

On a Moser-Steffensen type method for nonlinear systems of equations

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Abstract

This paper is devoted to the construction and analysis of a Moser-Steffensen iterative scheme. The method has quadratic convergence without evaluating any derivative nor inverse operator. We present a complete study of the order of convergence for systems of equations, hypotheses ensuring the local convergence and finally we focus our attention to its numerical behavior. The conclusion is that the method improves the applicability of both Newton and Steffensen methods having the same order of convergence.

Keywords: Steffensen's method, Moser's strategy, recurrence relations, local convergence, numerical analysis

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1 Introduction

One of the most studied problems in numerical analysis is the solution of nonlinear equations

$$F(x) = 0. \tag{1}$$

Many scientific and engineering problems can be written in the form of a nonlinear systems of equations, where F is a nonlinear operator defined on a non-empty open convex subset Ω of \mathbb{R}^m with values in \mathbb{R}^m . A powerful tool to solve these nonlinear systems of equations is by means of iterative methods.

It is well-known that Newton's method,

$$\begin{cases} x_0 \text{ given in } \Omega, \\ x_{n+1} = x_n - F'(x_n)^{-1}F(x_n), \quad n \geq 0, \end{cases} \tag{2}$$

is the one of the most used iterative method to approximate the solution x^* of (1). The quadratic convergence and the low operational cost of (2) ensure that Newton's method has a good computational efficiency. But the existence of the operator $F'(x_n)^{-1}$ is needed at each step or equivalently to solve $F'(x_n)(x_{n+1} - x_n) = -F(x_n)$. It is also known another feature of Newton's iteration: calculating inverse operators is not needed if the inverse of an operator is approximated; namely, to approximate P^{-1} , where $P \in \mathcal{L}(X, Y)$, the set of bounded linear operators from X into Y , we can phrase $G(Q) = Q^{-1} - P = 0$, so that Newton's method is reduced to $Q_{n+1} = 2Q_n - Q_n P Q_n, n \geq 0$, provided that Q_0 is given. So, in [17], Moser proposed, to solve nonlinear operator equations, the following iterative process:

$$\begin{cases} x_0, B_0 \text{ given}, \\ x_{n+1} = x_n - B_n F(x_n), \quad n \geq 0 \\ B_{n+1} = 2B_n - B_n F'(x_n) B_n, \quad n \geq 0. \end{cases}$$

This new iterative method, which can be considered as a Newton-type method, does not need to calculate inverse operators. It can be shown that the rate of convergence is $\frac{1+\sqrt{5}}{2}$, provided the root is simple (see [17]). This process uses the same amount of information per step as Newton's method, but it converges no faster than the secant method, so that this unsatisfactory from a numerical point of view. For that, Hald proposes in [16] the use of the following iteration:

$$\begin{cases} x_0, B_0 \text{ given,} \\ x_{n+1} = x_n - B_n F(x_n), \quad n \geq 0 \\ B_{n+1} = 2B_n - B_n F'(x_{n+1}) B_n, \quad n \geq 0. \end{cases} \quad (3)$$

Observe that the first equation is similar to the Newton's method in which case B_n is $F'(x_n)^{-1}$. The second equation is Newton's method applied to $G(P) = P^{-1} - F'(x_{n+1}) = 0$. We can stress two features of (4): it has the same rate of convergence of Newton's method and it does not need to solve nonlinear equations at each step (it is "inversion free"). Moreover, from the convergence of the sequence x_n , the convergence of the sequence B_n can be given, so that it also produces successive approximations B_n to the bounded right inverse of $F'(x^*)$ at the solution x^* , which is very helpful when sensitivity of solutions to small perturbations are investigated. However, as Newton's method, this method has the same serious shortcoming: the derivative $F'(x)$ has to be evaluated at each iteration. This makes it unapplicable to equations with nondifferentiable operators and in situations when evaluation of the derivative is too costly. The goal of this paper is to modify the previous two-step method in order to avoid the evaluation of any Fréchet derivative.

It is common to approximate derivatives by divided differences, so that iterative methods that use divided differences instead of derivatives are obtained. Remember that an operator $[u, v; F]$, $u, v \in \Omega$, is called a first order divided difference [20, 21], if it is a bounded linear operator such that

$$[u, v; F] : \Omega \subset \mathbb{R}^m \longrightarrow \mathbb{R}^m \quad \text{and} \quad [u, v; F](u - v) = F(u) - F(v).$$

In this paper, we will start with Steffensen's method [1, 4, 5, 6, 7, 8, 9, 11, 14, 19] to approximate a solution of the nonlinear system of equations $F(x) = 0$. It is a one-point iterative process given by the following algorithm:

$$\begin{cases} x_0 \text{ given,} \\ x_{n+1} = x_n - [x_n, x_n + F(x_n); F]^{-1} F(x_n), \quad n \geq 0, \end{cases} \quad (4)$$

The main interest of this iterative process lies in that the approximation of the derivative $F'(x_n)$, that appears in each step of Newton's method, by the divided difference $[x_n, x_n + F(x_n); F]^{-1}$ is good enough to keep the quadratic convergence [22] and, therefore, keeps the computational efficiency of Newton's method. However, in the Steffensen method remains an interesting problem to solve, its algorithm needs to solve a linear system of equations

at each step:

$$\begin{cases} x_{-1}, x_0 \text{ given,} \\ [x_n, x_n + F(x_n); F](x_{n+1} - x_n) = F(x_n), \quad n \geq 0. \end{cases} \quad (5)$$

In order to improve this fact, following the previous ideas applied in the case of Newton's method, we consider the following Moser-Steffensen type method

$$\begin{cases} x_0, B_0 \text{ given,} \\ x_{n+1} = x_n - B_n F(x_n), \quad n \geq 0 \\ B_{n+1} = 2B_n - B_n[x_{n+1}, x_{n+1} + F(x_{n+1}); F]B_n, \end{cases} \quad (6)$$

where we have changed the resolution of the linear system in every step by making several matrix multiplications.

Whereas the operational cost of both processes is similar, however the possibility of *ill-conditioned* linear systems appearing will be avoided simply taking appropriate initial matrix B_0 , and therefore this previous algorithm will be able to be stable more easily. The matrix given by the divided difference $[x_n, x_n + F(x_n); F]$, can be *ill-conditioned* and therefore the linear system of equations previously indicated (5), in the classical Steffensen method (4), should cause instabilities.

Remark 1.1 *Along the paper, we consider the following first order divided difference in \mathbb{R}^m : $[u, v; F] = ([u, v; F]_{ij})_{i,j=1}^m$, where*

$$[u, v; F]_{ij} = \frac{1}{u_j - v_j} (F_i(u_1, \dots, u_j, v_{j+1}, \dots, v_m) - F_i(u_1, \dots, u_{j-1}, v_j, \dots, v_m)), \quad (7)$$

$$u = (u_1, u_2, \dots, u_m)^T \text{ and } v = (v_1, v_2, \dots, v_m)^T.$$

The organization of the paper is the following. In Section 2 we study the local error equation, seeing his quadratic convergence. After, in Section 3, we obtain a local convergence result for this iterative process. Moreover, in the Section 4, the numerical behavior is analyzed. From this study, we can conclude that the considered method (6) improves the applicability of Steffensen method (4).

2 Local order of convergence

We assume that $F : \Omega \subseteq \mathbf{R}^m \rightarrow \mathbf{R}^m$ has at least 2-order derivatives with continuity on Ω for any $x \in \Omega$ lying in a neighborhood of a simple zero,

$x^* \in \Omega$, of the system $F(x) = 0$. We can apply Taylor's formulae to $F(x)$. By setting $e_k = x_k - x^*$, the local order, and assuming that $[F'(x^*)]^{-1}$ exists, we have

$$F(x_k) = F(x^* + e_k) = \Gamma(e_k + O(e_k^2)), \quad (8)$$

where $\Gamma = F'(x^*)$, $e_k^2 = (e_k, e_k) \in \mathbf{R}^m \times \mathbf{R}^m$. Moreover, from [13] we obtain

$$[x_k, y_k; F] = \Gamma(I + A_2(e_k + \varepsilon_k) + O_2(e_k, \varepsilon_k)), \quad (9)$$

where $\varepsilon_k = y_k - x^*$ and $A_2 = \frac{1}{2} \Gamma^{-1} F''(x^*) \in \mathfrak{L}_2(\Omega, \mathbf{R}^m)$. We say that an operator depending on e_k and ε_k is an $O_2(e_k, \varepsilon_k)$ if it is an $O(e_k^{q_0} \varepsilon_k^{q_1})$ with $q_0 + q_1 = 2$, $q_i \geq 0$, $i = 0, 1$.

If we expand in formal power series of e_k and ε_k , the inverse of the divided difference given in (9) is:

$$[x_k, y_k; F]^{-1} = (I - A_2(e_k + \varepsilon_k) + O_2(e_k, \varepsilon_k)) \Gamma^{-1}. \quad (10)$$

These developments of the divided difference operator (10) were previously used in the study of Grau *et al.* [13]. In particular, for the operator $\Theta_k = [x_k, x_k + F(x_k); F]$ we take

$$[x_k, x_k + F(x_k); F] = \Gamma(I + A_2(e_k + (2I + \Gamma)e_k) + O(e_k^2)),$$

Note that we have the following relation between $F(x_k)$ and $\Theta_k e_k$:

$$F(x_k) = \Theta_k e_k + O(e_k^2). \quad (11)$$

A first main local result is stated in the following theorem:

Theorem 2.1 $e_{k+1} = E_k e_k + O(e_k^2)$, where $E_k = I - B_k \Theta_k$.

Proof.

By subtracting x^* from both sides of the first step of (6) and taking into account (11) we obtain

$$\begin{aligned} e_{k+1} &= e_k - B_k F(x_k) \\ &= e_k - B_k \Theta_k e_k + O(e_k^2) \\ &= E_k e_k + O(e_k^2), \end{aligned} \quad (12)$$

and the proof is completed. ■

Other relations that are necessary to obtain a second theorem are the following ones:

$$\begin{aligned}
E_{k+1} &= I - B_{k+1} \Theta_{k+1} \\
&= I - 2 B_k \Theta_{k+1} + B_k \Theta_{k+1} B_k \Theta_{k+1} \\
&= (I - B_k \Theta_{k+1})^2.
\end{aligned} \tag{13}$$

and

$$\begin{aligned}
I - B_k \Theta_{k+1} &= I - B_k (\Theta_{k+1} - \Theta_k) B_k \Theta_k \\
&= E_k - B_k (\Theta_{k+1} - \Theta_k) \\
&= E_k - G_k e_k + O(e_{k+1}, e_k^2),
\end{aligned} \tag{14}$$

where $G_k = B_k A_2 (2I + \Gamma) \in \mathfrak{L}_2(\Omega, \mathbf{R})$.

A second main local result is stated in the following theorem:

Theorem 2.2 $E_{k+1} = (E_k + G_k e_k)^2 + O_2(E_k, e_k)$.

Proof.

By substituting (14) into (13) we have

$$\begin{aligned}
E_{k+1} &= (E_k - G_k e_k + O(E_k e_k, e_k^2))^2 \\
&= E_k^2 + (G_k e_k)^2 - E_k G_k e_k - G_k e_k E_k + o(E_k^2, E_k e_k).
\end{aligned} \tag{15}$$

The proof is complete. ■

In a more precise way we can write Theorems 1 and 2 (see (12) and (15) respectively) in norm terms. Namely,

$$\|e_{k+1}\| = O(\|E_k\| \|e_k\|) \tag{16}$$

$$\|E_{k+1}\| = O_2(\|E_k\|, \|e_k\|) = O(\|E_k\|^2, \|e_k\|^2, \|E_k\| \|e_k\|). \tag{17}$$

We have three possibilities:

- If $\|E_{k+1}\| = O(\|E_k\|^2)$, then $\|E_k\| = O(\|E_{k-1}\|^2)$, and from (16) we take $\|e_{k+1}\| = O(\|E_{k-1}\|^2 \|e_k\|)$, and applying (16) for $k-1$, we have $\|e_k\| = O(\|E_{k-1}\| \|e_{k-1}\|)$. Hence, $\|e_{k+1}\| = O(\|E_{k-1}\|^3 \|e_{k-1}\|)$. Taking into account that from (16) with $k-1$ we have $\|e_k\|^3 = O(\|E_{k-1}\|^3 \|e_{k-1}\|^3)$, finally, we obtain

$$\|e_{k+1}\| = O(\|e_k\|^3 \|e_{k-1}\|^{-2}). \tag{18}$$

The equation associated with (18) is $p_1(t) = t^2 - 3t + 2 = 0$. The real positive root that coincides with the local order of convergence in this case is $\rho = 2$ (see [18, 23]).

- If $\|E_{k+1}\| = O(\|e_k\|^2)$ and $E_k = O(\|e_{k-1}\|^2)$, then from (16) we have

$$\|e_{k+1}\| = O(\|e_k\|\|e_{k-1}\|^2). \quad (19)$$

In this case, the local order of convergence ρ is the unique real positive root of the indicial polynomial (see [18, 23, 24]) of the error difference equation (19) given by $p(t) = t^2 - t - 2$. That is, $\rho = 2$.

- If $\|E_{k+1}\| = O(\|E_k\|\|e_k\|)$ and we have (see (16)) $\|e_{k+1}\| = O(\|E_k\|\|e_k\|)$, then

$$\begin{aligned} \|e_{k+1}\| &= O(\|E_{k+1}\|) = O(\|E_k\|\|E_{k-1}\|\|e_{k-1}\|) \\ &= O(\|E_{k-1}\|^2\|e_{k-1}\|^2) \\ &= O(\|e_k\|^2). \end{aligned}$$

The method, as in the two first cases, presents quadratic order of convergence again.

We are now in a position to state the following theorem.

Theorem 2.3 *The iterative method defined by (6), from a local view of point, is a quadratic method. That is $\|e_{k+1}\| = O(\|e_k\|^2)$. ■*

3 Local convergence analysis

In this section, we prove the local convergence of the Moser-Steffensen type method given by (6). First, we establish a system of recurrence relations, from the real parameters that are introduced under some conditions for the pair (F, x_0) , where a sequence of positive real numbers is involved. After that, we can guarantee the semilocal convergence of the method in \mathbb{R}^m .

3.1 Recurrence relations

We suppose:

- (C1) Let x^* a zero of nonlinear system $F(x) = 0$ such that $\|F'(x^*)\| \leq M$ and there exists $r > 0$ with $B(x^*, r) \subseteq \Omega$.
- (C2) Let $B_0 \in \mathcal{L}(\mathbb{R}^m, \mathbb{R}^m)$ with $B_0 \neq 0$ such that $\|B_0\| = \beta$ and $\|I - B_0 F'(x^*)\| = \delta < 1$.
- (C3) Consider $x_0 \in B(x^*, r)$, such that there exists $\tilde{r} > 0$ such that $x_0 + F(x_0) \in B(x^*, \tilde{r})$, with $B(x^*, \tilde{r}) \subseteq \Omega$.
- (C4) For each pair of distinct points $x, y \in \Omega$, there exists a first order divided difference $[x, y; F]$ of F and $k \geq 0$, such that

$$\|[x, y; G] - F'(x^*)\| \leq k(\|x - x^*\| + \|y - x^*\|); \quad \forall x, y \in \Omega, \quad (20)$$

Notice that, in these conditions, the Fréchet derivative of F exists in Ω and satisfies $[x, x; F] = F'(x)$. On the other hand, to simplify the notation, we denote $L_n = [x_n, x^*; F]$ and $\Theta_n = [x_n, x_n + F(x_n); F]$, for all $n \in \mathbb{N}$.

From the above, we denote $\alpha_0 = r$, $\beta_0 = \beta$, $\delta_0 = \delta$, $\tilde{\alpha}_0 = \tilde{r}$ and define the scalar sequences:

$$\begin{aligned} \alpha_n &= (\delta_{n-1} + k \beta_{n-1} \alpha_{n-1}) \alpha_{n-1}, & \tilde{\alpha}_n &= (1 + M + k \alpha_n) \alpha_n \\ d_n &= \delta_n + k \beta_n (\alpha_{n+1} + \tilde{\alpha}_{n+1}), & \beta_n &= (1 + d_{n-1}) \beta_{n-1} \\ \delta_n &= \delta_{n-1}^2 + k M \beta_{n-1}^2 (\alpha_n + \tilde{\alpha}_n) \end{aligned} \quad (21)$$

Next, for $n = 1$, we prove the following recurrence relations for sequences (21) and $\{x_n\}$:

$$\begin{aligned} \|x_1 - x^*\| &< \alpha_1, \\ \|x_1 + F(x_1) - x^*\| &< \tilde{\alpha}_1, \\ \|I - B_1 \Theta_2\| &\leq d_1, \\ \|B_1\| &\leq \beta_1, \\ \|I - B_1 F'(x^*)\| &\leq \delta_1, \end{aligned}$$

provided that

$$x_0, x_0 + F(x_0) \in \Omega.$$

From the initial hypotheses, it follows that $x_1 = x_0 - B_0 F(x_0)$ is well defined and

$$\begin{aligned}
\|x_1 - x^*\| &= \|x_0 - B_0 F(x_0) - x^*\| \\
&= \|x_0 - x^* - B_0 L_0(x_0 - x^*)\| \\
&\leq \|I - B_0 L_0\| \|x_0 - x^*\| \\
&\leq (\|I - B_0 F'(x^*)\| + \|B_0\| \|L_0 - F'(x^*)\|) \|x_0 - x^*\| \\
&< (\delta_0 + \beta_0 k \alpha_0) \|x_0 - x^*\| \\
&< (\delta_0 + \beta_0 k \alpha_0) \alpha_0 = \alpha_1.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\|x_1 + F(x_1) - x^*\| &= \|x_1 + L_1(x_1 - x^*) - x^*\| \leq \|I + L_1\| \|x_1 - x^*\| \\
&\leq (\|I + F'(x^*)\| + \|F'(x^*) - L_1\|) \|x_1 - x^*\| \\
&\leq (1 + \|F'(x^*)\| + k \|x_1 - x^*\|) \|x_1 - x^*\| \\
&\leq (1 + M + k \|x_1 - x^*\|) \|x_1 - x^*\| \\
&\leq (1 + M + k \alpha_1) \alpha_1 = \tilde{\alpha}_1.
\end{aligned}$$

Assuming that $\alpha_1 < \alpha_0$ and $(1 + M + kr)r < \tilde{r}$, then $\tilde{\alpha}_1 < \tilde{\alpha}_0$ and therefore $x_1, x_1 + F(x_1) \in \Omega$. So, there exist $\Theta_1 = [x_1, x_1 + F(x_1); F]$ and $B_1 = 2B_0 - B_0 \Theta_1 B_0$. Then, we establish

$$\begin{aligned}
\|I - B_0 \Theta_1\| &\leq \|I - B_0 F'(x^*)\| + \|B_0\| \|\Theta_1 - F'(x^*)\| \\
&\leq \|I - B_0 F'(x^*)\| + \|B_0\| \|k(\|x_1 - x^*\| + \|x_1 + F(x_1) - x^*\|)\| \\
&\leq \delta_0 + \beta_0 k(\alpha_1 + \tilde{\alpha}_1) = d_0.
\end{aligned}$$

As a consequence,

$$\begin{aligned}
\|B_1\| &= \|2B_0 - B_0 \Theta_1 B_0\| \\
&\leq (1 + \|I - B_0 \Theta_1\|) \|B_0\| \\
&\leq (1 + d_0) \|B_0\| = \beta_1.
\end{aligned}$$

Moreover, to finish the first step, notice that

$$\begin{aligned}
\|I - B_1 F'(x^*)\| &= \|I - (2B_0 - B_0\Theta_1 B_0) F'(x^*)\| \\
&\leq \|I - B_0 F'(x^*)\|^2 + \|B_0\| \|\Theta_1 - F'(x^*)\| \|B_0 F'(x^*)\| \\
&\leq \|I - B_0 F'(x^*)\|^2 + \|B_0\|^2 \|F'(x^*)\| k (\|x_1 - x^*\| + \|x_1 + F(x_1) - x^*\|) \\
&< \delta_0^2 + \beta_0^2 M k (\alpha_1 + \tilde{\alpha}_1) = \delta_1.
\end{aligned}$$

Next, for $n = 2$, we prove the following recurrence relations for sequences (21) and $\{x_n\}$:

$$\begin{aligned}
\|x_2 - x^*\| &< \alpha_2, \\
\|x_2 + F(x_2) - x^*\| &< \tilde{\alpha}_2, \\
\|I - B_2\Theta_3\| &\leq d_2, \\
\|B_2\| &\leq \beta_2, \\
\|I - B_2 F'(x^*)\| &\leq \delta_2.
\end{aligned}$$

Now, by (6), $x_2 = x_1 - B_1 F(x_1)$, furthermore

$$\begin{aligned}
\|x_2 - x^*\| &\leq \|I - B_1 [x_1, x^*; F]\| \|x_1 - x^*\| \\
&= \|I - B_1 L_1\| \|x_1 - x^*\| \\
&\leq (\|I - B_1 F'(x^*)\| + \|B_1\| \|L_1 - F'(x^*)\|) \|x_1 - x^*\|. \\
&\leq (\delta_1 + \beta_1 k \alpha_1) \alpha_1 = \alpha_2.
\end{aligned}$$

Moreover, it is easy to check

$$\begin{aligned}
\|x_2 + F(x_2) - x^*\| &= \|x_2 + L_2(x_2 - x^*) - x^*\| \leq \|I + L_2\| \|x_2 - x^*\| \\
&\leq (\|I + F'(x^*)\| + \|F'(x^*) - L_2\|) \|x_2 - x^*\| \\
&\leq (1 + \|F'(x^*)\| + k \|x_2 - x^*\|) \|x_2 - x^*\| \\
&\leq (1 + M + k \|x_2 - x^*\|) \|x_2 - x^*\| \\
&\leq (1 + M + k \alpha_2) \alpha_2 = \tilde{\alpha}_2.
\end{aligned}$$

Assuming that $\alpha_2 < \alpha_1$, then $\tilde{\alpha}_2 < \tilde{\alpha}_1$ and therefore $x_2, x_2 + F(x_2) \in \Omega$. So, Θ_2 and B_2 are well defined.

Then, we have

$$\begin{aligned}
\|I - B_1 \Theta_2\| &\leq \|I - B_1 F'(x^*)\| + \|B_1\| \|\Theta_2 - F'(x^*)\| \\
&\leq \|I - B_1 F'(x^*)\| + \|B_1\| k(\|x_2 - x^*\| + \|x_2 + F(x_2) - x^*\|) \\
&\leq \delta_1 + \beta_1 k(\alpha_2 + \tilde{\alpha}_2) = d_1,
\end{aligned}$$

and we get

$$\begin{aligned}
\|B_2\| &= \|2B_1 - B_1 \Theta_2 B_1\| \\
&\leq (1 + \|I - B_1 \Theta_2\|) \|B_1\| \\
&\leq (1 + d_1) \|B_1\| \\
&\leq (1 + d_1) \beta_1 = \beta_2.
\end{aligned}$$

To finish the second step, we consider

$$\begin{aligned}
\|I - B_2 F'(x^*)\| &= \|I - (2B_1 - B_1 \Theta_2 B_1) F'(x^*)\| \\
&\leq \|I - B_1 F'(x^*)\|^2 + \|B_1\| \|\Theta_2 - F'(x^*)\| \|B_1 F'(x^*)\| \\
&\leq \|I - B_1 F'(x^*)\|^2 + \|B_1\|^2 \|F'(x^*)\| k(\|x_2 - x^*\| + \|x_2 + F(x_2) - x^*\|) \\
&< \delta_1^2 + \beta_1^2 M k(\alpha_2 + \tilde{\alpha}_2) = \delta_2.
\end{aligned}$$

At this time, we are able to obtain a general result that allows us to relate the sequences (21) and $\{x_n\}$.

Lemma 3.1 *In the previous conditions, if the sequence $\{\alpha_n\}$ is decreasing and $(1 + M + kr)r < \tilde{r}$, then*

$$(I) \quad \|x_n - x^*\| < \alpha_n,$$

$$(II) \quad \|x_n + F(x_n) - x^*\| < \tilde{\alpha}_n,$$

$$(III) \quad \|I - B_n \Theta_{n+1}\| \leq d_n,$$

$$(IV) \quad \|B_n\| \leq \beta_n,$$

$$(V) \quad \|I - B_n F'(x^*)\| \leq \delta_n,$$

for all $n \in N$.

Proof.

First, since $\{\alpha_n\}$ is a decreasing sequence and $(1 + M + kr)r < \tilde{r}$, then $\{\tilde{\alpha}_n\}$ is also decreasing. Therefore, we have that $x_k, x_k + F(x_k) \in \Omega$ is verified for $k = 0, 1, \dots, n$, and therefore there exist Θ_k, B_k such that $x_{k+1} = x_k - B_k F(x_k)$ is well defined.

Once shown the relationships (I) – (V) in their first two steps previously, we will use mathematical induction. Suppose that the relations (I) – (V) are true for $k = 1, \dots, n$ and we are going to show them for $k = n + 1$.

Observe that

$$F(x_n) = F(x_n) - F(x^*) = L_n (x_n - x^*)$$

and by (6)

$$x_{n+1} - x^* = x_n - B_n F(x_n) - x^* = (I - B_n L_n)(x_n - x^*),$$

furthermore

$$\begin{aligned} \|x_{n+1} - x^*\| &\leq \|I - B_n L_n\| \|x_n - x^*\| \\ &\leq (\|I - B_n F'(x^*)\| + \|B_n\| \|L_n - F'(x^*)\|) \|x_n - x^*\| \\ &\leq (\|I - B_n F'(x^*)\| + \|B_n\| k \|x_n - x^*\|) \|x_n - x^*\| \leq (\delta_n + \beta_n k \alpha_n) \|x_n - x^*\| \\ &\leq (\delta_n + \beta_n k \alpha_n) \alpha_n = \alpha_{n+1}. \end{aligned}$$

In addition

$$\begin{aligned} \|x_{n+1} + F(x_{n+1}) - x^*\| &\leq \|I + L_{n+1}\| \|x_{n+1} - x^*\| \\ &\leq (\|I + F'(x^*)\| + \|F'(x^*) - L_{n+1}\|) \|x_{n+1} - x^*\| \\ &\leq (1 + \|F'(x^*)\| + k \|x_{n+1} - x^*\|) \|x_{n+1} - x^*\| \\ &\leq (1 + M + k \|x_{n+1} - x^*\|) \|x_{n+1} - x^*\| \\ &\leq (1 + M + k \alpha_{n+1}) \alpha_{n+1} \\ &= \tilde{\alpha}_{n+1}. \end{aligned}$$

Assuming that $\alpha_{n+1} < \alpha_n$, then $\tilde{\alpha}_{n+1} < \tilde{\alpha}_n$ and $x_{n+1}, x_{n+1} + F(x_{n+1}) \in \Omega$. Consequently Θ_{n+1} and B_{n+1} are well defined.

So, we can consider

$$\begin{aligned} \|I - B_n \Theta_{n+1}\| &\leq \|I - B_n F'(x^*)\| + \|B_n\| \|\Theta_{n+1} - F'(x^*)\| \\ &\leq \|I - B_n F'(x^*)\| + \|B_n\| k (\|x_{n+1} - x^*\| + \|x_{n+1} + F(x_{n+1}) - x^*\|) \\ &\leq \delta_n + \beta_n k (\alpha_{n+1} + \tilde{\alpha}_{n+1}) = d_n, \end{aligned}$$

that implies

$$\|B_{n+1}\| = \|2B_n - B_n \Theta_{n+1} B_n\| \leq (1 + \|I - B_n \Theta_{n+1}\|) \|B_n\| \leq (1 + d_n) \beta_n = \beta_{n+1}.$$

Finally, to round off

$$\begin{aligned} \|I - B_{n+1} F'(x^*)\| &= \|I - (2B_n - B_n \Theta_{n+1} B_n) F'(x^*)\| \\ &\leq \|I - B_n F'(x^*)\|^2 + \|B_n\| \|\Theta_{n+1} - F'(x^*)\| \|B_n F'(x^*)\| \\ &\leq \|I - B_n F'(x^*)\|^2 + \|B_n\|^2 \|F'(x^*)\| k (\|x_{n+1} - x^*\| + \|x_{n+1} + F(x_{n+1}) - x^*\|) \\ &\leq \delta_n^2 + \beta_n^2 M k (\alpha_{n+1} + \tilde{\alpha}_{n+1}) = \delta_{n+1}. \end{aligned}$$

The proof is complete. \blacksquare

Once generalized the previous recurrence relations to every point of the sequence $\{x_n\}$, we have to guarantee that $\{x_n\}$ is a Cauchy sequence having into account these recurrence relations. For this, we first analyse the scalar sequences given by(21) in the next section.

3.2 Analysis of the scalar sequence

Now, we analyse the scalar sequence defined in (21) in order to prove later the semilocal convergence of the sequence $\{x_n\}$ in \mathbb{R}^m . For this, it suffices to see that $\{x_n\}$ is a Cauchy sequence. First, we give a technical lemma.

Lemma 3.2 *Let $\{\alpha_n\}$, $\{\tilde{\alpha}_n\}$, $\{d_n\}$ and $\{\delta_n\}$ be the sequences given by (21). If it is verified that*

$$(1 + M + kr)r < \tilde{r}, \quad \delta_1 < \delta_0 \quad \text{and} \quad (1 + d_0)^2(\delta_0 + k\beta\alpha_0) < 1, \quad (22)$$

then

- (a) $(\delta_0 + k\beta_0\alpha_0) < 1$ and $(1 + d_0)(\delta_0 + k\beta_0\alpha_0) < 1$,
- (b) the sequences $\{\alpha_n\}$, $\{n\}$, $\{d_n\}$ and $\{\delta_n\}$ are decreasing.

Proof.

Observe that as $(1 + d_0) > 1$, then $(1 + d_0)^2(\delta + k\beta\alpha) < 1$ implies that $(1 + d_0)(\delta + k\beta\alpha) < 1$. By the same reason $(\delta + k\beta\alpha) < 1$ and (a) holds.

We shall prove (b) by induction.

From (a), for $n = 1$, we have that $\alpha_1 = (\delta_0 + k\beta_0\alpha_0)\alpha_0 < \alpha_0$ and $\tilde{\alpha}_1 = (1 + M + k\alpha_1)\alpha_1 < (1 + M + k\alpha_0)\alpha_0 = \tilde{\alpha}_0$.

For $n = 2$, having into account that $\beta_1 \alpha_1 < (1+d_0)\beta_0 (\delta_0 + k \beta_0 \alpha_0) \alpha_0 < \beta_0 \alpha_0$, we obtain $\alpha_2 = (\delta_1 + k \beta_1 \alpha_1) \alpha_1 < (\delta_0 + k \beta_0 \alpha_0) \alpha_0 = \alpha_1$ and $\tilde{\alpha}_2 = (1 + M + k \alpha_2) \alpha_2 < (1 + M + k \alpha_1) \alpha_1 = \tilde{\alpha}_1$.

To analyze the sequences $\{d_n\}$ and $\{\delta_n\}$, we must also have in mind that

$$\begin{aligned} \beta_1^2 \alpha_2 &< (1 + d_0)^2 \beta_0^2 \alpha_2 < \beta_0^2 (1 + d_0)^2 (\delta_1 + k \beta_1 \alpha_1) \alpha_1 \\ &< \beta_0^2 (1 + d_0)^2 (\delta_0 + k \beta_0 \alpha_0) \alpha_1 < \beta_0^2 \alpha_1 \end{aligned}$$

and therefore it follows that $\beta_1^2 \tilde{\alpha}_2 < \beta_0^2 \tilde{\alpha}_1$, $\beta_1 \alpha_2 < \beta_0 \alpha_1$ and $\beta_1 \tilde{\alpha}_2 < \beta_0 \tilde{\alpha}_1$.

Then, to finish the case $n = 2$, taking into account that by hypothesis $\delta_1 < \delta_0$, we get $\delta_2 = \delta_1^2 + k M \beta_1^2 (\alpha_2 + \tilde{\alpha}_2) < \delta_0^2 + k M \beta_0^2 (\alpha_1 + \tilde{\alpha}_1) = \delta_1$ and $d_1 = \delta_1 + k \beta_1 (\alpha_2 + \tilde{\alpha}_2) < \delta + k \beta (\alpha_1 + \tilde{\alpha}_1) = d_0$.

From now, we suppose that $\alpha_0 > \alpha_1 > \dots > \alpha_n$, $\beta_0 \alpha_0 > \beta_1 \alpha_1 > \dots > \beta_n \alpha_n$ and $\beta_0^2 \alpha_1 > \beta_1^2 \alpha_2 > \dots > \beta_n^2 \alpha_{n+1}$ hold, which implies that the sequences $\{\tilde{\alpha}_k\}_{k=1}^n$, $\{\beta_k \tilde{\alpha}_k\}_{k=1}^n$, $\{\beta_k^2 \tilde{\alpha}_{k+1}\}_{k=1}^n$, $\{\beta_k \alpha_{k+1}\}_{k=1}^n$ and $\{\beta_k \tilde{\alpha}_{k+1}\}_{k=1}^n$ are decreasing, as well as $\{\delta_k\}_{k=1}^n$ and $\{d_k\}_{k=0}^{n-1}$ are.

We need to check the inductive step.

In first place, it is easy to prove:

$$\begin{aligned} \alpha_{n+1} &= (\delta_n + k \beta_n \alpha_n) \alpha_n < (\delta_{n-1} + k \beta_{n-1} \alpha_{n-1}) \alpha_{n-1} = \alpha_n, \\ \tilde{\alpha}_{n+1} &= (1 + M + k \alpha_{n+1}) \alpha_{n+1} < (1 + M + k \alpha_n) \alpha_n = \tilde{\alpha}_n, \\ d_n &= \delta_n + k \beta_n (\alpha_{n+1} + \tilde{\alpha}_{n+1}) < \delta_{n-1} + k \beta_{n-1} (\alpha_n + \tilde{\alpha}_n) = d_{n-1}, \\ \delta_{n+1} &= \delta_n^2 + k M \beta_n^2 (\alpha_{n+1} + \tilde{\alpha}_{n+1}) < \delta_{n-1}^2 + k M \beta_{n-1}^2 (\alpha_n + \tilde{\alpha}_n) = \delta_n. \end{aligned}$$

On the other hand

$$\begin{aligned} \beta_{n+1} \alpha_{n+1} < \beta_n \alpha_n &\Leftrightarrow (1 + d_n) \alpha_{n+1} < \alpha_n \Leftrightarrow (1 + d_n) (\delta_n + k \beta_n \alpha_n) \alpha_n < \alpha_n \\ &\Leftrightarrow (1 + d_n) (\delta_n + k \beta_n \alpha_n) < 1, \end{aligned}$$

which is true since that

$$(1 + d_n) (\delta_n + k \beta_n \alpha_n) < (1 + d_0) (\delta + k \beta \alpha_0) < 1.$$

Note that we also have

$$\alpha_{n+2} = (\delta_{n+1} + k \beta_{n+1} \alpha_{n+1}) \alpha_{n+1} < (\delta_n + k \beta_n \alpha_n) \alpha_n = \alpha_{n+1}$$

and therefore,

$$\begin{aligned} \beta_{n+1}^2 \alpha_{n+2} &< (1 + d_n)^2 \beta_n^2 \alpha_{n+2} < \beta_n^2 (1 + d_n)^2 (\delta_{n+1} + k \beta_{n+1} \alpha_{n+1}) \alpha_{n+1} \\ &< \beta_n^2 (1 + d_n)^2 (\delta_n + k \beta_n \alpha_n) \alpha_n < \beta_n^2 \alpha_{n+1}. \end{aligned}$$

Consequently $\{\alpha_n\}$, $\{\tilde{\alpha}_n\}$, $\{d_n\}$ and $\{\delta_n\}$ are decreasing.

The proof is complete. \blacksquare

3.3 A local convergence result

First of all, we notice that, fixed $x_0 \in B(x^*, r)$, if there is \tilde{r} , with the condition $(1 + M + kr)r < \tilde{r}$ (in order to verify $B(x^*, \tilde{r}) \subseteq \Omega$) and, in addition, r verifies the two other conditions given in (22), then $\{x_n\}$ will be convergent.

On the other hand, the conditions given in (22) can be written in the following way:

$$(1 + M + kr)r < \tilde{r}, \quad (23)$$

$$\delta_1 < \delta_0 \Leftrightarrow \delta^2 + kM\beta^2(\alpha_1 + \tilde{\alpha}_1) < \delta \Leftrightarrow 0 < \delta(1 - \delta) - rP_1(r), \quad (24)$$

$$\begin{aligned} (1 + d_0)^2(\delta_0 + k\beta\alpha_0) < 1 &\Leftrightarrow (1 + \delta + k\beta(\alpha_1 + \tilde{\alpha}_1))^2(\delta + k\beta r) < 1 \\ &\Leftrightarrow 0 < (1 - (1 + \delta)^2\delta) - rP_3(r), \end{aligned} \quad (25)$$

where P_1 is a polynomial of degree one and P_3 is a polynomial of degree three, both decreasing and concave in $(0, +\infty)$. In this situation, it is clear that if $1 - (1 + \delta)^2\delta > 0$, then there is always r checking (24) and (25).

Theorem 3.3

Using the above notations, under the initial conditions (C1) – (C4), we assume that there exists $r > 0$ verifying the conditions (23), (24), (25) and $B(x^, r) \subseteq \Omega$. Then, if we consider $x_0 \in B(x^*, r)$, the sequence $\{x_n\}$ given by (6) is well defined and converges to a solution x^* of $F(x) = 0$.*

Proof.

First, it is easy to prove from the hypothesis that $x_n, x_n + F(x_n) \in \Omega$ for $n \geq 1$. Then, the sequence $\{x_n\}$ given by (6) is well defined.

On the other hand, if we denote $L = \delta + k\beta r$, we have

$$\|x_1 - x^*\| < (\delta + k\beta r)\|x_0 - x^*\| = L\|x_0 - x^*\|$$

$$\|x_2 - x^*\| < (\delta_1 + k\beta_1\alpha_1)\|x_1 - x^*\| < (\delta + k\beta r)\|x_1 - x^*\| < L^2\|x_0 - x^*\|$$

So, in general, we obtain

$$\|x_n - x^*\| < (\delta_{n-1} + k\beta_{n-1}\alpha_{n-1})\|x_{n-1} - x^*\| < (\delta + k\beta r)\|x_{n-1} - x^*\| < L^n\|x_0 - x^*\|$$

Since $L < 1$ from lemma 3.2, it follows that the sequence $\{x_n\}$ given by (6) converges to a solution x^* of $F(x) = 0$. ■

Notice that, if $\Omega = \mathbb{R}^m$, the condition (23) it is not necessary.

3.4 An example

Next, we illustrate the previous result with the following example given in [10]. We choose the max-norm.

Let $F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ be defined as $F(x, y, z) = (x, y^2 + y, e^z - 1)$. It is obvious that the unique solution of the system is $x^* = (0, 0, 0)$.

From F , having into account (7), we have

$$F'(x, y, z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2y + 1 & 0 \\ 0 & 0 & e^z \end{pmatrix}$$

$$[(x, y, z), (u, v, w); F] = \begin{pmatrix} 1 & 0 & 0 \\ 0 & y + v + 1 & \\ 0 & 0 & \frac{e^z - e^w}{z - w} \end{pmatrix}.$$

So, $F'(x^*)$ is the identity matrix 3×3 . Then, $\|F'(x^*)\| = 1$ and consider $B_0 = \text{diag}\{\beta, \beta, \beta\}$ with $\beta = 0.75$ and $\delta = 0.25$. On the other hand, there exists $\tilde{r} = 1$, such that $B(0, \tilde{r}) = \{w \in \mathbb{R}^3 : \|w\| < 1\} \subset \mathbb{R}^3$, and it is easy to prove that

$$\begin{aligned} \|[(x, y, z), (u, v, w); F] - F'(0, 0, 0)\| &\leq \max\{|y + v|, |\frac{e^z - e^w}{z - w} - 1|\} \\ &\leq \|(x, y, z)\| + \|(u, v, w)\|, \end{aligned}$$

in $B(0, \tilde{r})$. Therefore, $M = 1$, $k = 1$ and considering $\alpha_0 = 0.246627$ we obtain:

$$(1 + M + kr)r = 0.554078 < \tilde{r}, \quad \alpha_1 = 0.107275, \quad \tilde{\alpha}_1 = 0.226058,$$

$$\delta - \delta_1 = 5.55112 \times 10^{-17}, \quad d_0 = 0.5, \quad 1 - (1 + d_0)^2(\delta_0 + k\beta\alpha_0) = 0.0213177$$

Therefore the iterative process (6) is convergent from any starting point belonging to $B(x^*, 0.246627)$.

4 Numerical experiments

In this section, we include two experiments to test the proposed algorithm (6). In the first one, we check numerically its order of convergence and its stability behavior. Moreover, we propose specific chooses of the initial matrix B_0 in order to improve the stability of the classical Steffensen method (4). In the final example, we apply our iterative method to solve the non-linear systems of equations that appear to approximate a stiff differential problem with an implicit method.

4.1 Academic example

We consider the academic system of equations $F(x, y) = (0, 0)$ given by:

$$\begin{aligned} \left(2x - \frac{x^2}{\epsilon}\right) + \left(y - \frac{y^2}{2\epsilon}\right) &= 0, \\ x + y &= 0. \end{aligned} \tag{26}$$

This system has as solution $(x^*, y^*) = (0, 0)$ and its Jacobian matrix is given by the following matrix

$$\begin{pmatrix} 2 - 2\frac{x}{\epsilon} & 1 - \frac{y}{\epsilon} \\ 1 & 1 \end{pmatrix}$$

On the other hand, having into account (7), the matrix $[x, \tilde{x}; F]$, with $x = (x_1, y_1)$ and $\tilde{x} = (x_2, y_2)$, is given by

$$\begin{pmatrix} 2 - \frac{x_1+x_2}{\epsilon} & 1 - \frac{y_1+y_2}{\epsilon} \\ 1 & 1 \end{pmatrix}$$

- Stability

The parameter ϵ (when $\epsilon \rightarrow 0$) increases the condition number of the difference divided matrix for a given initial guess and the Steffensen method (4) should have problems of convergence to the solution for small values of ϵ . Moreover, notice that $F'(\epsilon, \epsilon)$ is not invertible.

We compute the maximum of the condition numbers of the linear systems that appear in the application of the Steffensen method (4) ($\|A\| \cdot \|A^{-1}\|$) and the maximum of the conditions numbers in all the matrix multiplications in the Moser-Steffensen type method (6) ($\frac{\|A\| \cdot \|B\|}{\|AB\|}$).

In table 1, the vector (ϵ, ϵ) is inside of the ball containing the initial guess and the solution. The Steffensen method (4) diverges.

This numerical behavior is similar for smaller parameters of ϵ , as we can see in the table 2 ($\epsilon = 10^{-1}$). The maximum of the condition numbers for the Steffensen method (4) is $6.09 \cdot 10^2$ (too big) and for the Moser-Steffensen type method (6) smaller than 30. Moreover, the sequences of condition numbers for both methods are increasing and decreasing sequences.

For this example, the Steffensen method (4) has a small region of convergence. However, the method (6) only reduces a little its velocity.

Table 1: System (26). Errors for $(x_0, y_0) = (-1, 1)$, $\|B_0 F'(-1, 1)\| \leq 10^{-3}$ and $\epsilon = 1$.

n	Steffensen	Moser-Steffensen
1	$1.55 \cdot 10^1$	$1.00 \cdot 10^0$
2	$1.84 \cdot 10^1$	$3.76 \cdot 10^{-1}$
3	$2.12 \cdot 10^1$	$1.08 \cdot 10^{-1}$
4	$2.41 \cdot 10^1$	$1.80 \cdot 10^{-2}$
5	$2.69 \cdot 10^1$	$9.12 \cdot 10^{-4}$
6	$2.98 \cdot 10^1$	$3.61 \cdot 10^{-6}$
7	$3.26 \cdot 10^1$	$7.60 \cdot 10^{-11}$
8	$3.54 \cdot 10^1$	$4.18 \cdot 10^{-20}$

Table 2: System (26). Errors for $(x_0, y_0) = (-0.25, 0.25)$, $\|B_0 F'(-0.25, 0.25)\| \leq 10^{-3}$ and $\epsilon = 10^{-1}$.

n	Steffensen	Moser-Steffensen
1	$1.70 \cdot 10^0$	$6.84 \cdot 10^{-1}$
2	$1.98 \cdot 10^0$	$2.08 \cdot 10^{-1}$
3	$2.27 \cdot 10^0$	$8.90 \cdot 10^{-2}$
4	$2.55 \cdot 10^0$	$3.95 \cdot 10^{-2}$
5	$2.83 \cdot 10^0$	$6.80 \cdot 10^{-2}$
6	$3.12 \cdot 10^0$	$6.95 \cdot 10^{-4}$
7	$3.41 \cdot 10^0$	$1.22 \cdot 10^{-5}$
8	$3.69 \cdot 10^0$	$5.38 \cdot 10^{-9}$
9	$3.97 \cdot 10^0$	$1.33 \cdot 10^{-15}$
10	$4.25 \cdot 10^0$	$1.00 \cdot 10^{-28}$

This is the main advantage of the Moser-Steffensen type method (6). The condition number of the operations used in the classical Steffensen method (4) should be large (in the previous cases of divergence the condition number goes to infinity) and there is not a general strategy to find preconditioners for a given linear system. However, by construction, the condition number in the operations of the proposed method (6) (matrix multiplications) seems controlled with our election of B_0 .

In Moser-type algorithms, as (6), the sequence of matrices B_n converges to the inverse of the Jacobian at the solution. For this reason, a good candidate for B_0 is an approximation to the inverse of the Jacobian at the initial guess [12].

- Order of convergence

In table 3, the method obtains the results expected by our theoretical analysis and the second order convergence is clear. The vector (ϵ, ϵ) is outside the convergence region associated to the initial guess. We compute the maximum of the condition numbers of the linear systems that appear in the application of the Steffensen method (4) and the maximum of the conditions numbers in all the matrix multiplications in our method (6). In this case, the maximum for the Steffensen method (4) and for our method (6) are smaller than 10, and both methods work well.

Table 3: System (26). Errors for $(x_0, y_0) = (-1, 1)$, $\|B_0 F'(-1, 1)\| \leq 10^{-3}$ and $\epsilon = 3$.

n	Steffensen	Moser-Steffensen
1	$1.41 \cdot 10^0$	$3.55 \cdot 10^{-1}$
2	$7.61 \cdot 10^{-1}$	$5.09 \cdot 10^{-2}$
3	$2.40 \cdot 10^{-1}$	$1.86 \cdot 10^{-3}$
4	$2.60 \cdot 10^{-2}$	$3.74 \cdot 10^{-6}$
5	$3.11 \cdot 10^{-4}$	$2.01 \cdot 10^{-11}$
6	$4.56 \cdot 10^{-8}$	$7.10 \cdot 10^{-22}$
7	$9.79 \cdot 10^{-16}$	

The results in the table 4 are similar to the first case, both methods have second order of convergence.

In table 4 case, we consider a smaller ϵ but again the point (ϵ, ϵ) is outside the ball including the initial guess (closer also to the solution) and the solution. In this case, our method preserve the second order of convergence (condition number smaller than 10), however the Steffensen method diverges (with condition number $1.80 \cdot 10^2$ in the last iteration).

- Election of the initial matrix B_0

Table 4: System (26). Errors for $(x_0, y_0) = (-0.5, 0.5)$, $\|B_0 F'(-0.5, 0.5)\| \leq 10^{-3}$ and $\epsilon = 1$.

n	Steffensen	Moser-Steffensen
1	$1.49 \cdot 10^0$	$2.12 \cdot 10^{-1}$
2	$2.75 \cdot 10^0$	$4.21 \cdot 10^{-2}$
3	$3.35 \cdot 10^0$	$3.09 \cdot 10^{-3}$
4	$6.82 \cdot 10^0$	$2.68 \cdot 10^{-5}$
5	$9.80 \cdot 10^0$	$2.77 \cdot 10^{-9}$
6	$1.27 \cdot 10^1$	$3.75 \cdot 10^{-17}$
7	$1.56 \cdot 10^1$	$8.71 \cdot 10^{-33}$
8	$1.84 \cdot 10^1$	
9	$2.13 \cdot 10^1$	
10	$2.41 \cdot 10^1$	

In general, as we indicated before, a good candidate for B_0 is an approximation to the inverse of the Jacobian matrix at the initial guess.

On the other hand, it is not necessary to consider B_0 a really accurate approximation to the Jacobian at the initial guess, as we can see in table 5. In particular, we can take some iterations of some of the algorithms that appear for instance in [2].

Table 5: System (26). Errors for Moser-Steffensen, $(x_0, y_0) = (-2, 2)$ and $\epsilon = 3$.

n	$\ B_0 F'(-2, 2)\ \leq 1$	$\ B_0 F'(-2, 2)\ \leq 10^{-1}$	$\ B_0 F'(-2, 2)\ \leq 10^{-3}$
1	$1.84 \cdot 10^0$	$1.10 \cdot 10^0$	$9.44 \cdot 10^{-1}$
2	$8.75 \cdot 10^{-1}$	$2.83 \cdot 10^{-1}$	$2.24 \cdot 10^{-1}$
3	$2.53 \cdot 10^{-1}$	$3.56 \cdot 10^{-2}$	$2.43 \cdot 10^{-2}$
4	$3.29 \cdot 10^{-2}$	$9.86 \cdot 10^{-4}$	$4.87 \cdot 10^{-4}$
5	$8.61 \cdot 10^{-4}$	$1.12 \cdot 10^{-6}$	$2.82 \cdot 10^{-7}$
6	$8.37 \cdot 10^{-7}$	$1.89 \cdot 10^{-12}$	$1.21 \cdot 10^{-13}$
7	$1.01 \cdot 10^{-12}$	$6.57 \cdot 10^{-24}$	$2.71 \cdot 10^{-26}$
7	$1.83 \cdot 10^{-24}$		

Finally, in the table 7, we force the method to take the bad iteration

(ϵ, ϵ) (here the Jacobian is not invertible). Only with the new approach we are able to find the solution (the Steffensen method diverges).

Indeed, we consider $(x_0, y_0) = (\epsilon, \epsilon)$. For this situations, a possibility is to take the initial matrix $B_0 = \delta I_2$, where δ is a small parameter (10^{-2} in our experiments) and I_2 is the identity matrix. When the method leaves the conflict zone, it recovers its good properties (second order convergence).

Table 6: System (26). Errors for $(x_0, y_0) = (2, 2)$, $\epsilon = 2$ and $B_0 = 10^{-2} I_2$.

n	Moser-Steffensen
10	$1.13 \cdot 10^{-2}$
11	$2.81 \cdot 10^{-4}$
12	$2.07 \cdot 10^{-7}$
13	$1.30 \cdot 10^{-13}$
14	$5.88 \cdot 10^{-26}$

4.2 A stiff problem: Chapman atmosphere

This model represents the Chapman mechanism for the generation of the ozone and the oxygen singlet. In this example, the concentration of the oxygen $y_3 = [O_2]$ will be held constant. It is a severe test for a stiff ODE package [15] governed by the following equations:

$$\begin{aligned} y_1'(t) &= 2k_3(t)y_3 + k_4(t)y_2(t) - (k_1y_3 + k_2y_2(t))y_1(t), \\ y_2'(t) &= k_1y_1(t)y_3 - (k_2y_1(t) + k_4(t))y_2(t), \end{aligned}$$

with $y_3 = 3.7 \times 10^{16}$, $k_1 = 1.63 \times 10^{-16}$, $k_2 = 4.66 \times 10^{-16}$,

$$k_i(t) = \begin{cases} \exp\left(\frac{a_i}{\sin(\omega t)}\right), & \text{if } \sin(\omega t) > 0 \\ 0, & \text{otherwise} \end{cases}$$

for $i = 3, 4$, with $a_3 = 22.62$, $a_4 = 7.601$ and $\omega = \frac{\pi}{43200}$. The constant 43200 is 12 h measured in seconds. The initial conditions are $y_1(0) = 10^6$ and $y_2(0) = 10^{12}$.

This problem has important features like:

- The Jacobian matrix is not a constant.

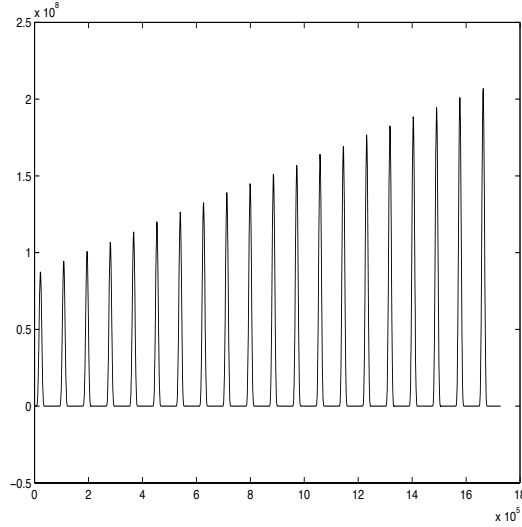


Figure 1: First component of the Chapman atmosphere problem

- The diurnal effect is present.
- The oscillations are fast.
- The time interval used is fairly long, $0 \leq t \leq 8.64 \cdot 10^5$, or 10 days.

Let $h > 0$. Given different coefficients c_i , $1 \leq i \leq s$ there is a (unique for h sufficiently small) polynomial of collocation $q(t)$ of degree less than or equal to s such that

$$q(t_0) = y_0, \quad q'(t_0 + c_i h) = f(t_0 + c_i h, q(t_0 + c_i h)) \quad \text{if } 1 \leq i \leq s. \quad (27)$$

The collocation methods are defined by an approximation $y(t) \simeq q(t)$, and are equivalent to implicit RK methods of s stages

$$\begin{aligned} k_i &= f(t_0 + c_i h, y_0 + h \sum_{j=1}^s a_{i,j} k_j), \\ y_1 &= y_0 + h \sum_{i=1}^s b_i k_i, \end{aligned} \quad (28)$$

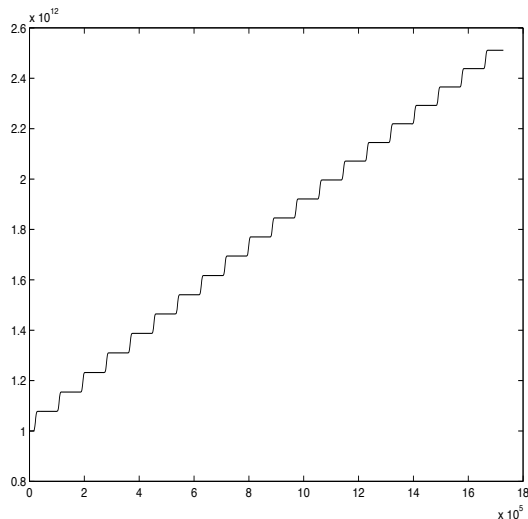


Figure 2: Second component of the Chapman atmosphere problem

for the coefficients

$$\begin{aligned}
 a_{i,j} &= \int_0^{c_i} \prod_{l \neq j} \frac{u - c_l}{c_j - c_l} du, \\
 b_i &= \int_0^1 \prod_{l \neq i} \frac{u - c_l}{c_i - c_l} du.
 \end{aligned}
 \tag{29}$$

The coefficients c_i play the role of the nodes of the quadrature formula, and the associated coefficients b_i are analogous to the weights. From (29) we can find implicit RK methods called Gauss of order $2s$, Radau IA and Radau IIA of order $2s - 1$ and Lobatto IIIA of order $2s - 2$. See [15] for more details.

We consider the implicit fourth order Gauss method ($s = 2$ as collocation method). We approximate the associated nonlinear systems of equations using our Moser-Steffensen's method as a black box. We obtain a good approximation as we can see in Figures 1 and 2. Note that $y_2 = [0_3]$ looks like a staircase with a rise at midday every day and $y_1 = [O]$ looks like a spike with its amplitude increases each day.

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