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On interpolation variants of Newton's method for functions of several variables ☆

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ABSTRACT

A generalization of the variants of Newton's method based on interpolation rules of quadrature is obtained, in order to solve systems of nonlinear equations. Under certain conditions, convergence order is proved to be $2d + 1$, where d is the order of the partial derivatives needed to be zero in the solution. Moreover, different numerical tests confirm the theoretical results and allow us to compare these variants with Newton's classical method, whose convergence order is $d + 1$ under the same conditions.

1. Introduction

Several modifications have been made to the classical Newton's method in order to accelerate the convergence or to reduce the number of operations and evaluations of functions in each step of the iterative process.

In dimension one, the variant developed by Weerakoon and Fernando in [1] use the trapezoidal quadrature formula in order to obtain the third order of convergence; Ozban extended this idea on [2], obtaining some new methods with third-order convergence. Moreover, some of the described methods are included in the family of modified Newton's methods of order three, defined by Frontini et al. in [3], by using a general interpolatory quadrature formula. The analysis made by Ford and Pennline in [4] shows that a modified Newton's method with order of convergence d can be found if all the derivatives at the solution, from order two to $d - 1$, are zero. In [5,6] the authors suggested the extension of the application of quadrature formulas in the development of new adjustments of Newton's method to functions of several variables, using open and closed quadrature formulas whose truncation error was up to $O(h^5)$, in order to improve the order of convergence. These methods are included in the family of modified Newton's methods of order three, defined by Frontini et al. in [7].

In this paper, a general interpolatory quadrature formula is used in order to obtain a family of modified Newton's methods for nonlinear systems, with order of convergence up to $2d + 1$ when the partial derivatives of each coordinate function in the solution, from order two until d, are zero.

Let us consider the problem of finding a real zero of a function $F : D \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}^n$, that is, a real solution α, of the nonlinear system $F(x) = 0$, of n equations with n unknowns. In Section 2, we analyze a general iterative formula for a nonlinear system and we study the additional conditions that certain parameters must satisfy in order to obtain a method with a particular order of convergence. To get this aim, we study the convergence of the different methods by using the following result.

Theorem 1 (*See [8]*). *Let $G(x)$ be a fixed point function with continuous partial derivatives of order p with respect to all components of x. The iterative method $x^{(k+1)} = G(x^{(k)})$ is of order p if*

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$$G(\alpha) = \alpha;$$
$$\frac{\partial^k g_i(\alpha)}{\partial x_{j_1} \partial x_{j_2} \cdots \partial x_{j_k}} = 0, \quad \textit{for all } 1 \le k \le p-1,\ 1 \le i, j_1, \ldots, j_k \le n;$$
$$\frac{\partial^p g_i(\alpha)}{\partial x_{j_1} \partial x_{j_2} \cdots \partial x_{j_p}} \neq 0, \quad \textit{for at least one value of } i, j_1, \ldots, j_p$$

where g_i, $i = 1, 2, \ldots, n$, *are the component functions of* G.

In order to compare the different methods, we consider the order of convergence and the *efficiency index* defined in [9] as $p^{1/d}$, where p is the order of convergence and d is the total number of new function evaluations (per iteration) required by the method. We will use these indices as well as $CE = p^{1/(d+op)}$, which we call *computational efficiency index*, where op is the number of operations per iteration. We recall that the number of products and quotients that we need for solving a linear system, by using Gaussian elimination, is

$$\frac{1}{3}n^3 + n^2 - \frac{1}{3}n,$$

where n is the size of the system.

The last section is devoted to numerical results obtained by applying some of the described methods to several systems of nonlinear equations. From these results, we compare the different methods, confirming the theoretical results and improving them, in some cases.

2. Description and convergence analysis of the method

Let $F : D \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}^n$ be a sufficiently differentiable function and α be a zero of the nonlinear system $F(x) = 0$. The following result will be used to describe the Newton method and the family of modified methods; its proof can be found in [10].

Lemma 1. *Let* $F : D \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}^n$ *be continuously differentiable on a convex set D. Then, for any* $x, y \in D$, *F satisfies*

$$F(y) - F(x) = \int_0^1 J_F(x + t(y - x))(y - x)\mathrm{d}t. \tag{1}$$

From iterate $x^{(k)}$ and (1), we have

$$F(y) = F(x^{(k)}) + \int_0^1 J_F(x^{(k)} + t(y - x^{(k)}))(y - x^{(k)})\mathrm{d}t. \tag{2}$$

If we estimate $J_F(x^{(k)} + t(y - x^{(k)}))$ in $[0, 1]$ by its value in $t = 0$, that is by $J_F(x^{(k)})$, and take $y = \alpha$, then

$$0 \approx F(x^{(k)}) + J_F(x^{(k)})(\alpha - x^{(k)}),$$

is obtained, and a new approximation of α can be done by

$$x^{(k+1)} = x^{(k)} - J_F(x^{(k)})^{-1}F(x^{(k)}),$$

which is the classical *Newton's method* (CN) for $k = 0, 1, \ldots$.

In this context, an estimation of (2) can be done by means of any quadrature formula, and if $y = \alpha$ is taken, then

$$0 \approx F(x^{(k)}) + \left[\sum_{h=1}^{m} A_h J_F(\eta_h(x^{(k)}))\right](\alpha - x^{(k)}),$$

is obtained, where $A_h \in \mathbb{R}$, $h \in \{1, \ldots, m\}$ are the coefficients of the quadrature rule and $\eta_h(x) = x - \tau_h J_F^{-1}(x)F(x)$, being τ_h, $h = 1, 2, \ldots, m$, the knots in $[0, 1]$. So, a new approximation $x^{(k+1)}$ of α is given by

$$x^{(k+1)} = x^{(k)} - \left[\sum_{h=1}^{m} A_h J_F(\eta_h(x^{(k)}))\right]^{-1} F(x^{(k)}). \tag{3}$$

Let us remark that the first condition that the parameters A_h must satisfy is

$$\sum_{h=1}^{m} A_h = 1, \tag{4}$$

as far as being A_h the weights of an interpolatory quadrature formula.

We proceed to study the convergence order of this collection of iterative methods for nonlinear systems, which is closely related to the value of the parameters A_h and τ_h. In the following, we consider $x \in \mathbb{R}^n$, $n > 1$, and denote by $J_{ij}(x)$ the (i, j)-entry of the Jacobian matrix, and by $H_{ij}(x)$ the respective entry of its inverse, so

$$\sum_{j=1}^{n} H_{ij}(x)J_{jk}(x) = \delta_{ik}, \tag{5}$$

where δ_{ik} is the Kronecker symbol. We also denote by $f_j(x)$, $j = 1, 2, \ldots, n$, the coordinate functions of $F(x)$. Moreover, it can be easily proved that:

$$\sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} \frac{\partial f_i(x)}{\partial x_r} = -\sum_{i=1}^{n} H_{ji}(x) \frac{\partial^2 f_i(x)}{\partial x_l \partial x_r}, \tag{6}$$

$$\sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_s \partial x_l} \frac{\partial f_i(x)}{\partial x_r} = -\sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} \frac{\partial^2 f_i(x)}{\partial x_s \partial x_r} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_s} \frac{\partial^2 f_i(x)}{\partial x_r \partial x_l} - \sum_{i=1}^{n} H_{ji}(x) \frac{\partial^3 f_i(x)}{\partial x_s \partial x_r \partial x_l}, \tag{7}$$

and

$$\begin{aligned}\sum_{i=1}^{n} \frac{\partial^3 H_{ji}(x)}{\partial x_u \partial x_s \partial x_l} \frac{\partial f_i(x)}{\partial x_r} = & -\sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_s \partial x_l} \frac{\partial^2 f_i(x)}{\partial x_u \partial x_r} - \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_u \partial x_l} \frac{\partial^2 f_i(x)}{\partial x_s \partial x_r} - \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_u \partial x_s} \frac{\partial^2 f_i(x)}{\partial x_l \partial x_r} \\ & - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} \frac{\partial^3 f_i(x)}{\partial x_u \partial x_s \partial x_r} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_s} \frac{\partial^3 f_i(x)}{\partial x_u \partial x_r \partial x_l} \\ & - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_u} \frac{\partial^3 f_i(x)}{\partial x_s \partial x_r \partial x_l} - \sum_{i=1}^{n} H_{ji}(x) \frac{\partial^4 f_i(x)}{\partial x_u \partial x_s \partial x_r \partial x_l}.\end{aligned} \tag{8}$$

The following result, partially proved in [8], will be useful in the proof of the main theorem.

Lemma 2. *Let $\lambda(x)$ be the iteration function of classical Newton's method, whose coordinates are:*

$$\lambda_j(x) = x_j - \sum_{i=1}^{n} H_{ji}(x) f_i(x),$$

for $j = 1, \ldots, n$. Then,

$$\frac{\partial \lambda_j(\alpha)}{\partial x_l} = 0, \tag{9}$$

$$\frac{\partial^2 \lambda_j(\alpha)}{\partial x_r \partial x_l} = \sum_{i=1}^{n} H_{ji}(\alpha) \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}, \tag{10}$$

$$\frac{\partial^3 \lambda_j(\alpha)}{\partial x_s \partial x_r \partial x_l} = \sum_{i=1}^{n} \left[\frac{\partial H_{ji}(\alpha)}{\partial x_r} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_l} + \frac{\partial H_{ji}(\alpha)}{\partial x_s} \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l} + \frac{\partial H_{ji}(\alpha)}{\partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_r} \right] + 2 \sum_{i=1}^{n} H_{ji}(\alpha) \frac{\partial^3 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l}, \tag{11}$$

and

$$\begin{aligned}\frac{\partial^4 \lambda_j(\alpha)}{\partial x_u \partial x_s \partial x_r \partial x_l} = & \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_s \partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_u} + \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_r \partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_u} + \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_r \partial x_s} \frac{\partial^2 f_i(\alpha)}{\partial x_l \partial x_u} + \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_u \partial x_r} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_l} \\ & + \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_u \partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_r} + \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(\alpha)}{\partial x_u \partial x_s} \frac{\partial^2 f_i(\alpha)}{\partial x_l \partial x_r} + 2 \sum_{i=1}^{n} \frac{\partial H_{ji}(\alpha)}{\partial x_r} \frac{\partial^3 f_i(\alpha)}{\partial x_u \partial x_s \partial x_l} \\ & + 2 \sum_{i=1}^{n} \frac{\partial H_{ji}(\alpha)}{\partial x_s} \frac{\partial^3 f_i(\alpha)}{\partial x_u \partial x_r \partial x_l} + 2 \sum_{i=1}^{n} \frac{\partial H_{ji}(\alpha)}{\partial x_l} \frac{\partial^3 f_i(\alpha)}{\partial x_u \partial x_s \partial x_r} + 2 \sum_{i=1}^{n} \frac{\partial H_{ji}(\alpha)}{\partial x_u} \frac{\partial^3 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l} \\ & + 3 \sum_{i=1}^{n} H_{ji}(\alpha) \frac{\partial^4 f_i(\alpha)}{\partial x_u \partial x_s \partial x_r \partial x_l},\end{aligned} \tag{12}$$

for $i, j, l, r, s, u \in \{1, 2, \ldots, n\}$.

Proof. Let us note that by direct differentiation, if j and l are arbitrary and fixed,

$$\frac{\partial \lambda_j(x)}{\partial x_l} = \delta_{jl} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} f_i(x) - \sum_{i=1}^{n} H_{ji}(x) J_{il}(x),$$

and applying (5)

$$\frac{\partial \lambda_j(x)}{\partial x_l} = -\sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} f_i(x).$$

We set now $x = \alpha$. Hence,

$$\frac{\partial \lambda_i(\alpha)}{\partial x_k} = -\sum_{i=1}^{n} \frac{\partial H_{ji}(\alpha)}{\partial x_l} f_i(\alpha) = 0,$$

since $f_i(\alpha) = 0$. If the second derivative of $\lambda_j(x)$ is analyzed for j, l and r arbitrary and fixed, we have

$$\frac{\partial^2 \lambda_j(x)}{\partial x_r \partial x_l} = -\sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_r \partial x_l} f_i(x) - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} \frac{\partial f_i(x)}{\partial x_r}. \tag{13}$$

Setting $x = \alpha$ in (13) and using (6), we have

$$\frac{\partial^2 \lambda_j(\alpha)}{\partial x_r \partial x_l} = \sum_{i=1}^{n} H_{ji}(\alpha) \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}.$$

Again, by direct differentiation on (13), being s arbitrary and fixed, and using expression (7), we obtain

$$\frac{\partial^3 \lambda_j(x)}{\partial x_s \partial x_r \partial x_l} = -\sum_{i=1}^{n} \frac{\partial^3 H_{ji}(x)}{\partial x_s \partial x_r \partial x_l} f_i(x) + \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} \frac{\partial^2 f_i(x)}{\partial x_r \partial x_s} + \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_r} \frac{\partial^2 f_i(x)}{\partial x_s \partial x_l} + \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_s} \frac{\partial^2 f_i(x)}{\partial x_r \partial x_l}$$
$$+ 2\sum_{i=1}^{n} H_{ji}(x) \frac{\partial^3 f_i(x)}{\partial x_s \partial x_r \partial x_l}. \tag{14}$$

And, evaluating in $x = \alpha$, relation (11) is obtained. Finally, if we evaluate in $x = \alpha$ the expression obtained by direct differentiation on (14), with u arbitrary and fixed, and using (8), the relation (12) is obtained. □

Let us note that, by applying Theorem 1 and using expressions (9) and (10) in Lemma 2, it can be concluded that the convergence order of Newton's method is $p = 2$.

With a similar proof to the previous result we can establish the next lemma that describes some partial results about the iteration function of the method described in (3).

Lemma 3. *Let $\eta_k(x)$ be the iteration function*

$$\eta_k(x) = x - \tau_k J_F^{-1}(x) F(x),$$

for $k = 1, \ldots, m$, where τ_k are the knots in $[0, 1]$. *Then,*

$$\left.\frac{\partial (\eta_k(x))_q}{\partial x_l}\right|_{x=\alpha} = (1 - \tau_k)\delta_{ql}, \tag{15}$$

$$\left.\frac{\partial^2 (\eta_k(x))_q}{\partial x_r \partial x_l}\right|_{x=\alpha} = \sum_{i=1}^{n} \tau_k H_{qi}(\alpha) \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}, \tag{16}$$

and

$$\left.\frac{\partial^3 (\eta_k(x))_q}{\partial x_s \partial x_r \partial x_l}\right|_{x=\alpha} = \tau_k \sum_{i=1}^{n} \left(\frac{\partial H_{qi}(\alpha)}{\partial x_r} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_l} + \frac{\partial H_{qi}(\alpha)}{\partial x_s} \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l} + \frac{\partial H_{qi}(\alpha)}{\partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_r} \right) + 2\tau_k \sum_{i=1}^{n} H_{qi}(\alpha) \frac{\partial^3 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l}, \tag{17}$$

for $q, l, r, s \in \{1, 2, \ldots, n\}$.

Finally, it is easy to prove the following result.

Lemma 4. *Let $\eta_k(x)$ be the iteration function*

$$\eta_k(x) = x - \tau_k J_F^{-1}(x) F(x),$$

for $k = 1, \ldots, m$, where τ_k are the knots in $[0, 1]$. *Then,*

$$\left.\frac{\partial J_{ij}(\eta_k(x))}{\partial x_l}\right|_{x=\alpha} = (1 - \tau_k) \frac{\partial^2 f_i(\alpha)}{\partial x_l \partial x_j}, \tag{18}$$

$$\left.\frac{\partial^2 J_{ij}(\eta_k(x))}{\partial x_r \partial x_l}\right|_{x=\alpha} = (1 - \tau_k)^2 \frac{\partial^3 f_i(\alpha)}{\partial x_r \partial x_l \partial x_j} + \sum_{q=1}^{n} \frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_j} H_{qi}(\alpha) \tau_k \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}, \tag{19}$$

and

$$\left.\frac{\partial^3 J_{ij}(\eta_k(x))}{\partial x_s \partial x_r \partial x_l}\right|_{x=\alpha} = (1-\tau_k)^3 \frac{\partial^4 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l \partial x_j} + \sum_{q=1}^{n} \frac{\partial^3 f_i(\alpha)}{\partial x_q \partial x_l \partial x_j} H_{qi}(\alpha)\tau_k(1-\tau_k)\frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_r}$$
$$+ \sum_{q=1}^{n} \frac{\partial^3 f_i(\alpha)}{\partial x_q \partial x_r \partial x_j} H_{qi}(\alpha)\tau_k(1-\tau_k)\frac{\partial^2 f_i(\alpha)}{\partial x_l \partial x_s} + \sum_{q=1}^{n} \frac{\partial^3 f_i(\alpha)}{\partial x_q \partial x_s \partial x_j} H_{qi}(\alpha)\tau_k(1-\tau_k)\frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}$$
$$+ \sum_{q=1}^{n} \frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_j} \tau_k \left(\frac{\partial H_{qi}(\alpha)}{\partial x_r} \frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_l} + \frac{\partial H_{qi}(\alpha)}{\partial x_s} \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l} \right)$$
$$+ \sum_{q=1}^{n} \frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_j} \tau_k \left(\frac{\partial H_{qi}(\alpha)}{\partial x_l} \frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_s} + 2H_{qi}(\alpha) \frac{\partial^3 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l} \right), \tag{20}$$

for $i, j, l, r, s \in \{1, 2, \ldots, n\}$.

By using the previous results, we analyze the convergence of the methods described by (3).

Theorem 2. *Let* $F : D \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}^n$ *be sufficiently differentiable at each point of an open neighborhood* D *of* $\alpha \in \mathbb{R}^n$, *that is a solution of the system* $F(x) = 0$. *Let us suppose that* $J_F(x)$ *is continuous and nonsingular in* α. *Then the sequence* $\{x^{(k)}\}_{k\geq 0}$ *obtained using the iterative expression* (3) *converges to* α *with convergence order:*

- $2d+1$ *if*

$$\sum_{k=1}^{m} A_k(1-\tau_k)^h = \frac{1}{h+1}, \quad h = 0, 1, \ldots, 2d-1$$

and

$$\frac{\partial^j f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2} \cdots \partial x_{a_j}} = 0, \quad 1 \leq i, a_1, \ldots, a_j \leq n, \ j = 2, 3, \ldots, d.$$

- $2d$ *if*

$$\sum_{k=1}^{m} A_k(1-\tau_k)^h = \frac{1}{h+1}, \quad h = 0, 1, \ldots, 2d-2$$

and

$$\frac{\partial^j f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2} \cdots \partial x_{a_j}} = 0, \quad 1 \leq i, a_1, \ldots, a_j \leq n, \ j = 2, 3, \ldots, d.$$

Proof. Let us consider the solution $\alpha \in \mathbb{R}^n$ of the nonlinear system $F(x) = 0$ as a fixed point of the iteration function $G : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ described in (3). Let us denote by $g_i : \mathbb{R}^n \longrightarrow \mathbb{R}$, $i = 1, 2, \ldots, n$, the coordinate functions of G.

Expanding $g_i(x)$, $x \in \mathbb{R}^n$, in a Taylor series about α yields

$$g_i(x) = g_i(\alpha) + \sum_{a_1=1}^{n} \frac{\partial g_i(\alpha)}{\partial x_{a_1}} e_{a_1} + \frac{1}{2}\sum_{a_1=1}^{n}\sum_{a_2=1}^{n} \frac{\partial^2 g_i(\alpha)}{\partial x_{a_1}\partial x_{a_2}} e_{a_1}e_{a_2} + \frac{1}{6}\sum_{a_1=1}^{n}\sum_{a_2=1}^{n}\sum_{a_3=1}^{n} \frac{\partial^3 g_i(\alpha)}{\partial x_{a_1}\partial x_{a_2}\partial x_{a_3}} e_{a_1}e_{a_2}e_{a_3} + \cdots \tag{21}$$

where $e_{a_k} = x_{a_k} - \alpha_{a_k}$, $1 \leq a_1, \ldots, a_k \leq n$.

We denote by $L_{ij}(x)$ the (i,j)-entry of matrix $L(x) = \sum_{k=1}^{m} A_k J_F(\eta_k(x))$, by $H_{ij}(x)$ the (i,j)-entry of $J_F^{-1}(x)$ and by $M_{ij}(x)$ the (i,j)-entry of $L^{-1}(x)$. Thus, the jth component of the iteration function is

$$g_j(x) = \lambda_j(x) + \sum_{i=1}^{n} H_{ji}(x) f_i(x) - \sum_{i=1}^{n} M_{ji}(x) f_i(x). \tag{22}$$

Since $M_{ji}(x)$ and $L_{ij}(x)$ are the elements of inverse matrices, (22) can be rewritten as

$$\sum_{j=1}^{n} L_{ij}(x) \left(g_j(x) - \lambda_j(x) - \sum_{i=1}^{n} H_{ji}(x) f_i(x) \right) + f_i(x) = 0 \tag{23}$$

and, by direct differentiation of (23), being j and l arbitrary and fixed,

$$\sum_{j=1}^{n} \frac{\partial L_{ij}(x)}{\partial x_l}\left(g_j(x) - \lambda_j(x) - \sum_{i=1}^{n} H_{ji}(x) f_i(x)\right) + \sum_{j=1}^{n} L_{ij}(x)\left(\frac{\partial g_j(x)}{\partial x_l} - \frac{\partial \lambda_j(x)}{\partial x_l} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} f_i(x) - \delta_{jl}\right) + \frac{\partial f_i(x)}{\partial x_l} = 0. \tag{24}$$

When $x = \alpha$, by applying Lemma 2, expression (9), and taking into account that $g_j(\alpha) = \alpha$, $\lambda(\alpha) = \alpha$ and $f_i(\alpha) = 0$, we have

$$\sum_{j=1}^{n} \frac{\partial L_{ij}(\alpha)}{\partial x_l}\left(\alpha_j - \alpha_j\right) + \sum_{j=1}^{n} L_{ij}(\alpha)\frac{\partial g_j(\alpha)}{\partial x_l} - L_{il}(\alpha) + \frac{\partial f_i(\alpha)}{\partial x_l} = 0.$$

So,

$$\sum_{j=1}^{n}\left(\sum_{k=1}^{m} A_k J_{ij}(\alpha)\right)\frac{\partial g_j(\alpha)}{\partial x_l} - \sum_{k=1}^{m} A_k J_{il}(\alpha) + \frac{\partial f_i(\alpha)}{\partial x_l} = 0$$

and

$$\sum_{j=1}^{n}\left(\sum_{k=1}^{m} A_k J_{ij}(\alpha)\right)\frac{\partial g_j(\alpha)}{\partial x_l} + \frac{\partial f_i(\alpha)}{\partial x_l}\left(1 - \sum_{k=1}^{m} A_k\right) = 0.$$

Moreover, it is known that $\sum_{k=1}^{m} A_k = 1$. In addition, j and l are arbitrary, and $J_F(\alpha)$ is nonsingular, so

$$\frac{\partial g_j(\alpha)}{\partial x_l} = 0. \tag{25}$$

By direct differentiation of (24), being r arbitrary and fixed,

$$\sum_{j=1}^{n} \frac{\partial^2 L_{ij}(x)}{\partial x_r \partial x_l}\left(g_j(x) - \lambda_j(x) - \sum_{i=1}^{n} H_{ji}(x) f_i(x)\right) + \sum_{j=1}^{n}\sum_{k=1}^{m} A_k \frac{\partial J_{ij}(\eta_k(x))}{\partial x_l}\left(\frac{\partial g_j(x)}{\partial x_r} - \frac{\partial \lambda_j(x)}{\partial x_r} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_r} f_i(x) - \delta_{jr}\right)$$
$$+ \sum_{j=1}^{n}\sum_{k=1}^{m} A_k \frac{\partial J_{ij}(\eta_k(x))}{\partial x_r}\left(\frac{\partial g_j(x)}{\partial x_l} - \frac{\partial \lambda_j(x)}{\partial x_l} - \sum_{i=1}^{n} \frac{\partial H_{ji}(x)}{\partial x_l} f_i(x) - \delta_{jl}\right)$$
$$+ \sum_{j=1}^{n}\sum_{k=1}^{m} A_k J_{ij}(\eta_k(x))\left(\frac{\partial^2 g_j(x)}{\partial x_r \partial x_l} - \frac{\partial^2 \lambda_j(x)}{\partial x_r \partial x_l} - \sum_{i=1}^{n} \frac{\partial^2 H_{ji}(x)}{\partial x_r \partial x_l} f_i(x) + \sum_{i=1}^{n} H_{ji}(x)\frac{\partial^2 f_i(x)}{\partial x_r \partial x_l}\right) + \frac{\partial^2 f_i(x)}{\partial x_r \partial x_l} = 0. \tag{26}$$

Let us substitute $x = \alpha$ and apply (18) from Lemma 4, and (9), (10) from Lemma 2. Then,

$$\frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l}\left(1 - 2\sum_{k=1}^{m} A_k(1 - \tau_k)\right) + \sum_{j=1}^{n} J_{ij}(\alpha)\frac{\partial^2 g_j(\alpha)}{\partial x_r \partial x_l} = 0.$$

So, if parameters A_k satisfy

$$\sum_{k=1}^{m} A_k(1 - \tau_k) = 1/2 \tag{27}$$

it can be concluded that

$$\frac{\partial^2 g_j(\alpha)}{\partial x_r \partial x_l} = 0. \tag{28}$$

In order to analyze the conditions that guarantee convergence order higher than three, it is necessary to differentiate (24), being s arbitrary and fixed, and evaluate the resulting expression in $x = \alpha$. Then, the following expression is obtained, by using (18) and (19) from Lemma 4, (9)–(11) from Lemma 2, and conditions (4) and (27):

$$\frac{\partial^3 f_i(\alpha)}{\partial x_s \partial x_r \partial x_l}\left(1 - 3\sum_{k=1}^{m} A_k(1 - \tau_k)^2\right) + \sum_{j=1}^{n} J_{ij}(\alpha)\frac{\partial^3 g_j(\alpha)}{\partial x_s \partial x_r \partial x_l}$$
$$- \frac{1}{2}\sum_{j=1}^{n}\sum_{q=1}^{n}\left(\frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_s} H_{qi}(\alpha)\frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_l} + \frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_r} H_{qi}(\alpha)\frac{\partial^2 f_i(\alpha)}{\partial x_s \partial x_l} + \frac{\partial^2 f_i(\alpha)}{\partial x_q \partial x_l} H_{qi}(\alpha)\frac{\partial^2 f_i(\alpha)}{\partial x_r \partial x_s}\right) = 0.$$

So, if

$$\frac{\partial^2 f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2}} = 0, \tag{29}$$

for any $a_1, a_2 \in \{1, 2, \dots, n\}$ and conditions (4), (27) and

$$\sum_{k=1}^{m} A_k (1-\tau_k)^2 = 1/3 \tag{30}$$

are satisfied, we conclude that

$$\frac{\partial^3 g_j(\alpha)}{\partial x_s \partial x_r \partial x_l} = 0. \tag{31}$$

Again, being u arbitrary and fixed and using conditions (4), (27), (29) and (30), Lemma 2 (expressions from (9)–(12)) and Lemma 4 (expressions from (18)–(20)), it can be proved that

$$\frac{\partial^4 f_i(\alpha)}{\partial x_u \partial x_s \partial x_r \partial x_l} \left(1 - 4\sum_{k=1}^{m} A_k (1-\tau_k)^3\right) + \sum_{j=1}^{n} J_{ij}(\alpha) \frac{\partial^4 g_j(\alpha)}{\partial x_u \partial x_s \partial x_r \partial x_l} = 0.$$

So, if condition

$$\sum_{k=1}^{m} A_k (1-\tau_k)^3 = 1/4 \tag{32}$$

is also satisfied, we conclude that

$$\frac{\partial^4 g_j(\alpha)}{\partial x_u \partial x_s \partial x_r \partial x_l} = 0. \tag{33}$$

In general, it can be proved that:

$$\frac{\partial^{2d-1} f_i(\alpha)}{\partial x_{a_1} \cdots \partial x_{a_{2d-1}}} \left(1 - (2d-1)\sum_{k=1}^{m} A_k (1-\tau_k)^{2d-2}\right) + \sum_{j=1}^{n} J_{ij}(\alpha) \frac{\partial^{2d-1} g_j(\alpha)}{\partial x_{a_1} \cdots \partial x_{a_{2d-1}}} + P(\alpha) = 0$$

where $P(\alpha)$ is a linear combination of partial derivatives of f_i, of order d, evaluated in α, and

$$\frac{\partial^{2d} f_i(\alpha)}{\partial x_{a_1} \cdots \partial x_{a_{2d}}} \left(1 - 2d\sum_{k=1}^{m} A_k (1-\tau_k)^{2d-1}\right) + \sum_{j=1}^{n} J_{ij}(\alpha) \frac{\partial^{2d} g_j(\alpha)}{\partial x_{a_1} \cdots \partial x_{a_{2d}}} = 0$$

where $1 \le i, a_1, \dots, a_{2d} \le n$.

Therefore, if parameters A_k and τ_k verify

$$\sum_{k=1}^{m} A_k (1-\tau_k)^h = \frac{1}{h+1}, \quad h = 0, 1, \dots, 2d-1$$

and the partial derivatives of the coordinate functions of $F(x)$ at the root α verify

$$\frac{\partial^j f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2} \cdots \partial x_{a_j}} = 0, \quad 1 \le i, a_1, \dots, a_j \le n\, j = 2, 3, \dots, d$$

by using Taylor series (21) and applying Theorem 1, we conclude that an iterative method of the family described by (3), is of order $2d+1$.

Moreover, if parameters A_k and τ_k verify

$$\sum_{k=1}^{m} A_k (1-\tau_k)^h = \frac{1}{h+1}, \quad h = 0, 1, \dots, 2d-2$$

and the following partial derivatives of the coordinate functions of $F(x)$ at α are zero

$$\frac{\partial^j f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2} \cdots \partial x_{a_j}} = 0, \quad 1 \le i, a_1, \dots, a_j \le n,\ j = 2, 3, \dots, d,$$

we conclude that an iterative method like (3) is of order $2d$. □

Table 1
Efficiency indices.

n	C_N	C_{MN}	C_{N3}	C_{M1}	C_{M2}
1	1.414214	1.442250	1.732051	1.587401	1.495349
2	1.122462	1.116123	1.200937	1.148698	1.121828
3	1.059463	1.053707	1.095873	1.068242	1.055113
4	1.035265	1.030987	1.056467	1.039259	1.031435
5	1.023374	1.020176	1.037299	1.025526	1.020322
6	1.016640	1.014184	1.026503	1.017932	1.014218
7	1.012455	1.010518	1.019812	1.013290	1.010506
8	1.009674	1.008111	1.015376	1.010245	1.008080
9	1.007731	1.006445	1.012282	1.008140	1.006407
10	1.006321	1.005245	1.010037	1.006623	1.005205

It is necessary to analyze the set of methods described in Theorem 2, in order to establish the optimal relationship between the order of convergence and the efficiency index. A key element is, for this aim, the number m of parameters used.

In fact, it is not surprising that the optimal relation for convergence of order two is that of the classical Newton's method, with $m = 1, A_1 = 1$ and $\tau_1 = 0$. The efficiency index of Newton's method, and the reference for evaluating the rest of the methods, is $2^{\frac{1}{n^2+n}}$, where n is the size of the system. Indeed, it is possible to find a method with only $m = 1$ and convergence order three: the middle-point method (MN), described in [5,7], with $A_1 = 1$ and $\tau_1 = \frac{1}{2}$ whose efficiency index is $3^{\frac{1}{2n^2+n}}$. The method based on the trapezoidal rule of quadrature (described also in [5,7]) that appears when $m = 2, A_1 = A_2 = \frac{1}{2}$ and $\tau_1 = 0$, $\tau_2 = 1$, also has convergence order three, and its efficiency index is the same as the one of MN method.

It is interesting to note that, if we fix $m = 2$ in order to limit the number of functional evaluations, a whole family of methods is found (that includes the trapezoidal method but not the middle-point method), with order of convergence three:

$$x^{(k+1)} = x^{(k)} - 4(1 - 3\tau_1 + 3\tau_1^2)\left[J_F(\eta_1(x^{(k)})) + 3(1 - 4\tau_1 + 4\tau_1^2)J_F(\eta_2(x^{(k)}))\right]^{-1} F(x^{(k)}), \tag{34}$$

where

$$\eta_1(x^{(k)}) = x^{(k)} - \tau_1 J_F(x^{(k)})^{-1}F(x^{(k)})$$

and

$$\eta_2(x^{(k)}) = x^{(k)} - \frac{3\tau_1 - 2}{6\tau_1 - 3} J_F(x^{(k)})^{-1}F(x^{(k)}).$$

Nevertheless, if an additional condition is required to the parameters in order to obtain order of convergence four, we obtain exactly the same family of methods under a restriction: the system must verify that

$$\frac{\partial^2 f_i(\alpha)}{\partial x_{a_1} \partial x_{a_2}} = 0, \quad 1 \le i, a_1, a_2 \le n. \tag{35}$$

The efficiency of these methods depends on the number of functional evaluations needed; the optimal relationship is obtained if we consider $\tau_1 = 0$. Then, a new method is found whose iterative expression is:

$$x^{(k+1)} = x^{(k)} - \left[\frac{1}{4} J_F(x^{(k)}) + \frac{3}{4} J_F\left(x^{(k)} - \frac{2}{3} J_F(x^{(k)})^{-1}F(x^{(k)})\right)\right]^{-1} F(x^{(k)}), \tag{36}$$

and it will be denoted by M1. For general nonlinear systems, M1 has the same efficiency index as middle-point and trapezoidal methods, but if condition (35) is satisfied, then its efficiency index is better. If $\tau_1 \neq 0$ is considered, other methods are found but they need more functional evaluations; so, their efficiency indices are worse.

When fifth-order approximations are looked for, there are two methods with the same optimal efficiency index: one of them is new and is obtained by fixing $m = 2$, resulting $A_1 = A_2 = \frac{1}{2}$ and $\tau_1 = \frac{3+\sqrt{3}}{6}$, $\tau_2 = \frac{3-\sqrt{3}}{6}$; it will be denoted by M2. The second one corresponds to the Simpson's–Newton method (NS), described in [6], with third order of convergence (under no additional restriction over the system). In this case, $m = 3$, we get $\tau_1 = 0$, $\tau_2 = \frac{1}{2}$, $\tau_3 = 1$ and then the only coefficients verifying conditions of fifth order of convergence are $A_1 = A_3 = \frac{1}{6}$, $A_2 = \frac{2}{3}$. Assuming the additional condition (35), fifth order of convergence is obtained for both methods and their efficiency index is $5^{\frac{1}{3n^2+n}}$.

We can observe in Table 1 that, for $n = 1$, the efficiency indices of the third-order methods, as MN or M1, without additional conditions over the system, improve the efficiency of Newton's method. This will not be the case when nonlinear systems of equations are considered. With respect to the new methods, M1 methods appear to be more efficient than M2, but, unfortunately, their efficiency indices do not improve the ones of Newton, under the same restrictions of the system, that, in this case, we denote by N3.

Table 2
Computational efficiency indices.

n	CE_{N}	CE_{MN}	CE_{N3}	CE_{M1}	CE_{M2}
1	1.259921	1.245731	1.442250	1.319508	1.307660
2	1.059463	1.051205	1.095873	1.065041	1.063858
3	1.024190	1.020176	1.038610	1.025526	1.025466
4	1.012455	1.010224	1.019812	1.012919	1.013064
5	1.007323	1.005956	1.011631	1.007522	1.007693
6	1.004694	1.003796	1.007451	1.004792	1.004949
7	1.003199	1.002576	1.005076	1.003252	1.003387
8	1.002283	1.001833	1.003620	1.002313	1.002427
9	1.001688	1.001352	1.002677	1.001707	1.001802
10	1.001284	1.001027	1.002037	1.001296	1.001377

Table 3
Numerical results for nonlinear systems.

$F(x)$	$x^{(0)}$	Iterations					p				
		CN	MN	M1	M2	NS	CN	MN	M1	M2	NS
(a)	$(0.4, 0.4)^T$	6	6	5	5	5	3.0	3.0	5.0	–	5.0
	$(0.8, 0.8)^T$	9	6	5	5	5	3.0	3.0	5.0	4.3	5.0
(b)	$(-0.5, 0.5)^T$	6	6	5	5	5	3.0	3.0	4.0	–	5.0
	$(-0.8, 0.8)^T$	7	7	6	6	5	3.0	3.0	4.0	5.0	5.0
(c)	$(-1, -2)^T$	7	6	5	5	5	3.0	3.0	4.0	5.0	5.0
	$(2, 2)^T$	8	7	6	6	6	3.0	3.0	4.0	–	5.0
(d)	$(0.2, 0.2)^T$	10	9	7	7	7	2.0	2.0	3.0	3.0	3.0
	$(3, 2)^T$	11	10	7	8	7	2.0	2.0	3.0	–	3.0
(e)	$x_1^{(0)}$	7	6	5	5	5	2.0	2.0	3.0	3.0	3.0
	$x_2^{(0)}$	8	6	6	6	6	2.0	2.0	3.0	3.0	3.0

If the computational effort of the methods is taken into account, it can be observed in Table 2 that the most efficient method in these terms is also the classical Newton's method. Nevertheless, a difference is noted with respect to the new methods: for $n \geq 4$, method (M2) shows a better behavior than (M1), in terms of computational efficiency index.

Finally, using the general result of Theorem 2, it is possible to define higher order iterative formulas, but the computational effort can make them less efficient than the previous ones.

3. Numerical results

In this section, we will check the effectiveness, in order to estimate the zeros of several nonlinear functions, of some of the known numerical methods of the family (3) (in particular, MN, NS methods and also the classical Newton's method, CN) but also the new methods: M1 from the family (34) and the fifth-order method M2.

(a) $F(x_1, x_2) = (\sin(x_1) + x_2\cos(x_1), x_1 - x_2), \alpha = (0, 0)^T$.
(b) $F(x_1, x_2) = (\exp(x_1^2) - \exp(\sqrt{2}x_1), x_1 - x_2), \alpha = (0, 0)^T$.
(c) $F(x_1, x_2) = \left(-\frac{x_2^2}{2} + \exp(x_2) + x_1 - 2, x_2 - 2x_1 + 2\right), \alpha = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)^T$.
(d) $F(x_1, x_2) = \left(x_1^2 + x_2^2 - 1, x_1^2 - x_2^2 + \frac{1}{2}\right), \alpha = (1, 0)^T$.
(e) $F(x) = (f_1(x), f_2(x), \ldots, f_n(x))$, where $x = (x_1, x_2, \ldots, x_n)^T$ and $f_i : \mathbb{R}^n \to \mathbb{R}$, $i = 1, 2, \ldots, n$, such that

$$f_i(x) = x_i x_{i+1} - 1, \quad i = 1, 2, \ldots, n-1$$
$$f_n(x) = x_n x_1 - 1.$$

When n is odd, the exact zeros of $F(x)$ are $\alpha_1 = (1, 1, \ldots, 1)$ and $\alpha_2 = (-1, -1, \ldots, -1)$; they are obtained for $x_1^{(0)} = (2, \ldots, 2)$ and $x_2^{(0)} = (-0.2, \ldots, -0.2)$, respectively. Results appearing in Table 3 are obtained for $n = 101$.

Numerical computations have been carried out in MATLAB, with variable precision arithmetic that uses floating point representation of 200 decimal digits of mantissa. Every iterate is obtained from the previous one by means of an iterative expression

$$x^{(k+1)} = x^{(k)} - A^{-1}b,$$

where $x^{(k)} \in \mathbb{R}^n$, A is a real $n \times n$ matrix and $b \in \mathbb{R}^n$. Matrix A and vector b are different according to the method used, but in any case the inverse calculation $-A^{-1}b$ is carried out solving the linear system $Ay = -b$, using Gaussian elimination with partial pivoting. So, the new estimation is easily obtained by the addition of the solution of the linear system and the previous iterate: $x^{(k+1)} = x^{(k)} + y$.

The stopping criterion used is $\|x^{(k+1)} - x^{(k)}\| + \|F(x^{(k)})\| < 10^{-100}$. Therefore, we check that iterates converge to a limit and moreover that this limit is a solution of the system of nonlinear equations. For every method, we analyze the number of iterations needed to converge to the solution and the order of convergence will be estimated by means of the computational order of convergence p (see [1]),

$$p \approx \frac{\ln\left(\left\|x^{(k+1)} - x^{(k)}\right\| / \left\|x^{(k)} - x^{(k-1)}\right\|\right)}{\ln\left(\left\|x^{(k)} - x^{(k-1)}\right\| / \left\|x^{(k-1)} - x^{(k-2)}\right\|\right)}.$$

The value of p that appears in Table 3 is the last coordinate of vector p when the variation between its coordinates is small.

It can be observed in Table 3 that several results were obtained using the previously described methods in order to estimate the zeros of functions from (a) to (e). For every function, the following items are specified: the initial estimation $x^{(0)}$, the solution and, for each method, the number of iterations needed and the estimated computational order of convergence p.

In practice, it can be seen that in case of $\frac{\partial^2 f_i(\alpha)}{\partial x_a \partial x_b} = 0$ for all i, a, b, as in (a), (b) and (c), the convergence of classical Newton's method is of order $p = 3$ while M1 and NS method obtain a computational order near to 4 and 5, respectively (although M1 sometimes improves the theoretical results, as in case (a)). If this condition is not verified, the computational order of convergence of the modified methods is about 3. Moreover, it can be observed in (e) that the efficiency of the methods remain although the system of equations is large.

4. Conclusions

In this paper we present a generalization of all variants of Newton's method based on interpolation rules of quadrature, for solving nonlinear systems. These methods have order of convergence three, but under certain conditions of the system this order increases.

All methods of the family (3) have an efficiency index and a computational efficiency index better than the ones of Newton for $n = 1$, but their efficiency indices do not improve the ones of Newton for $n \geq 2$. However, the existence of an extensive literature on higher order methods for solving nonlinear systems (see, for example, [11–13]) reveals that they are only limited by the nature of the problem to be solved: in particular, numerical solution of quadratic equations and nonlinear integral equations are needed in the study of dynamical models of chemical reactors [14], or in radioactive transfer [15]. Moreover, many of these numerical applications use high precision in their computations; the results of these numerical experiments show that the high order methods associated with a multiprecision arithmetic floating point is very useful, because it yields a clear reduction in iterations.

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