t^*)$, for $n \geq 0$.

Since $\lim_n t_n = t^*$, $\{t_n\}$ is a Cauchy sequence, then $\{x_n\}$ is also a Cauchy sequence and thus convergent. So, $\lim_n x_n = x^*$ and $\|x^* - x_n\| \leq t^* - t_n$, for $n \geq 0$. Moreover, as $\|F(x_n)\| \leq \psi_1(t_n)$, for $n \geq 0$, then, by letting $n \to +\infty$, it follows $F(x^*) = 0$ by the continuities of F and ψ_1.

To prove the uniqueness of x^*, we suppose that $t^* < t^{**}$ and y^* is a solution of $F(x) = 0$ in $B(x_0, t^{**}) \cap \Omega$ different from x^*. Then, taking into account that $t_0 = 0$, we have

$$\|y^* - x_0\| \leq \rho(t^{**} - t_0) \quad \text{with} \quad \rho \in (0, 1).$$

We now suppose $\|y^* - x_i\| \leq \rho^{2^i}(t^{**} - t_i)$ for $i = 0, 1, \ldots, n$. In addition,

$$\begin{aligned}
\|y^* - x_{n+1}\| &= \|-\Gamma_n \left(F(y^*) - F(x_n) - F'(x_n)(y^* - x_n)\right)\| \\
&= \left\|-\Gamma_n \int_0^1 F''(x_n + \tau(y^* - x_n))(y^* - x_n)^2 (1-\tau)\, d\tau\right\| \\
&= \left\|-\Gamma_n \int_0^1 \left(F''(x_n + \tau(y^* - x_n)) - F''(\widetilde{x})\right)(y^* - x_n)^2 (1-\tau)\, d\tau\right. \\
&\quad \left. + \frac{1}{2} F''(\widetilde{x})(y^* - x_n)^2\right\| \\
&\leq \|\Gamma_n\| \int_0^1 \|F''(x_n + \tau(y^* - x_n)) - F''(\widetilde{x})\|(1-\tau)\, d\tau \|y^* - x_n\|^2 \\
&\quad + \frac{1}{2}\|F''(\widetilde{x})\|\|y^* - x_n\|^2 \\
&\leq -\frac{\mu}{\psi_1'(t_n)}\|y^* - x_n\|^2,
\end{aligned}$$

where $\mu = \int_0^1 \psi_1''\left(t_n + \tau(t^{**} - t_n)\right)(1-\tau)\, d\tau$.

On the other hand, we also have

$$t^{**} - t_{n+1} = -\frac{1}{\psi_1'(t_n)} \int_{t_n}^{t^{**}} \psi_1''(\xi)(t^{**} - \xi)\, d\xi = -\frac{\mu}{\psi_1'(t_n)}(t^{**} - t_n)^2.$$

Therefore, it follows

$$\|y^* - x_{n+1}\| \leq \frac{t^{**} - t_{n+1}}{(t^{**} - t_n)^2}\|y^* - x_n\|^2 \leq \rho^{2^{n+1}}(t^{**} - t_{n+1}),$$

so that $y^* = x^*$.

If $t^{**} = t^*$ and y^* is another solution of $F(x) = 0$, different from x^*, in $\overline{B(x_0, t^{**})}$, then $\|y^* - x_0\| \leq t^* - t_0 = t^*$. Proceeding similarly to the previous case, we can prove by mathematical induction on n that $\|y^* - x_n\| \leq t^{**} - t_n$. Since $t^{**} = t^*$ and $\lim_n t_n = t^*$, the uniqueness of the solution is now easy to follow. ■

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2.2 On the convergence domain

Following to Huang [6] and Gutiérrez [5], a sufficient condition to satisfy (E3) is:

$$3\beta^2\eta\widetilde{L}_1^2 + 3\beta^2\delta_0\widetilde{L}_1 + \beta^3\delta_0^3 \leq \left(\beta^2\delta_0^2 + 2\beta\widetilde{L}_1\right)^{\frac{3}{2}}.$$

As a consequence, we obtain the following domain of parameters

$$D(\widetilde{L}_1) = \left\{x_0 \in \Omega : 3\beta^2\eta\widetilde{L}_1^2 + 3\beta^2\delta_0\widetilde{L}_1 + \beta^3\delta_0^3 \leq \left(\beta^2\delta_0^2 + 2\beta\widetilde{L}_1\right)^{\frac{3}{2}}\right\} \tag{14}$$

associated with Theorem 2. In this case, once parameter $\widetilde{L}_1$ is fixed, it is obvious that we can find different starting points for Newton's method, such as we can see in the following example. So, by keeping a condition centered on the second derivative of the operator involved, we obtain that the convergenc domain is not reduced to a single point, or the empty set, as in the case of Gutiérrez in [5]. Observe that we obtain Gutiérrez's result as a particular case of our result if the auxiliary point $\widetilde{x}$ is chosen as the starting point x_0.

2.3 Example

We illustrate Section 2.1 with the following nonlinear Fredholm integral equation

$$x(s) = \frac{1}{2}\sin(\pi s) + \int_0^1 \cos(\pi s)\sin(\pi t)x(t)^5\,dt, \tag{15}$$

where $s \in [0, 1]$ and $x(s)$ is a solution to be determined.

Observe that solving equation (15) is equivalent to solving $\mathcal{F}(x) = 0$, where $\mathcal{F} : \Omega \subseteq \mathcal{C}([0, 1]) \longrightarrow \mathcal{C}([0, 1])$ is such that

$$[\mathcal{F}(x)](s) = x(s) - \frac{1}{2}\sin(\pi s) - \int_0^1 \cos(\pi s)\sin(\pi t)x(t)^5\,dt.$$

In addition, a solution $x^*(s)$ of equation (15) always satisfies

$$\|x^*(s)\| - \frac{1}{2}\|\sin(\pi s)\| - \frac{2}{\pi}\|x^*(s)\|^5 \leq 0,$$

which is true provided that $\|x^*(s)\| \leq \rho_1 = 0.5255\ldots$ or $\|x^*(s)\| \geq \rho_2 = 0.9203\ldots$, where ρ_1 and ρ_2 are the two real positive roots of the scalar equation deduced from the last expression and given by $\frac{2}{\pi}t^5 - t + \frac{1}{2} = 0$. Thus, we can consider the domain

$$\Omega = \{x \in \mathcal{C}([0, 1]) :\ \|x\| < \rho\},$$

with $\rho \in (\rho_1, \rho_2)$, as domain for the operator $\mathcal{F}$.

Besides, as

$$[\mathcal{F}'(x)y](s) = y(s) - 5\int_0^1 \cos(\pi s)\sin(\pi t)x(t)^4 y(t)\,dt,$$

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$$[\mathcal{F}''(x)(yz)](s) = -20\int_0^1 \cos(\pi s)\sin(\pi t)x(t)^3 z(t)y(t)\,dt,$$

we have

$$\|\mathcal{F}'(x) - \mathcal{F}'(x_0)\| \leq \frac{10}{\pi}\left(\sum_{i=0}^{3}\rho^i\|x_0\|^{3-i}\right)\|x - x_0\|,$$

$$\|\mathcal{F}''(x) - \mathcal{F}''(\widetilde{x})\| \leq \frac{40}{\pi}\left(\sum_{i=0}^{2}\rho^i\|\widetilde{x}\|^{2-i}\right)\|x - \widetilde{x}\|,$$

so that $\mathcal{F}'(x)$ is center Lipschitz continuous at x_0 with constant $K_0 = \frac{10}{\pi}\left(\sum_{i=0}^{3}\rho^i\|x_0\|^{3-i}\right)$ and $\mathcal{F}''(x)$ is center Lipschitz continuous at $\widetilde{x}$ with constant $\widetilde{L}_1 = \frac{40}{\pi}\left(\sum_{i=0}^{2}\rho^i\|\widetilde{x}\|^{2-i}\right)$ and we can then apply Theorem 2 for guaranteeing the convergence of the method.

Hence, if we consider, as it is usually done, the starting point $x_0(s) = \frac{1}{2}\sin(\pi s)$ for Newton's method, then $\beta = 1.1061\ldots$, $\eta = 0.0108\ldots$. If we now choose $\rho = 3/5$ and $\widetilde{x}(s) = x_0(s)$, then $\gamma = 0$, $\delta_0 = \frac{15}{16}$,

$$\psi_1(t) = (0.0097\ldots) - (0.9040\ldots)t + (0.4687\ldots)t^2 + (1.9310\ldots)t^3,$$

$\alpha_1 = 0.3223\ldots$, $\psi_1(\alpha_1) = -0.1682\ldots < 0$ and $B(x_0, s^*) \subset \Omega$, where $s^* = 0.0108\ldots$ is the smallest positive zero of $\psi_1(t)$. Therefore, the convergence of Newton's method is guaranteed by Theorem 2 and taking into account the point $\widetilde{x}(s)$, where $\mathcal{F}''(x)$ is center Lipschitz continuous, as starting point for the method.

In addition, we can also guarantee the convergence of Newton's method starting at other points different from the point $\widetilde{x}(s)$ where $\mathcal{F}''(x)$ is center Lipschitz continuous, so that the domain of starting points is then increased when center conditions are required. For example, if we choose the starting point $x_0(s) = \frac{9}{20}\sin(\pi s)$, then $\gamma = \|\widetilde{x}(s) - x_0(s)\| = \frac{1}{20}$, $\beta = 1.0696\ldots$, $\eta = 0.0061\ldots$, $\delta_0 = 1.5168\ldots$,

$$\psi_1(t) = (0.0057\ldots) - (0.9349\ldots)t + (0.7584\ldots)t^2 + (1.9310\ldots)t^3,$$

$\alpha_1 = 0.2916\ldots$, $\psi_1(\alpha_1) = -0.1544\ldots < 0$ and $B(x_0, t^*) \subset \Omega$, where $t^* = 0.0061\ldots$ is the smallest positive zero of the last $\psi_1(t)$. Thus, the convergence of Newton's method can be also guaranteed when the method starts at $x_0(s) \neq \widetilde{x}(s)$. Moreover, the domains of existence and uniqueness of solution are respectively

$$\{\nu \in \Omega : \|\nu(s) - x_0(s)\| \leq 0.0061\ldots\} \quad \text{and} \quad \{\nu \in \Omega : \|\nu(s) - x_0(s)\| < 0.5226\ldots\}.$$

After that, we apply Newton's method from $x_0(s) = \frac{9}{20}\sin(\pi s)$ to approximate a solution $x^*(s)$ of integral equation (15) and obtain the approximation

$$x^*(s) = (0.0097\ldots)\cos\pi s + \frac{1}{2}\sin\pi s$$

after three iterations with stopping criterion $\|x_n(s) - x_{n-1}(s)\| < 10^{-16}$. In Table 1, we show errors $\|x^*(s) - x_n(s)\|$ and sequence $\{\|[\mathcal{F}(x_n)](s)\|\}$. From the last, observe that $x^*(s)$ is a good approximation of a solution of equation (15).

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n	$\|x^*(s) - x_n(s)\|$	$\|[\mathcal{F}(x_n)](s)\|$
1	$8.0297\ldots \times 10^{-4}$	$8.0179\ldots \times 10^{-4}$
2	$5.0494\ldots \times 10^{-8}$	$5.0417\ldots \times 10^{-8}$

Table 1: Absolute errors and $\{\|[\mathcal{F}(x_n)](s)\|\}$ for (15)

2.4 Remark

Note that Theorem 2 is reduced to the theorem given in [4] if the center condition for the first Fréchet derivative on the starting point is dropped, since $\delta_0 = \delta + \gamma \widetilde{L}_1$ and $\widetilde{L}_1 = \widetilde{L}$. In [4], condition (D2) is used instead of (E2), the center condition for the first Fréchet derivative of F on the starting point x_0 given in (E1),

$$\|F'(x) - F'(x_0)\| \leq K_0\|x - x_0\| \quad \text{for} \quad x \in \Omega,$$

is dropped and polynomial

$$\psi(t) = \frac{\widetilde{L}}{6}t^3 + \frac{1}{2}\left(\delta + \gamma\widetilde{L}\right)t^2 - \frac{t}{\beta} + \frac{\eta}{\beta}$$

is used instead of $\psi_1(t)$. Observe then that

$$\widetilde{L}_1 \leq \widetilde{L}$$

holds in general, since $\Omega_0 \subseteq \Omega$. Moreover, the iterates $\{x_n\}$ lie within Ω_0, which is a more precise location than Ω. Furthermore,

$$\alpha_1 = \frac{2}{\beta\left(\delta_0 + \sqrt{\delta_0^2 + \dfrac{2\widetilde{L}_1}{\beta}}\right)}$$

and the smallest positive root of $\psi'(t) = 0$ is

$$\alpha = \frac{2}{\beta\left(\delta + \gamma\widetilde{L} + \sqrt{\left(\delta + \gamma\widetilde{L}\right)^2 + \dfrac{2\widetilde{L}}{\beta}}\right)}.$$

In addition, if

$$\delta_0 \leq \delta + \gamma\widetilde{L},$$

then

$$\alpha \leq \alpha_1, \qquad \psi_1(t) \leq \psi(t)$$

and

$$\psi(\alpha) \leq 0 \qquad \Rightarrow \qquad \psi_1(\alpha_1) \leq 0.$$

Hence, we obtain weaker sufficient semilocal convergence conditions than in [4] for the semilocal convergence of Newton's method.

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2.5 Example

Now, we illustrate the idea written in the previous remark on the following chemical equilibrium problem from [10], that describes the fraction of the nitrogen-hydrogen feed that gets converted to ammonia, called fractional conversion [2]. For 250 atm and 500°C, this equation takes the form:

$$f(x) = x^4 - 7.79075x^3 + 14.7445x^2 + 2.511x - 1.674 = 0. \tag{16}$$

If we choose $x_0 = 0.5$ and $\Omega = B(x_0, 0.75)$, then $\beta = 0.0839\ldots$ and $\eta = 0.1978\ldots$ Moreover, if $\widetilde{x} = 0.31$, then $\gamma = 0.19$, $\delta = 16.1514\ldots$ and $\widetilde{L} = 46.0245\ldots$, so that

$$\psi(t) = (2.3562\ldots) - (11.9124\ldots)t + (12.4480\ldots)t^2 + (7.6707\ldots)t^3,$$

$\alpha = 0.3592\ldots$, $\psi(\alpha) = 0.0389\ldots > 0$ and, as a consequence, the main condition of Theorem given in [4] is not satisfied and we cannot then guarantee the semilocal convergence of Newton's method from that work. However, we can do it if we apply the present work, as we can see below.

Indeed, for the last values, we also obtain $K_0 = 24.3959\ldots$, so that the restricted domain $\Omega_0 = \Omega \cap B(x_0, \frac{1}{\beta K_0}) = (0.0117\ldots, 0.9882\ldots)$ allows us to guarantee the semilocal convergence of Newton's method from Theorem 2, since $\widetilde{L}_1 = 42.8841\ldots$, $\delta_0 = K_0$,

$$\psi_1(t) = (2.3562\ldots) - (11.9124\ldots)t + (12.1979\ldots)t^2 + (7.1473\ldots)t^3,$$

$\alpha_1 = 0.3687\ldots$, $\psi_1(\alpha_1) = -0.0194\ldots < 0$ and $B(x_0, t^*) \subset \Omega$, where $t^* = 0.3375\ldots$ is the smallest positive zero of $\psi_1(t)$. In addition, the domains of existence and uniqueness of solution are respectively

$$\{s \in \Omega : |s - x_0| \leq 0.3375\ldots\} \quad \text{and} \quad \{s \in \Omega : |s - x_0| < 0.3996\ldots\}.$$

Finally, we apply Newton's method from $x_0 = 0.5$ and approximate the solution $x^* = 0.2777\ldots$, which is the only solution physically meaningful, since, by definition, the fractional conversion is a number between 0 and 1. In Table 2, we show errors $|x^* - x_n|$ and sequence $\{|f(x_n)|\}$. From the last, observe that x^* is a good approximation of a solution of equation (16).

3 A priori error bounds and quadratic convergence of Newton's method

Finally, from the following theorem which provides some a priori error estimates for Newton's method, we deduce the quadratic convergence of the method under conditions (E1)–(E3). The proof of the theorem follows from Ostrowski's technique [9] and is analogous to that given in [3].

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n	$\lvert x^* - x_n \rvert$	$\lvert f(x_n) \rvert$
1	$2.4440\ldots \times 10^{-2}$	$2.2469\ldots \times 10^{-1}$
2	$5.3328\ldots \times 10^{-4}$	$4.7937\ldots \times 10^{-3}$
3	$2.7537\ldots \times 10^{-7}$	$2.4740\ldots \times 10^{-6}$
4	$7.3561\ldots \times 10^{-14}$	$6.6090\ldots \times 10^{-13}$
5	$5.2494\ldots \times 10^{-27}$	$4.7162\ldots \times 10^{-26}$
6	$2.6731\ldots \times 10^{-53}$	$2.4016\ldots \times 10^{-52}$

Table 2: Absolute errors and $\{\lvert f(x_n)\rvert\}$ for (16)

Notice first that if $\psi_1(t)$ has two real zeros t^* and t^{**} such that $0 < t^* \leq t^{**}$, we can then write

$$\psi_1(t) = \left(\frac{\widetilde{L}_1}{6}t + \varepsilon\right)(t^* - t)(t^{**} - t)$$

with $t^* \neq \dfrac{6\epsilon}{\widetilde{L}_1}$ and $t^{**} \neq \dfrac{6\epsilon}{\widetilde{L}_1}$.

Theorem 3. *Suppose that conditions (E1)–(E3) are satisfied and $\psi_1(\alpha_1) \leq 0$, where α_1 is a positive root of $\psi_1'(t) = 0$ and ψ_1 is given in (6).*

(a) *If $t^* < t^{**}$ and $t^* > \frac{6\varepsilon}{\widetilde{L}_1}$, then*

$$\frac{(t^{**} - t^*)\theta^{2^n}}{P - \theta^{2^n}} \leq t^* - t_n \leq \frac{(t^{**} - t^*)\Delta^{2^n}}{Q - \Delta^{2^n}}, \quad n \geq 0,$$

where $\theta = \frac{t^*}{t^{**}}P$, $\Delta = \frac{t^*}{t^{**}}Q$, $P = \frac{\widetilde{L}_1 t^{**} - 6\varepsilon}{\widetilde{L}_1 t^* + 6\varepsilon}$, $Q = \frac{\widetilde{L}_1(2t^* - t^{**}) + 6\varepsilon}{\widetilde{L}_1 t^* + 6\varepsilon}$ and provided that $\theta < 1$ and $\Delta < 1$.

(b) *If $t^* = t^{**}$ and $t^* > \frac{12\varepsilon}{\widetilde{L}_1}$, then*

$$\left(\frac{\widetilde{L}_1 t^* - 6\varepsilon}{\widetilde{L}_1 t^* - 12\varepsilon}\right)^n t^* \leq t^* - t_n \leq \frac{t^*}{2^n}, \quad n \geq 0.$$

Proof. Let $t^* < t^{**}$ and denote $a_n = t^* - t_n$ and $b_n = t^{**} - t_n$ for all $n \geq 0$. Then

$$\psi_1(t_n) = \frac{1}{6}\left(\widetilde{L}_1 t_n + 6\varepsilon\right) a_n b_n, \quad \psi_1'(t_n) = \frac{\widetilde{L}_1}{6}\, a_n b_n - \frac{1}{6}\left(\widetilde{L}_1 t_n + 6\varepsilon\right)(a_n + b_n)$$

and

$$a_{n+1} = t^* - t_{n+1} = t^* - t_n + \frac{\psi_1(t_n)}{\psi_1'(t_n)} = \frac{a_n^2\left(\widetilde{L}_1 b_n - 6\varepsilon - \widetilde{L}_1 t_n\right)}{\widetilde{L}_1\, a_n b_n - \left(\widetilde{L}_1 t_n + 6\varepsilon\right)(a_n + b_n)}.$$

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From $\dfrac{a_{n+1}}{b_{n+1}} = \dfrac{a_n^2\left(\widetilde{L}_1\,b_n - \left(\widetilde{L}_1 t_n + 6\varepsilon\right)\right)}{b_n^2\left(\widetilde{L}_1\,a_n - \left(\widetilde{L}_1 t_n + 6\varepsilon\right)\right)}$ and taking into account function $d(t) = \frac{\widetilde{L}_1 t^{**} - 6\varepsilon - 2\widetilde{L}_1 t}{\widetilde{L}_1 t^{*} - 6\varepsilon - 2\widetilde{L}_1 t}$, $P \le \min\{d(t); t \in [0, t^*]\} = d(0)$ and $Q = \max\{d(t); t \in [0, t^*]\} = d(t^*)$ it follows

$$P\left(\frac{a_n}{b_n}\right)^2 \le \frac{a_{n+1}}{b_{n+1}} \le Q\left(\frac{a_n}{b_n}\right)^2.$$

In addition,

$$\frac{a_{n+1}}{b_{n+1}} \le Q^{2^{n+1}-1}\left(\frac{a_0}{b_0}\right)^{2^{n+1}} = \frac{\Delta^{2^{n+1}}}{Q} \qquad \text{and} \qquad \frac{a_{n+1}}{b_{n+1}} \ge P^{2^{n+1}-1}\left(\frac{a_0}{b_0}\right)^{2^{n+1}} = \frac{\theta^{2^{n+1}}}{P}.$$

Taking then into account that $b_{n+1} = (t^{**} - t^*) + a_{n+1}$, it follows:

$$\frac{(t^{**} - t^*)\theta^{2^{n+1}}}{P - \theta^{2^{n+1}}} \le t^* - t_{n+1} \le \frac{(t^{**} - t^*)\Delta^{2^{n+1}}}{Q - \Delta^{2^{n+1}}}.$$

If $t^* = t^{**}$, then $a_n = b_n$ and

$$a_{n+1} = \frac{a_n\left(\widetilde{L}_1\,a_n - \left(\widetilde{L}_1 t_n + 6\varepsilon\right)\right)}{\widetilde{L}_1\,a_n - 2\left(\widetilde{L}_1 t_n + 6\varepsilon\right)}.$$

As a consequence, $\left(\frac{\widetilde{L}_1 t^* - 6\varepsilon}{\widetilde{L}_1 t^* - 12\varepsilon}\right) a_n \le a_{n+1} \le \frac{a_n}{2}$ and

$$\left(\frac{\widetilde{L}_1 t^* - 6\varepsilon}{\widetilde{L}_1 t^* - 12\varepsilon}\right)^{n+1} t^* \le t^* - t_{n+1} \le \frac{t^*}{2^{n+1}}.$$

The proof is complete. ■

From the last theorem, it follows that the convergence of Newton's method is quadratic if $t^* < t^{**}$ and linear if $t^* = t^{**}$.

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