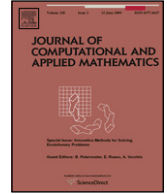




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An extension of Gander's result for quadratic equations

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ABSTRACT

In the study of iterative methods with high order of convergence, Gander provides a general expression for iterative methods with order of convergence at least three in the scalar case. Taking into account an extension of this result, we define a family of iterations in Banach spaces with R -order of convergence at least four for quadratic equations.

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1. Introduction

Gander writes in [1] that solving a nonlinear equation is a problem that has occupied mathematicians for many centuries. At the moment this could be generalized to every researcher who studies scientific and engineering problems. It is well known that there are physical, chemical and engineering problems that employ numerical methods to approximate a solution of a nonlinear equation [2–5]. In [1] Gander provides an algebraic technique to obtain the iteration of Halley's method and other third order iterative methods in the scalar case. In this paper, Section 2, we extend the technique developed by Gander to obtain a family of iterations with order of convergence at least four when they are applied to solve quadratic equations.

In Section 3, the iterations given in Section 2 are generalized to Banach spaces in order to consider more general problems than scalar quadratic equations and prove the semilocal convergence of them by using majorant sequences [6]. Besides, we provide domains of existence and uniqueness of solutions and give some a priori error estimates, which are obtained from a similar technique to the one developed in [7] and used later by other authors [8,9].

The study of quadratic equations is interesting, since there are problems which can be expressed by means of them. For example, equations which appears in the theory of dynamics of gases [10] and equations related with Chandrasekhar's work [11], which arise in the theories of radiative transfer, neutron transport and the kinetic theory of gases. An extensive literature exists on equations of this type, see [12] and the references therein. To finish, two applications are presented, where known quadratic equations are considered: an equation of molecular interaction [10] and an integral equation of

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Chandrasekhar type [11]. For the integral equation, as a consequence of the high operational cost when the second derivative is used, we use a modification of one of the methods considered previously, which has the same order of convergence and less operational cost.

2. A family of iterations with order of convergence at least four for quadratic equations

We consider a real function $f \in C^{(6)}[a, b]$, such that f has a simple zero $s \in (a, b)$, and the following iterative methods

$$\begin{cases} x_0 \in [a, b] \text{ given,} \\ x_{n+1} = G(x_n) = x_n - H(L_f(x_n)) \frac{f(x_n)}{f'(x_n)}, \quad n \geq 0, \end{cases} \tag{1}$$

where $L_f(x) = f(x)f''(x)/f'(x)^2$ is the degree of logarithmic convexity [13] and H is an analytic real function defined in a real domain D such that $\text{Im}(L_f) \subseteq D$. It is well known that method (1) has order of convergence at least four if the zero s satisfies $s = G(s)$, $G'(s) = G''(s) = G'''(s) = 0$ and $G^{(4)}(s) \neq 0$ [14]. Following Gander, we impose these conditions to (1) for obtaining an expression for the function H . From the conditions $s = G(s)$ and $G'(s) = G''(s) = 0$, it follows that $H(0) = 1$ and $H'(0) = 1/2$, so that (1) has order of convergence at least three.

Moreover, if f is a quadratic function, then $f''(x) = C \in \mathbb{R}$, $f^{(n)}(x) = 0$, for all $n \geq 3$, $n \in \mathbb{N}$, and it is easy to prove that:

$$\begin{aligned} L'_f(x) &= \frac{f''(x)}{f'(x)} (1 - 2L_f(x)), \\ L''_f(x) &= -3 \frac{f''(x)^2}{f'(x)^2} (1 - 2L_f(x)). \end{aligned}$$

In this case,

$$G'''(s) = 3 (H'(0) - H''(0)) L'_f(s)^2 + (H(0) - 3H'(0)) L''_f(s),$$

so that $G'''(s) = 0$ if and only if $H''(0) = 1/2$. If we now consider the analytic real function H , which appears in (1), defined by

$$H(L_f(x)) = 1 + \frac{1}{2}L_f(x) + \frac{1}{2}L_f(x)^2 + \sum_{k \geq 3} A_k L_f(x)^k, \quad A_k \in \mathbb{R}, \quad k \geq 3 \quad (k \in \mathbb{N}), \tag{2}$$

where $\{A_k\}_{k \geq 3}$ is a positive non-increasing real sequence, iterations (1) have order of convergence at least four when they are applied to solve quadratic equations.

Notice that (1) is reduced to the Super-Halley method [15,16]:

$$x_{n+1} = x_n - \left(1 + \frac{L_f(x_n)}{2(1 - L_f(x_n))} \right) \frac{f(x_n)}{f'(x_n)}, \quad n \geq 0, \tag{3}$$

if $A_0 = 1$ and $A_k = 1/2$, for all $k \in \mathbb{N}$, in (2). And (1) is reduced to the following Chebyshev-like method [17,18]:

$$x_{n+1} = x_n - \left(1 + \frac{1}{2}L_f(x_n) + \frac{1}{2}L_f(x_n)^2 \right) \frac{f(x_n)}{f'(x_n)}, \quad n \geq 0, \tag{4}$$

if $A_0 = 1$, $A_1 = A_2 = 1/2$ and $A_k = 0$, for all $k \geq 3$ ($k \in \mathbb{N}$), in (2).

3. Semilocal convergence in Banach spaces

Since the main goal of the paper is to solve more general quadratic equations than the scalar ones by means of iterations (1), we generalize the previous situation to Banach spaces. To do this, we now consider the problem of approximating a locally unique solution x^* of the nonlinear equation

$$F(x) = 0, \tag{5}$$

where $F : \Omega \subseteq X \rightarrow Y$ is a quadratic operator defined on a non-empty open convex subset Ω of a Banach space X with values in a Banach space Y . From the result given in [1] and the expressions of well-known one-point iterative methods of R -order of convergence [19] at least three, we consider in Banach spaces the family of iterations:

$$\begin{cases} x_{n+1} = G(x_n) = x_n - H(L_F(x_n)) \Gamma_n F(x_n), \quad n \geq 0, \\ H(L_F(x_n)) = \sum_{k \geq 0} A_k L_F(x_n)^k, \end{cases} \tag{6}$$

where $\Gamma_n = [F'(x_n)]^{-1}$, $L_F(x) = 0$, $A_0 = 1$, $A_1 = A_2 = 1/2$ and $\{A_k\}_{k \geq 0}$ is a positive non-increasing real sequence such that $\sum_{k \geq 0} A_k t^k < +\infty$ for $|t| < r$. Note that $L_F(x) \in \mathcal{L}(\Omega)$ is known as the operator “degree of logarithmic convexity” [13], where $\mathcal{L}(\Omega)$ is the set of bounded linear operators from Ω into Ω . If $L_F(x_n)$ exists and $\|L_F(x_n)\| < r$, then (6) is well defined [20]. We assume that the operator $H : \mathcal{L}(\Omega) \rightarrow \mathcal{L}(\Omega)$ is analytical in a neighborhood of zero and the Taylor series

has a special form. Family of iterations (6) is well defined if the operator H exists. This operator, defined in (6), is such that

$$H(L_F(_)) : \Omega \xrightarrow{L_F} \mathcal{L}(\Omega) \xrightarrow{H} \mathcal{L}(\Omega),$$

where $H(L_F(x_n)) = \sum_{k \geq 0} A_k L_F(x_n)^k$ and $L_F(x)^k$ is a linear operator in Ω , which denotes the composition of the operator $L_F(x)$ k times.

Notice that iterations (6) with $A_0 = 1$ and $A_1 = 1/2$ have R -order of convergence at least three, see [21].

One of the more used techniques in Banach spaces to prove the convergence of a sequence $\{x_n\}$, given by an iterative method, is based on majorant real sequences:

$$\|x_{n+1} - x_n\| \leq t_{n+1} - t_n, \quad n \geq 0,$$

where $\{t_n\}$ is a non-negative real increasing sequence [6]. The interesting feature of this technique is that the convergence of the majorant real sequence $\{t_n\}$ implies the convergence of $\{x_n\}$. In fact, if $\{t_n\}$ converges to t^* , there exists x^* such that $\{x_n\}$ converges to x^* and

$$\|x^* - x_n\| \leq t^* - t_n, \quad n \geq 0.$$

Moreover, from the last inequality, we can obtain error estimates for the sequence $\{x_n\}$ in terms of the sequence $\{t_n\}$.

The presented results provide sufficient conditions in order to define the sequence given in (6), guarantee its semilocal convergence to x^* and provide error estimates at each step. Moreover, domains of existence and uniqueness of solutions are also given.

To prove the semilocal convergence and establish the R -order of converge of iterations (6) in Banach spaces, we assume the following:

(C1) there exists a point $x_0 \in \Omega$ where the operator $\Gamma_0 \in \mathcal{L}(Y, \Omega)$ is defined and such that $\|\Gamma_0 F(x_0)\| \leq \eta$,

(C2) $\|\Gamma_0 F''(x)\| \leq \alpha$, for all $x \in \Omega$,

(C3) $\beta = \alpha\eta < \min\{1/2, r\}$, where r is the radius of convergence of the power series $\sum_{k \geq 0} A_k t^k$,

(C4) $B(x_0, t^*) = \{x \in X; \|x - x_0\| \leq t^*\} \subseteq \Omega$, where $t^* = \frac{1 - \sqrt{1 - 2\beta}}{\beta} \eta$.

Note that $\|F''(x)\| = M \in \mathbb{R}$, for all $x \in \Omega$, since F is a quadratic operator.

Next, we prove that the sequence given in (6) is well defined and converges to a solution x^* of Eq. (5). Firstly, we have

$$\|L_F(x_0)\| \leq \|\Gamma_0 F''(x_0)\| \|\Gamma_0 F(x_0)\| \leq \beta,$$

so that $H(L_F(x_0))$ is well defined, since $x_0 \in \Omega$ and $\Gamma_0 F(x_0) \in \Omega$. Now taking into account that the real sequence $\{A_k\}_{k \geq 0}$ is non-increasing, it follows that

$$\|x_1 - x_0\| \leq \left(\sum_{k \geq 0} A_k \beta^k \right) \eta < \left(1 + \frac{\beta}{2(1 - \beta)} \right) \eta < t^*.$$

Therefore, $x_1 \in B(x_0, t^*) \subset \Omega$.

A simple form of finding a majorant sequence $\{t_n\}$ is to consider the sequence obtained when iterations (6) are applied to the scalar quadratic equation $p(t) = 0$, where

$$p(t) = \frac{\alpha}{2} t^2 - t + \eta \tag{7}$$

is a polynomial which satisfies conditions (C1)–(C2) for $t_0 = 0$, see [6]. In this case, the majorant real sequence is

$$\begin{cases} t_{n+1} = P(t_n) = t_n - h(L_p(t_n)) \frac{p(t_n)}{p'(t_n)}, & n \geq 0, \\ h(L_p(t_n)) = \sum_{k \geq 0} A_k L_p(t_n)^k, \end{cases} \tag{8}$$

where $\{A_k\}_{k \geq 0}$ is the sequence defined previously. It is easy to prove that (8), starting at $t_0 = 0$, is an increasing sequence and converges to the smallest root t^* of $p(t) = 0$. From

$$t_1 - t_0 = -h(L_p(t_0)) \frac{p(t_0)}{p'(t_0)} = \left(\sum_{k \geq 0} A_k \beta^k \right) \eta,$$

it follows that $\|x_1 - x_0\| \leq t_1 - t_0$.

To prove that (6) is well defined and convergent, we take into account the following decompositions of the operator F and polynomial p , which are obtained from their corresponding Taylor's series.

Lemma 3.1. *We suppose that conditions (C1)–(C4) are satisfied. Then,*

$$F(x_{n+1}) = \frac{1}{2} F''(x_n) \Gamma_n F(x_n) \left(\sum_{k \geq 3} 2(A_{k-1} - A_k) L_F(x_n)^{k-1} \right) \Gamma_n F(x_n) + \frac{1}{8} F''(x_n) \left(L_F(x_n) \tilde{H}(L_F(x_n)) \Gamma_n F(x_n) \right)^2,$$

where $\tilde{H}(z) = I + \sum_{k \geq 2} 2A_k z^{k-1}$. \square

Lemma 3.2. Let p be polynomial (7). Then,

$$p(t_{n+1}) = \frac{1}{2}p(t_n) \sum_{k \geq 3} 2(A_{k-1} - A_k)L_p(t_n)^k + \frac{1}{8}p(t_n)L_p(t_n)^3 \tilde{h}(L_p(t_n))^2,$$

where $\tilde{h}(t) = 1 + \sum_{k \geq 2} 2A_k t^{k-1}$. \square

We next observe that, for all $x \in B(x_0, t^*)$, we have

$$\begin{aligned} \|I - \Gamma_0 F'(x)\| &\leq \|\Gamma_0 [F'(x_0) - F'(x)]\| \leq \int_{x_0}^x \|\Gamma_0 F''(z)\| dz \leq \alpha \|x - x_0\| \\ &< \alpha t^* = 1 - \sqrt{1 - 2\beta} < 1, \end{aligned}$$

and by the Banach lemma [6], the inverse operator of $\Gamma_0 F'(x)$ exists and

$$\|[\Gamma_0 F'(x)]^{-1}\| \leq \frac{1}{1 - \|I - \Gamma_0 F'(x)\|} < \frac{1}{1 - \alpha t^*}.$$

From Lemmas 3.1 and 3.2 and using norms, it follows that

$$\begin{aligned} \|\Gamma_0 F(x_1)\| &\leq \|L_F(x_0)\| \|\Gamma_0 F(x_0)\| \left\| \sum_{k \geq 3} 2(A_{k-1} - A_k)L_F(x_0)^{k-1} \right\| \\ &\quad + \frac{1}{8} \|\Gamma_0 F''(x_0)\| \|L_F(x_0)\|^2 \|\tilde{H}(L_F(x_0))\|^2 \|\Gamma_0 F(x_0)\|^2 \\ &\leq \eta \left(\sum_{k \geq 3} (A_{k-1} - A_k)\beta^k + \frac{\beta}{2} \left(\sum_{k \geq 1} A_k \beta^k \right)^2 \right) = -\frac{p(t_1)}{p'(t_0)}, \end{aligned}$$

and consequently,

$$\|\Gamma_1 F(x_1)\| = \|\Gamma_1 F'(x_0)\Gamma_0 F(x_1)\| \leq -\frac{p(t_1)}{p'(t_1)}.$$

Moreover,

$$\begin{aligned} \|L_F(x_1)\| &\leq \frac{\alpha}{1 - \alpha t_1} \left(-\frac{p(t_1)}{p'(t_1)} \right) = L_p(t_1) < r, \\ \|\tilde{H}(L_F(x_1))\| &\leq 1 + \sum_{k \geq 2} 2A_k L_p(t_1)^{k-1} = \tilde{h}(L_p(t_1)), \end{aligned}$$

x_2 is well defined and

$$\|x_2 - x_1\| \leq \left(1 + \frac{1}{2}L_p(t_1)\tilde{h}(L_p(t_1)) \right) \left(-\frac{p(t_1)}{p'(t_1)} \right) = t_2 - t_1.$$

Furthermore,

$$\|x_2 - x_0\| \leq \|x_2 - x_1\| + \|x_1 - x_0\| \leq t_2 - t_1 + t_1 - t_0 = t_2 - t_0 < t^*$$

and $x_2 \in B(x_0, t^*) \subset \Omega$.

Then invoke the induction hypothesis and see that Γ_n exists, $\|\Gamma_n F(x_n)\| \leq -p(t_n)/p'(t_n)$ and $\|\Gamma_n F''(x_n)\| \leq -p''(t_n)/p'(t_n)$, for all $x_n \in B(x_0, t^*)$. In consequence,

$$\|L_F(x_n)\| \leq L_p(t_n) < r.$$

Following the same procedure as above, we prove that x_{n+1} ,

$$x_{n+1} = x_n - \left(I + \frac{1}{2}L_F(x_n)\tilde{H}(L_F(x_n)) \right) \Gamma_n F(x_n),$$

is well defined, since x_n and $\Gamma_n F(x_n)$ belong to Ω and $\tilde{H}(L_F(x_n))$ is well defined.

Besides,

$$\begin{aligned} \|\tilde{H}(L_F(x_n))\| &\leq 1 + \sum_{k \geq 2} 2A_k L_p(t_n)^{k-1} = \tilde{h}(L_p(t_n)), \\ \|x_{n+1} - x_n\| &\leq \left(1 + \frac{1}{2}L_p(t_n)\tilde{h}(L_p(t_n)) \right) \left(-\frac{p(t_n)}{p'(t_n)} \right) = t_{n+1} - t_n, \end{aligned}$$

$$\|x_{n+1} - x_0\| \leq \|x_{n+1} - x_n\| + \|x_n - x_0\| \leq t_{n+1} - t_n + t_n - t_0 = t_{n+1} - t_0 < t^*.$$

So, $x_{n+1} \in B(x_0, t^*) \subset \Omega$ and $\{x_n\}$ is majorized by $\{t_n\}$.

In consequence,

$$\|x_{n+m} - x_n\| \leq t_{n+m} - t_n, \quad n, m \in \mathbb{N}, \tag{9}$$

and $\{x_n\}$ is then a Cauchy sequence. Therefore, $\{x_n\}$ is convergent and $\lim_{n \rightarrow +\infty} x_n = l$. Now, since $\|F(x_n)\| \leq p(t_n)$, we obtain

$$\lim_{n \rightarrow +\infty} \|F(x_n)\| \leq \lim_{n \rightarrow +\infty} p(t_n) = p(t^*) = 0.$$

Consequently, $\lim_{n \rightarrow +\infty} F(x_n) = 0$ and, from the continuity of the operator F , $l = x^*$, where x^* is a solution of Eq. (5). Moreover, if $m \rightarrow \infty$ and take $n = 0$ in (9), we have $\|x^* - x_0\| < t^*$ and $x^* \in B(x_0, t^*)$.

On the other hand, we prove the uniqueness of the solution x^* in $B(x_0, t^{**}) \cap \Omega$, where t^{**} is the biggest root of the polynomial (7). To do this, we suppose that y^* is another solution of (5) in $B(x_0, s) \cap \Omega$. From

$$0 = \Gamma_0[F(y^*) - F(x^*)] = \left[\int_0^1 \Gamma_0 F'(x^* + t(y^* - x^*)) dt \right] (y^* - x^*) = T(y^* - x^*),$$

it suffices to prove that the operator T is invertible, and consequently, $x^* = y^*$. So,

$$\begin{aligned} \|I - T\| &\leq \int_0^1 \|\Gamma_0 (F'(x^* + t(y^* - x^*)) - F'(x_0))\| dt \\ &\leq \alpha \int_0^1 \|x^* + t(y^* - x^*) - x_0\| dt, \end{aligned}$$

and, since $\|y^* - x_0\| < s$ and $\|x^* - x_0\| \leq t^*$, it follows that

$$\|I - T\| < \alpha(s + t^*)/2.$$

Now, we look for s such that $\alpha(s + t^*)/2 \leq 1$ (namely, $s = 2/\alpha - t^* = t^{**}$). Hence, x^* is the unique solution of Eq. (5) in $B(x_0, t^{**}) \cap \Omega$.

Now, from the above-mentioned facts, we establish in the following theorem the semilocal convergence and the domains of existence and uniqueness of solutions for iterations (6). We also give error estimates for sequence (6) in terms of real sequence (8).

Theorem 3.3. *Let $F : \Omega \subseteq X \rightarrow Y$ be a twice Fréchet-differentiable quadratic operator, defined on a non-empty open convex subset Ω of a Banach space X with values in a Banach space Y . Suppose (C1)–(C4). Then, sequence $\{x_n\}$, defined by (6) and starting at x_0 , converges to a solution x^* of (5) in $B(x_0, t^*)$, and the solution x^* is unique in $B(x_0, t^{**}) \cap \Omega$, where t^* and t^{**} are the two roots of polynomial (7). Moreover,*

$$\|x^* - x_n\| \leq t^* - t_n, \quad n \geq 0. \quad \square \tag{10}$$

Finally, we use Ostrowski’s technique to obtain a priori error estimates for iterations (6) from polynomial (7), so that the terms of the real sequence $\{t_n\}$ do not need to be calculated. From these error estimates, if $t^* \neq t^{**}$, we conclude that iterations (6) have R -order of convergence at least four when they are applied to quadratic equations.

Theorem 3.4. *If polynomial (7) has two positive roots t^* and t^{**} , such that $t^* \leq t^{**}$, and $\{t_n\}$ is the sequence defined in (8), then (a) if $t^* < t^{**}$ and $\sqrt[3]{5}\phi < 1$, where $\phi = t^*/t^{**}$, we have*

$$(t^{**} - t^*) \frac{\phi^{4^n}}{1 - \phi^{4^n}} \leq t^* - t_n \leq (t^{**} - t^*) \frac{(\sqrt[3]{5}\phi)^{4^n}}{\sqrt[3]{5} - (\sqrt[3]{5}\phi)^{4^n}}, \quad n \geq 0; \tag{11}$$

(b) if $t^* = t^{**}$ and $C = \frac{5}{16} - \sum_{k \geq 3} \frac{A_k}{2^{k+1}} < 1$, we have

$$t^* - t_n = t^* C^n, \quad n \geq 0. \tag{12}$$

Proof. Let (8), $a_n = t^* - t_n$ and $b_n = t^{**} - t_n$, for all $n \geq 0$. Then,

$$p(t_n) = \frac{\alpha}{2} a_n b_n, \quad p'(t_n) = -\frac{\alpha}{2} (a_n + b_n).$$

From (8), it follows that

$$\begin{aligned} a_{n+1} &= \frac{a_n^4}{(a_n + b_n)^5} \left(a_n^2 + 4a_n b_n + 5b_n^2 - 8b_n^4 \sum_{k \geq 0} 2^k A_{k+3} \frac{a_n^k b_n^k}{(a_n + b_n)^{2k+2}} \right), \\ b_{n+1} &= \frac{b_n^4}{(a_n + b_n)^5} \left(5a_n^2 + 4a_n b_n + b_n^2 - 8a_n^4 \sum_{k \geq 0} 2^k A_{k+3} \frac{a_n^k b_n^k}{(a_n + b_n)^{2k+2}} \right). \end{aligned}$$

If $t^* < t^{**}$, then $\phi = t^*/t^{**} < 1$ and

$$\frac{a_{n+1}}{b_{n+1}} = \left(\frac{a_n}{b_n}\right)^4 h(a_n),$$

where

$$h(x) = \frac{10x^2 + 14dx + 5d^2 - 8(x+d)^4 S(x)}{10x^2 + 6dx + d^2 - 8x^4 S(x)}, \quad S(x) = \sum_{k \geq 0} 2^k A_{k+3} \frac{x^k (x+d)^k}{(2x+d)^{2k+2}}$$

and $d = t^{**} - t^*$. Observe that $1 \leq h(x) \leq 5$, so that

$$\phi^{4^n} \leq \dots \leq \left(\frac{a_{n-1}}{d + a_{n-1}}\right)^4 \leq \frac{a_n}{a_n + d} \leq 5 \left(\frac{a_{n-1}}{a_{n-1} + d}\right)^4 \leq \dots \leq \frac{1}{\sqrt[3]{5}} \left(\sqrt[3]{5} \phi\right)^{4^n}$$

and (11) is satisfied, since $\sqrt[3]{5} \phi < 1$.

On the other hand, if $t^* = t^{**}$, then $a_n = b_n$,

$$a_n = \frac{a_{n-1}}{16} \left(5 - 8 \sum_{k \geq 3} \frac{A_k}{2^k}\right)$$

and (12) is satisfied, since $C < 1$. \square

Remark 3.5. From Theorem 3.4, more precise a priori error estimates can be given for particular iterations (6) in Banach spaces:

- if (6) is reduced to the Super-Halley method, we have

$$t^* - t_n = (t^{**} - t^*) \frac{\phi^{4^n}}{1 - \phi^{4^n}}, \quad n \geq 0,$$

where $\phi = t^*/t^{**}$ and $t^* < t^{**}$, and if $t^* = t^{**}$, we have

$$t^* - t_n = t^* (1/4)^n, \quad n \geq 0;$$

- if (6) is reduced to Chebyshev-like method (4), we have

$$(t^{**} - t^*) \frac{\phi^{4^n}}{1 - \phi^{4^n}} \leq t^* - t_n \leq (t^{**} - t^*) \frac{(\sqrt[3]{5} \phi)^{4^n}}{\sqrt[3]{5} - (\sqrt[3]{5} \phi)^{4^n}}, \quad n \geq 0,$$

where $\phi = t^*/t^{**}$ and $t^* < t^{**}$, and if $t^* = t^{**}$, we have

$$t^* - t_n = t^* (5/16)^n, \quad n \geq 0.$$

In both cases we deduce that the R -order of convergence of the methods is at least four when they are applied to solve quadratic equations, which is well known, see [4,18].

4. Applications

In this section, we illustrate the previous results with two applications, where two quadratic equations are shown: an equation of molecular interaction and a Chandrasekhar's equation.

In the equation of molecular interaction, we have to solve a boundary value problem with a partial differential equation. To do this, we consider a discretization procedure and use two different iterations (6) to solve the corresponding system of equations. Moreover, a priori error estimates are obtained according to Theorems 3.3 and 3.4 and the speed of convergence is computationally justified.

For Chandrasekhar's equation, we first provide domains of existence and uniqueness of solution by using Theorem 3.3, and secondly we discretize the problem to approximate a solution of the equation by means of Chebyshev-like method (4). In this case, due to the expression of the corresponding operator F'' in the application of (4), whose operational cost is high, we use a modification of (4) to reduce the operational cost, where F'' is not used, but preserves the speed of convergence.

4.1. Equation of molecular interaction

Firstly, we consider the following equation of molecular interaction, that appears in the theory of dynamics of gases [10]:

$$u_{xx} + u_{yy} = u^2,$$

with the boundary conditions:

$$\begin{cases} u(x, 0) = 2x^2 - x + 1, & 0 \leq x \leq 1, \\ u(1, y) = 2, & 0 \leq y \leq 1, \\ u(x, 1) = 2, & 0 \leq x \leq 1, \\ u(0, y) = 2y^2 - y + 1, & 0 \leq y \leq 1. \end{cases}$$

We first discretize the problem, then define a uniform mesh with knots

$$P_{i,j} = (ih, jh), \quad h = \frac{1}{n+1}, \quad i, j = 0, 1, \dots, n+1,$$

and we approach the second derivatives of u in the points $P_{i,j}$ by the following formulas:

$$u_{xx}(P_{i,j}) = \frac{u(P_{i+1,j}) - 2u(P_{i,j}) + u(P_{i-1,j}))}{h^2}, \quad i, j = 1, \dots, n,$$

$$u_{yy}(P_{i,j}) = \frac{u(P_{i,j+1}) - 2u(P_{i,j}) + u(P_{i,j-1}))}{h^2}, \quad i, j = 1, \dots, n.$$

We denote $x_{i,j} = u(P_{i,j})$, $i, j = 0, 1, \dots, n+1$, and obtain the system

$$-x_{i+1,j} - x_{i-1,j} - x_{i,j+1} - x_{i,j-1} + 4x_{i,j} = -h^2 x_{i,j}^2, \quad i, j = 1, \dots, n. \tag{13}$$

Observe that the values $x_{0,j}$, $x_{n+1,j}$, $x_{i,0}$ and $x_{i,n+1}$ are given by the boundary conditions. Let $m = n^2$ and we order $x_{i,j}$ ($i, j = 1, \dots, n$) in the following way

$$x_1 = x_{1,1}, \dots, x_n = x_{n,1}, x_{n+1} = x_{1,2}, \dots, x_m = x_{n,n}.$$

System (13) can be written as

$$A\bar{x} + \Phi(\bar{x}) = \bar{b},$$

where

$$A = \begin{pmatrix} B & -I & 0 & \dots & 0 \\ -I & B & -I & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -I \\ 0 & \dots & 0 & -I & B \end{pmatrix} \in M(m \times m),$$

$$B = \begin{pmatrix} 4 & -1 & 0 & \dots & 0 \\ -1 & 4 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \dots & 0 & -1 & 4 \end{pmatrix} \in M(n \times n).$$

I is the identity matrix in \mathbb{R}^n , $\bar{x} = (x_1 \dots, x_m)^t$, $\Phi(\bar{x}) = h^2(x_1^2 \dots, x_m^2)^t$ and \bar{b} is a vector formed from the boundary conditions. The systems in the previous way are known as almost linear systems. Although in general the use of iterative processes that bear the computation of the second derivative is not viable (mainly for big dimensions), they can be taken into account in this type of systems, since the second derivative of the operator is constant.

If for example we now consider the case $n = 3$ (and $m = 9$), the vector \bar{b} is given by

$$\bar{b} = (7/4, 1, 27/8, 1, 0, 2, 27/8, 2, 4)^t,$$

and (13) can be written as

$$F(\bar{x}) = A\bar{x} + \Phi(\bar{x}) - \bar{b} = \bar{0},$$

so that $F'(\bar{x})$ is the linear operator given by the matrix

$$A + \frac{1}{8} \begin{pmatrix} x_1 & 0 & \dots & 0 \\ 0 & x_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & x_9 \end{pmatrix}$$

Table 1
A priori error estimates (10).

n	Chebyshev-like method (4)	Super-Halley method (3)
1	$5.40570 \dots \times 10^{-4}$	$1.27736 \dots \times 10^{-4}$
2	$1.48624 \dots \times 10^{-16}$	$9.26994 \dots \times 10^{-20}$
3	$8.49486 \dots \times 10^{-67}$	$2.57121 \dots \times 10^{-80}$

Table 2
A priori error estimates (11).

n	Chebyshev-like method (4)	Super-Halley method (3)
1	$6.38706 \dots \times 10^{-4}$	$1.27736 \dots \times 10^{-4}$
2	$2.89685 \dots \times 10^{-16}$	$9.26994 \dots \times 10^{-20}$
3	$1.22605 \dots \times 10^{-65}$	$2.57121 \dots \times 10^{-80}$

and $F''(\bar{x})$ is the constant bilinear operator:

$$F''(\bar{x})\bar{u}\bar{v} = \frac{1}{8}\bar{u}\bar{v}, \quad \bar{u}, \bar{v} \in \mathbb{R}^9.$$

For the finite dimensional case, the computation of the Chebyshev-like method (4) is obtained according to the following stages:

1. Stage: Compute one LR-decomposition of F' by the Gauss elimination.
2. Stage: Solve the linear system: $F'(\bar{x}_k)\bar{c}_k = -F(\bar{x}_k)$.
3. Stage: Solve the linear system: $F'(\bar{x}_k)\bar{z}_k = F''(\bar{x}_k)(\bar{c}_k)^2$.
4. Stage: Solve the linear system: $F'(\bar{x}_k)\bar{w}_k = F''(\bar{x}_k)\bar{c}_k\bar{z}_k$.
5. Stage: Define: $\bar{x}_{k+1} = \bar{x}_k + \bar{c}_k - \frac{1}{2}(\bar{z}_k - \bar{w}_k)$.

If we use the Super-Halley method, then the stages are now:

1. Stage: Compute one LR-decomposition of F' by the Gauss elimination.
2. Stage: Solve the linear system: $F'(\bar{x}_k)\bar{c}_k = -F(\bar{x}_k)$.
3. Stage: Compute one LR-decomposition of $F'(\bar{x}_k) + F''(\bar{x}_k)\bar{c}_k$ by the Gauss elimination.
4. Stage: Solve the linear system:

$$[F'(\bar{x}_k) + F''(\bar{x}_k)\bar{c}_k]\bar{d}_k = -F(\bar{x}_k) + \frac{1}{2}F''(\bar{x}_k)\bar{c}_k^2.$$

5. Stage: Define: $\bar{x}_{k+1} = \bar{x}_k + \bar{d}_k$.

In view of the previous algorithms, we note that the application of Chebyshev-like method (4) only uses one LR-decomposition, whereas the Super-Halley method uses two LR-decompositions.

On the other hand, we notice that $F''(\bar{x})\bar{y}$ is a linear application and the associated matrix is diagonal. If $\bar{x} = (x_1, \dots, x_m)$ and $\bar{y} = (y_1, \dots, y_m)$, the matrix associated to $F''(\bar{x})\bar{y}$ is

$$2h^2 \text{diag}\{y_1, \dots, y_m\},$$

so that the application of $F''(\bar{x})\bar{y}$ is simple.

We consider the following norms of \bar{x} and A :

$$\|\bar{x}\|_\infty = \max_{1 \leq i \leq m} |x_i|, \quad \|A\| = \sup_{\substack{\bar{x} \in \mathbb{R}^m \\ \bar{x} \neq 0}} \frac{\|A\bar{x}\|_\infty}{\|\bar{x}\|_\infty} = \max_{1 \leq i \leq m} \left(\sum_{j=1}^{n-1} |a_{ij}| \right),$$

where $\bar{x} \in \mathbb{R}^m$ and $A \in M(m \times m)$. On the other hand, we denote the n th iteration by $\bar{x}_n = (x_1^{(n)}, x_2^{(n)}, \dots, x_9^{(n)})^t$. If we choose $x_i^{(0)} = 1$, for $i = 1, 2, \dots, 9$, the hypotheses of convergence Theorem 3.3 are satisfied, $\alpha\eta = 0.0984298 \dots < 1/2$, so that method (6) converges to a solution of system (13). Moreover, the domains of existence and uniqueness of solution of (13) are respectively $\{\bar{u} \in \mathbb{R}^9 \mid \|\bar{u} - \bar{x}_0\|_\infty \leq 0.823331 \dots\}$ and $\{\bar{u} \in \mathbb{R}^9 \mid \|\bar{u} - \bar{x}_0\|_\infty \leq 15.0375 \dots\}$.

In Tables 1 and 2, the error estimates obtained when Chebyshev-like method (4) and Super-Halley method (3) are applied to solve system (13) are shown. Notice that they are similar. However, observe that Ostrowski's technique used in Table 2 has the advantage of not having to calculate the terms of the scalar sequence $\{t_n\}$ if we know the roots of majorant polynomial (7). In Table 1, we obtain a priori error estimates (10) using the majorizing sequence. Observe that the a priori error estimates given in Tables 1 and 2 are rather sharp and the ones for the Super-Halley method are the same, as we can see from Remark 3.5.

After four iterations applying Chebyshev-like method (4) and using stopping criterion $\|\bar{x}_n - \bar{x}^*\|_\infty < 10^{-150}$, we obtain the numerical solution \bar{x}^* of (13), which is given in Table 3.

Table 3
Numerical solution \bar{x}^* of system (13).

x_1^*	1.02591171169 ...
x_2^*	1.20971388713 ...
x_3^*	1.51670303095 ...
x_4^*	1.20971388713 ...
x_5^*	1.38770378643 ...
x_6^*	1.62587249195 ...
x_7^*	1.51670303095 ...
x_8^*	1.62587249195 ...
x_9^*	1.76429948544 ...

Table 4
Errors and the computational order of convergence for the Chebyshev-like and Super-Halley methods.

n	Chebyshev-like method (4)	Super-Halley method (3)	ρ_{CH-L}	ρ_{S-H}
1	$4.48909 \dots \times 10^{-5}$	$8.80779 \dots \times 10^{-6}$	3.91068 ...	3.92133 ...
2	$1.27535 \dots \times 10^{-21}$	$3.79989 \dots \times 10^{-25}$	4.01161 ...	4.01240 ...
3	$5.33834 \dots \times 10^{-88}$	$7.57164 \dots \times 10^{-103}$		

Considering the same stopping criterion in Table 4, we obtain the errors $\|\bar{x}_n - \bar{x}^*\|_\infty$. If we now consider the computational order of convergence [22]:

$$\rho \approx \ln \frac{\|\bar{x}_{n+1} - \bar{x}^*\|_\infty}{\|\bar{x}_n - \bar{x}^*\|_\infty} \bigg/ \ln \frac{\|\bar{x}_n - \bar{x}^*\|_\infty}{\|\bar{x}_{n-1} - \bar{x}^*\|_\infty}, \quad n \in \mathbb{N}, \tag{14}$$

Chebyshev-like method (4) and the Super-Halley method reach computationally the R -order of convergence at least four obtained in Remark 3.5. See Table 4, where ρ_{CH-L} and ρ_{S-H} denote respectively the computational orders of convergence of the Chebyshev-like and Super-Halley methods.

4.2. Chandrasekhar's equation

Secondly, we use the results obtained previously to obtain domains of existence and uniqueness of solutions and some error estimates for a particular quadratic integral equation of the type:

$$x(s) = f(s) + \lambda x(s) \int_0^1 \kappa(s, t)x(t)dt. \tag{15}$$

Eq. (15) appears in [11] and arise from the study of the radiative transfer theory, the transport of neutrons and the kinetic theory of the gases. It is studied in [12] and, under certain conditions for the kernel, in [23,4].

We consider the max-norm, the kernel $\kappa(s, t)$ as a continuous function in $s, t \in [0, 1]$ such that $0 < \kappa(s, t) < 1$ and $\kappa(s, t) + \kappa(t, s) = 1$. Moreover, we assume that $f(s) \in C[0, 1]$ is a given function and λ is a real constant.

Notice that finding a solution of (15) is equivalent to solving the equation $F(x) = 0$, where $F : C[0, 1] \rightarrow C[0, 1]$ and

$$F(x)(s) = x(s) - f(s) - \lambda x(s) \int_0^1 \kappa(s, t)x(t)dt, \quad x \in C[0, 1], s \in [0, 1].$$

In particular, we consider

$$F(x)(s) = x(s) - 1 - \frac{x(s)}{4} \int_0^1 \frac{s}{s+t} x(t)dt, \quad x \in C[0, 1], s \in [0, 1]. \tag{16}$$

Note that the operator F' is such that $F'(x) \in \mathcal{L}(C[0, 1])$, for every $x \in C[0, 1]$, and $F'(x)y$ is a continuous function given by

$$[F'(x)y](s) = y(s) - \frac{x(s)}{4} \int_0^1 \frac{s}{s+t} y(t)dt - \frac{y(s)}{4} \int_0^1 \frac{s}{s+t} x(t)dt, \quad s \in [0, 1],$$

for every $x, y \in C[0, 1]$, and the second Fréchet derivative is given by

$$[F''(x)(y, z)](s) = -\frac{y(s)}{4} \int_0^1 \frac{s}{s+t} z(t)dt - \frac{z(s)}{4} \int_0^1 \frac{s}{s+t} y(t)dt, \quad s \in [0, 1],$$

where $x, y, z \in C[0, 1]$.

Notice that a reasonable choice of the starting point is $x_0(s) = 1$, for all $s \in [0, 1]$, since $x(0) = 1$. Next, we calculate the constants η and α . Since,

$$F(x_0)(s) = -\frac{1}{4} \int_0^1 \frac{s}{s+t} dt = -\frac{s}{4} \ln \frac{s+1}{s}$$

Table 5
Weights and knots for the Gauss–Legendre formula ($m = 8$).

j	t_j	β_j
1	0.0198550717512 ...	0.101228536290 ...
2	0.101666761293 ...	0.222381034453 ...
3	0.237233795041 ...	0.313706645877 ...
4	0.408282678752 ...	0.362683783378 ...
5	0.591717321247 ...	0.362683783378 ...
6	0.762766204958 ...	0.31370664587 ...
7	0.898333238706 ...	0.222381034453 ...
8	0.980144928248 ...	0.101228536290 ...

and

$$\max_{s \in [0,1]} \left| \int_0^1 \frac{s}{s+t} dt \right| = \max_{s \in [0,1]} \left(s \ln \frac{s+1}{s} \right) = \ln 2,$$

it follows that

$$\|F(x_0)\| \leq \frac{\ln 2}{4}.$$

Moreover,

$$\|I - F'(x_0)\| \leq \frac{1}{2} \ln 2 < 1,$$

and therefore there exists $\Gamma_0 = F'(x_0)^{-1}$ and

$$\|\Gamma_0\| \leq \frac{1}{1 - \|I - F'(x_0)\|} \leq \frac{2}{2 - \ln 2}.$$

In consequence, conditions (C1) and (C2) are satisfied, since

$$\|\Gamma_0 F(x_0)\| \leq \frac{\ln 2}{4 - 2 \ln 2} = \eta, \quad \|\Gamma_0 F''(x)\| \leq \frac{\ln 2}{2 - \ln 2} = \alpha, \quad x \in C[0, 1].$$

Moreover, conditions (C3), $\alpha\eta = 0.140659 \dots < 1/2$, and (C4) are also satisfied, and consequently operator (16) has a zero in $\{x \in C[0, 1] \mid \|x - 1\|_\infty \leq 0.287048 \dots\}$ and is unique in $\{x \in C[0, 1] \mid \|x - 1\|_\infty \leq 3.48373 \dots\}$.

Finally, we approximate numerically a solution of $F(x) = 0$, where F is given in (16) by means of a discretization procedure. We then approach the integral which appears in (16) by the Gauss–Legendre quadrature formula:

$$\int_0^1 f(t) dt \approx \frac{1}{2} \sum_{j=1}^m \beta_j f(t_j),$$

where β_j are the weights and t_j the knots tabulated in Table 5 for $m = 8$.

If we denote by x_i the approximations of $x(t_i)$, $i = 1, \dots, 8$, we obtain the following nonlinear system:

$$x_i \approx 1 + \frac{1}{8} x_i \sum_{j=1}^8 a_{ij} x_j, \quad \text{where } a_{ij} = \frac{t_i \beta_j}{8(t_i + t_j)}, \quad i = 1, \dots, 8. \tag{17}$$

Now, we denote $\bar{x} = (x_1, \dots, x_8)^T$, $\bar{1} = (1, \dots, 1)^T$, $A = (a_{ij})$ and we can write nonlinear system (17) in the matrix form:

$$F(\bar{x}) = \bar{x} - \bar{1} - \bar{x} \odot A \bar{x},$$

where \odot denotes the scalar product. $F'(\bar{x})$ is then the linear operator given by

$$F'(\bar{x})\bar{y} = \bar{y} - (\bar{x} \odot A\bar{y} + \bar{y} \odot A\bar{x}),$$

and $F''(\bar{x})$ is the bilinear operator:

$$F''(\bar{x})\bar{y}\bar{z} = -(\bar{z} \odot A\bar{y} + \bar{y} \odot A\bar{z}).$$

Contrary to the previous equation of molecular interaction, we observe for this equation that it is necessary to calculate two scalar products and two matrix products, so that the operational cost is increased considerably when Chebyshev-like method (4) is applied. The efficiency of this method in Banach spaces can be improved without any additional computations if F'' is replaced in each step by Taylor's formula using F' , since the order of convergence of the method is preserved. So, from Taylor's formula, we have

$$F'(y_n) = F'(x_n) + F''(x_n)(y_n - x_n),$$

Table 6
Numerical solution \bar{x}^* of system (17).

x_1^*	1.02171973146 ...
x_2^*	1.07318638173 ...
x_3^*	1.12572489365 ...
x_4^*	1.16975331216 ...
x_5^*	1.20307175130 ...
x_6^*	1.22649087463 ...
x_7^*	1.24152460059 ...
x_8^*	1.24944851669 ...

Table 7
Errors and the computational order of convergence for method (18).

n	method (18)	ρ
1	$4.20528 \dots \times 10^{-5}$	4.13255 ...
2	$1.07373 \dots \times 10^{-20}$	4.02218 ...
3	$2.05799 \dots \times 10^{-83}$	

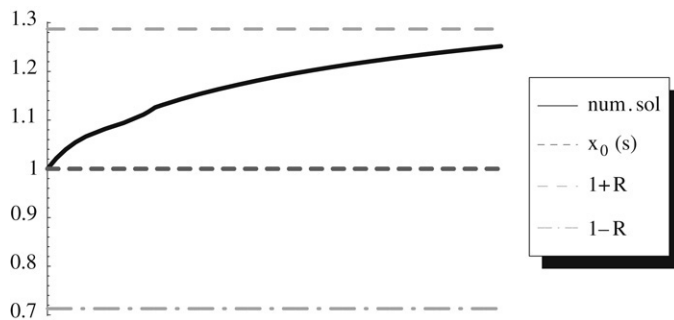


Fig. 1. Approximated solution and domain of existence of solutions.

where $y_n = x_n - \Gamma_n F(x_n)$, since F is a quadratic operator ($F^{(n)}(x) = 0$, for all $n \geq 3$). Then,

$$F''(x_n)\Gamma_n F(x_n) = F'(x_n) - F'(y_n), \quad L_F(x_n) = I - \Gamma_n F'(y_n).$$

Consequently, Chebyshev-like method (4) for quadratic operators can be written as:

$$x_{n+1} = x_n - \left(2I - \frac{3}{2}\Gamma_n F'(y_n) + \frac{1}{2}(\Gamma_n F'(y_n))^2 \right) \Gamma_n F(x_n), \quad n \geq 0. \tag{18}$$

Starting at \bar{x}_n , for the finite dimensional case, the computation of the $(n + 1)$ -step of (18) proceeds as follows:

1. Stage: Compute one LR -decomposition of F' by the Gauss elimination.
2. Stage: Solve the linear system: $F'(\bar{x}_n)\bar{z}_n = -F(\bar{x}_n)$.
3. Stage: Set $\bar{y}_n = \bar{x}_n + \bar{z}_n$.
4. Stage: Solve the linear system: $F'(\bar{x}_n)\bar{u}_n = F'(\bar{y}_n)\bar{z}_n$.
5. Stage: Solve the linear system: $F'(\bar{x}_n)\bar{v}_n = F'(\bar{y}_n)\bar{u}_n$.
6. Stage: Set $\bar{x}_{n+1} = \bar{x}_n + 2\bar{z}_n - \frac{3}{2}\bar{u}_n + \frac{1}{2}\bar{v}_n$.

Notice that the linear systems considered above have the same associated matrix and then we only need one LR -decomposition of the matrix $F'(x_n)$ in each step and it is not necessary to consider F'' .

Iteration (18) reaches the numerical solution appearing in Table 6 after four iterations, using stopping criterion $\|\bar{x}_{n+1} - \bar{x}_n\|_\infty < 10^{-150}$ and starting at $\bar{x}_0 = \bar{1}$. Observe that the R -order of convergence at least four is computationally reached by method (18), see Table 7.

Now, we denote the ratio of existence domain obtained above by $R = 0.287048 \dots$, and observe that the interpolated approximation shown in Fig. 1, along with the starting function $\bar{x}_0 = \bar{1}$, lie in the domain of existence.

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