A Class of Maximally Efficient Sixth-Order Iterative Schemes for Systems of Nonlinear Equations

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1 Introduction

The main method used for approximate solutions of systems of nonlinear equations with form $F(x)=0$, where $F:D\subset\mathbb{R}^n\to\mathbb{R}^n$, with $n\in\mathbb{N}$, is a function that is defined on a convex domain D, is N2S. Its iterative procedure is

$$x^{(k+1)}=x^{(k)}-F'\left(x^{(k)}\right)^{-1}F\left(x^{(k)}\right),k=0,1,\ldots, \tag{1}$$

where $F'(x)\in\mathscr{L}\left(\mathbb{R}^n,\mathbb{R}^n\right)$ is the linear operator called the Jacobian matrix. It has quadratic convergence order, or speed with which it tends to the solution that depends on the initial approximation, among other factors. Its computational cost is low: it only needs a functional evaluation, a Jacobian evaluation and solving a linear system per iteration.

We consider $e^{(k)}=x^{(k)}-\xi$ as the local error at the k^{th} iteration, we can estimate the order of convergence p for an iterative method from the error equation

$$e^{(k+1)}=Le^{(k)^p}+O\left(e^{(k)^{p+1}}\right),$$

where $L\in\mathscr{L}(\overbrace{\mathbb{R}^n\times\cdots\times\mathbb{R}^n}^{p-\text{ times}},\mathbb{R}^n)$ is a p-linear operator and $\mathscr{L}$ is a set of bounded linear operators.

Not a few researchers have tried to improve it [1, 2], taking it as a first step of new schemes, managing to increase the convergence order and maintaining a good relationship between convergence order and computational cost.

Kung and Traub in [3] established a conjecture about optimal methods for nonlinear equations. Similarly, Cordero and Torregrosa state in [4] on vectorial case that for any multistep method for nonlinear systems of equations, the order of convergence cannot exceed $2^{k_1+k_2-1}$, where k_1 is the total of evaluations of the Jacobian matrix and k_2 the number of evaluations of the nonlinear function per iteration, and $k_1\le k_2$. Therefore, $2^{k_1+k_2-1}$ is the optimal order.

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Until this work, the only optimal methods for systems, to the best of our knowledge, are N2S and EH4S in [2], with scheme:

$$x^{(k+1)} = y^{(k)} - F'\left(x^{(k)}\right)^{-1}\left(\rho_k\, F\left(y^{(k)}\right) + q_k\, F\left(x^{(k)}\right)\right), \quad k = 0, 1, \ldots, \tag{2}$$

being $y^{(k)}$ the N2S scheme and

$$(\lambda, \psi) \in \mathbb{R}^2, \quad \nu_k = \frac{\left\|F(y^{(k)})\right\|^2}{\left\|F(x^{(k)})\right\|^2}, \quad \rho_k = \frac{1+\psi\nu_k}{1+\lambda\nu_k}, \quad q_k = \frac{2\nu_k}{1+\lambda\nu_k}.$$

Arroyo et al. proposed in [4] a very efficient fifth-order method, which we denote by ACT5S. Its iterative expression is

$$\begin{aligned} z^{(k)} &= y^{(k)} - F'\left(x^{(k)}\right)^{-1}\left[5\, F\left(y^{(k)}\right)\right], \\ x^{(k+1)} &= y^{(k)} - F'\left(x^{(k)}\right)^{-1}\left[-\frac{16}{5} F\left(y^{(k)}\right) + \frac{1}{5} F\left(z^{(k)}\right)\right], \end{aligned} \tag{3}$$

where $y^{(k)}$ is N2S.

Soleymani et al. developed in [5] a sixth-order Jarratt-type iterative method for solving nonlinear problems, which we denote by S6S, whose iterative expression is

$$\begin{aligned} z^{(k)} &= x^{(k)} - \frac{1}{2} S F'\left(x^{(k)}\right)^{-1} F\left(x^{(k)}\right), \\ x^{(k+1)} &= z^{(k)} - \frac{1}{4} S^2 F'\left(x^{(k)}\right)^{-1} F\left(z^{(k)}\right), \end{aligned} \tag{4}$$

where $w^{(k)}$ is the first step of Jarratt's scheme, and

$$S = \left[3F'\left(w^{(k)}\right) - F'\left(x^{(k)}\right)\right]^{-1}\left[3F'\left(w^{(k)}\right) + F'\left(x^{(k)}\right)\right].$$

Hueso et al. created in [6] a sixth-order iterative method, requiring two evaluations of the function F and two of the Jacobian F' per iteration, which we denote by H6S:

$$\begin{aligned} z^{(k)} &= x^{(k)} - \left(\frac{5}{8} I + \frac{3}{8} M^2(w^{(k)}, x^{(k)})\right) N(x^{(k)}, x^{(k)}), \\ x^{(k+1)} &= z^{(k)} - \left(-\frac{9}{4} I + \frac{15}{8} M(w^{(k)}, x^{(k)}) + \frac{11}{8} M(x^{(k)}, w^{(k)})\right) N(w^{(k)}, z^{(k)}), \end{aligned} \tag{5}$$

where $w^{(k)}$ is the first step of Jarratt's scheme, I denotes the identity matrix of size $n \times n$, $M(s,r) = F'(s)^{-1} F'(r)$ and $N(s,r) = F'(s)^{-1} F(r)$.

Singh et al. in [1] presented a fifth-order highly efficient method, which we denote by S5S, whith iterative scheme

$$x^{(k+1)} = z^{(k)} - \left(1 + \frac{F\left(z^{(k)}\right)^T F\left(z^{(k)}\right)}{F\left(x^{(k)}\right)^T F\left(x^{(k)}\right)}\right) F'\left(z^{(k)}\right)^{-1} F\left(z^{(k)}\right), \tag{6}$$

being $z^{(k)}$ the *k-th* iteration of N2S.

Cordero et al. in [7] have proposed an eighth-order method, which we denote by CGT8S, with the following iterative scheme

$$\begin{aligned} w^{(k)} &= v^{(k)} - \left[\frac{5}{4} I - \frac{1}{2} M(v^{(k)}, x^{(k)}) + \frac{1}{4} M^2(v^{(k)}, x^{(k)})\right] F'\left(v^{(k)}\right)^{-1} F\left(v^{(k)}\right), \\ x^{(k+1)} &= w^{(k)} - \left[\frac{3}{2} I - M(v^{(k)}, x^{(k)}) + \frac{1}{2} M^2(v^{(k)}, x^{(k)})\right] F'\left(v^{(k)}\right)^{-1} F\left(w^{(k)}\right), \end{aligned} \tag{7}$$

where $v^{(k)}$ is N2S and $M(s,r) = F'(s)^{-1} F'(r)$.

Some authors [8] define Computational Cost (or Effort) as the total number of evaluations and operations in an iterative process. We calculate it by using

$$Effort = iter \times (d + op), \tag{8}$$

where d, iter and op indicate the quantity of evaluations, iterations and operations, respectively.

Ostrowski efficiency index is calculated by using

$$I = p^{1/d}, \tag{9}$$

where p indicates the order of convergence and d is the total quantity of new functional evaluations required by the method per iteration.

2 New concepts about the efficiency

Proposition 1. *The minimum total number of functional and Jacobian matrix evaluations of a multi-step Newton-type iterative method will always exceed the number of steps.*

Definition 2. *Any method with m steps and $m+1$ evaluations in total is called low-eval-cost (LOE). We say a method is least-eval- cost (LEC) if it has frozen Jacobian matrix and as many functional evaluations as steps. All least-eval-cost methods are low-eval-cost.*

Definition 3. *Given two iterative methods Θ and Γ with Ostrowski efficiency indexes $I(\Theta)$ and $I(\Gamma)$, respectively. We say that Θ is more efficient than Γ if and only if $I(\Theta) > I(\Gamma)$. In such a case we will represent it as $\Theta \succ \Gamma$.*

Proposition 4. *The most efficient iterative methods, among all those that have the same order of convergence and the same number of steps, are LEC.*

Proposition 5. *The order of a damped composed Newton-type LOE scheme is at most equal to composed Newton that same number of steps.*

Proposition 6. *The minimum number of steps for a LEC method to reach a predetermined $Pth-$order is $\lceil \frac{lnP}{ln2} \rceil$.*

Definition 7. *An iterative method $Pth-$order Φ_P of damped composed Newton-type is said to be Maximally Efficient if no other method with the same order is more efficient, that is $\Phi_P \succeq \theta_P$ for any iterative method $Pth-$order θ_P.*

Proposition 8. *The following statements are equivalent about the iterative scheme P-order Φ_P:*

1. *Φ_P is Maximally Efficient.*
2. *Φ_P is LEC and it has $\lceil \frac{lnP}{ln2} \rceil$ steps.*

Thus, the methods N2S, Traub in [9], EH4S (including their particular cases: Ostrowski, King's family, Chun, KLAM family, among others) and ACT5S in iterative expression (3), are all maximally efficient of orders 2, 3, 4 and 5, respectively.

As far as we know to date, there has been no maximally efficient sixth-order method.

3 Methods

A new class of iterative procedures can be obtained by extending to the vector case the Ermakov's Hyperfamily for the scalar case presented in [10], distinct from the EH4S extension of optimal fourth ordn schemes. If we add a step and conjecture that there exists a weight function $H(\mu_k)$ satisfying certain conditions, with "frozen" Jacobian matrix, such that we can obtain better order. The new iterative scheme is

$$\begin{aligned} z^{(k)} &= y^{(k)} - \quad \omega_k \, F'(x^{(k)})^{-1} F(y^{(k)}), \\ x^{(k+1)} &= z^{(k)} - H(\mu_k) \, F'(x^{(k)})^{-1} F(z^{(k)}), \quad k = 0, 1, \ldots \end{aligned} \tag{10}$$

where $y^{(k)}$ is the *k-th* iteration of Newton's scheme for systems, and

$$\begin{aligned} \omega_k &= \tfrac{1+2\mu_k+\psi\nu_k}{1+\lambda\nu_k}, \quad \mu_k = \tfrac{F(x^{(k)})^T F(y^{(k)})}{\left\| F(x^{(k)}) \right\|^2}, \\ \nu_k &= \tfrac{\left\| F(y^{(k)}) \right\|^2}{\left\| F(x^{(k)}) \right\|^2}, \quad (\lambda, \psi) \in \mathbb{R}^2. \end{aligned}$$

Now, we can establish the following result. We base its proof on Taylor expansions around the solution, whose notation was introduced by Cordero et al. in [11], and the Taylor expansion series of the scalar product introduced by Singh et al. in [1], and an innovation we introduce here, to extend $f(y_k)/f(x_k)$ to the vectorial context.

Theorem 9. *Let $F : E \subseteq \mathbb{R}^m \to \mathbb{R}^m$ be a sufficiently differentiable function in an open convex neighborhood E of a solution ξ of the nonlinear system $F(x) = 0$. Suppose that $F'(x)$ is non-singular in ξ and an initial guess $x^{(0)}$ close enough to solution ξ. The biparametric family defined by (10) converges to ξ with fourth order of convergence if we only use the first two steps, and its convergence is order six with the third step for each weight function $H : \mathbb{R} \longrightarrow \mathbb{R}$ sufficiently differentiable, such that $H(0) = 1$ and $H'(0) = 2$.*

The biparametric class described by (10) satisfying the hypothesis of Theorem 9, is referred to hereafter as CRTV Hyperfamily. It is clear that it is Maximally Efficient.

3.1 Optimal fourth-order iterative schemes

Let us remark that we get new optimal fourth-order classes of methods, according to the Cordero-Torregrosa Conjecture, by taking only the first two steps of iterative scheme (10):

- If $\psi = 0$, we have an uniparametric class, we call CRTV4S$_\lambda$. Furthermore, it is an extension to vectorial case of the KLAM Family of fourth-order optimal methods for equations presented in [10], with second step:

$$x^{(k+1)} = y^{(k)} - \frac{1 + 2\mu_k}{1 + \lambda\nu_k} \, F'(x^{(k)})^{-1} \, F(y^{(k)}), \quad k = 0, 1, \ldots \tag{11}$$

- If $\lambda = -\beta^2$ and $\psi = -\beta(\beta + 2)$, we have a new extension of the King's Family for systems, with second step:

$$x^{(k+1)} = y^{(k)} - \frac{1 + 2\mu_k - \beta(\beta + 2)\nu_k}{1 - \beta^2\nu_k} \, F'(x^{(k)})^{-1} \, F(y^{(k)}), \quad k = 0, 1, \ldots$$

3.2 Maximally efficient sixth-order methods

We have a new maximally efficient uniparametric sixth-order class of methods, if $\psi = 0$ and $H(\mu_k) = 1 + 2\mu_k$ in (10), and denote it by CRTV6S$_\lambda$. Its third step is

$$x^{(k+1)} = z^{(k)} - (1 + 2\mu_k)\, F'(x^{(k)})^{-1}\, F(z^{(k)}), \quad k = 0, 1, \ldots \tag{12}$$

where $y^{(k)}$ is Newton's scheme and $z^{(k)}$ is the second step of CRTV4S$_\lambda$.

4 Efficiency Analysis

In addition to the Ostrowski efficiency index, defined in expression (9), we consider the Computational Efficiency Index, proposed by Cordero et al. in [11] defined as $CI = p^{1/op}$, where op is the quantity of products/quotients per iteration. The number of products and quotients needed to solve m linear systems using the same matrix of coefficients, applying the LU factorization, is $\frac{1}{3}n^3 + mn^2 - \frac{1}{3}n$, where n is the size of each system.

4.1 Maximally Efficient Class vs. other LOC Class

Among the maximally efficient class methods of order P, which we will call MAXP, $n \in \mathbb{N}$, whose Ostrowski efficiency index is

$$I_{\text{MAXP}} = P^{\frac{1}{n^2+mn}},$$

with $m = \lceil \frac{lnP}{ln2} \rceil$ steps, the following holds

1. $I_{\text{MAX4}} > I_{\text{MAX3}} > I_{\text{MAX2}}$,
2. $I_{\text{ MAX6}} > I_{\text{MAX5}}$,
3. $I_{\text{ MAX6}} > I_{\text{MAX4}}$.

Now we compare with other methods that are not maximally efficient.

Let us compare with methods that require two evaluations of the Jacobian matrix. Let 2JP be a class of Pth-order methods, with $k_1 = 2$ and $k_2 = m - 1$, per step, with $m = \lceil \frac{lnP}{ln2} \rceil$ steps, thus it has minimum number of $m + 1$ evaluations. Therefore, any member of $2JP$ is LOE with two Jacobians, but not LEC and any member of MAXP is LEC. Both they have $m = \lceil \frac{lnP}{ln2} \rceil$ steps.

The Ostrowski efficiency index of $2JP$ is

$$I_{\text{2JP}} = P^{\frac{1}{2n^2+(m-1)n}},$$

respect to those of maximum efficiency, then

1. $I_{\text{MAX4}} > I_{\text{2JP}},\ n > 2,\ P \leq 12$,
2. $I_{\text{MAX6}} > I_{\text{2JP}}, n > 2,\ P \leq 21$.

We observe that some maximally efficient methods outperform even others that are higher order optimal methods.

Table 1: Efficiency Index Comparison

Method	Order	NFE	I
N2S	2	n^2+n	$2^{1/\left(n^2+n\right)}$
S6S	6	$2\ \mathrm{n}^2+2n$	$6^{1/\left(2n^2+2n\right)}$
H6S	6	$2\ \mathrm{n}^2+2n$	$6^{1/\left(2n^2+2n\right)}$
CGT8S	8	$2\ \mathrm{n}^2+3n$	$8^{1/\left(2n^2+3n\right)}$
CRTV4S$_\lambda$	4	n^2+2n	$4^{1/\left(n^2+2n\right)}$
CRTV6S$_\lambda$	6	n^2+3n	$6^{1/\left(n^2+3n\right)}$

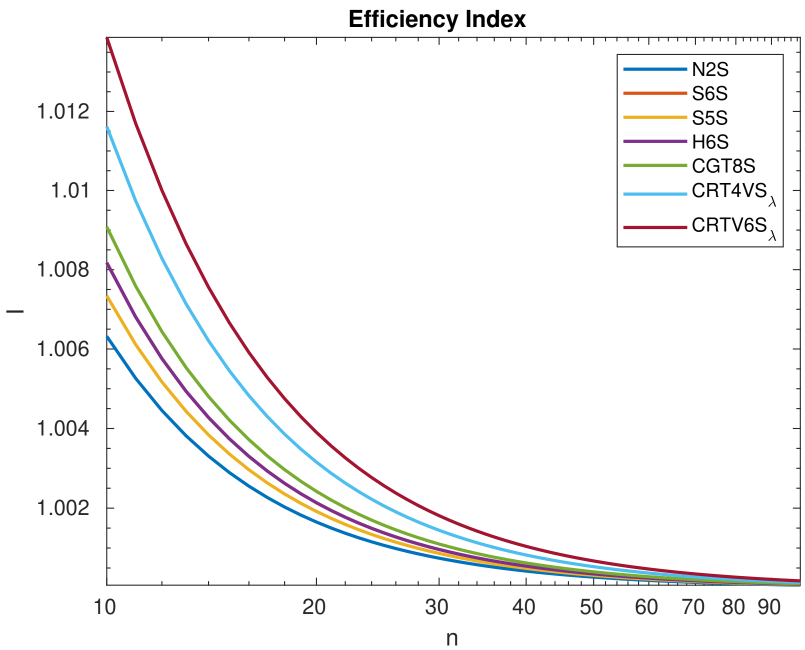

Figure 1: Efficiency Index for $n = 10$ to 100 (logarithmic scale)

Table 2: Computational Efficiency Index Comparison

Method	Order	NFE + op	CI
N2S	2	$(1/3)\mathrm{n}^3+2n^2+(2/3)n$	$2^{1/((1/3)n^3+2n^2+(2/3)n)}$
S6S	6	$(2\ /\ 3)\ \mathrm{n}^3+10n^2+(4/3)n$	$6^{1/\left((2/3)n^3+10n^2+(4/3)n\right)}$
H6S	6	$(2\ /\ 3)\ \mathrm{n}^3+12n^2+(4/3)n$	$6^{1/\left((2/3)n^3+12n^2+(4/3)n\right)}$
CGT8S	8	$(2\ /\ 3)\ \mathrm{n}^3+13n^2+(7/3)n$	$8^{1/\left((2/3)n^3+13n^2+(7/3)n\right)}$
CRTV4S$_\lambda$	4	$(1/3)\mathrm{n}^3+3n^2+(5/3)n$	$4^{1/((1/3)n^3+3n^2+(5/3)n)}$
CRTV6S$_\lambda$	6	$(1/3)\mathrm{n}^3+4n^2+(8/3)n$	$6^{1/((1/3)n^3+4n^2+(8/3)n)}$

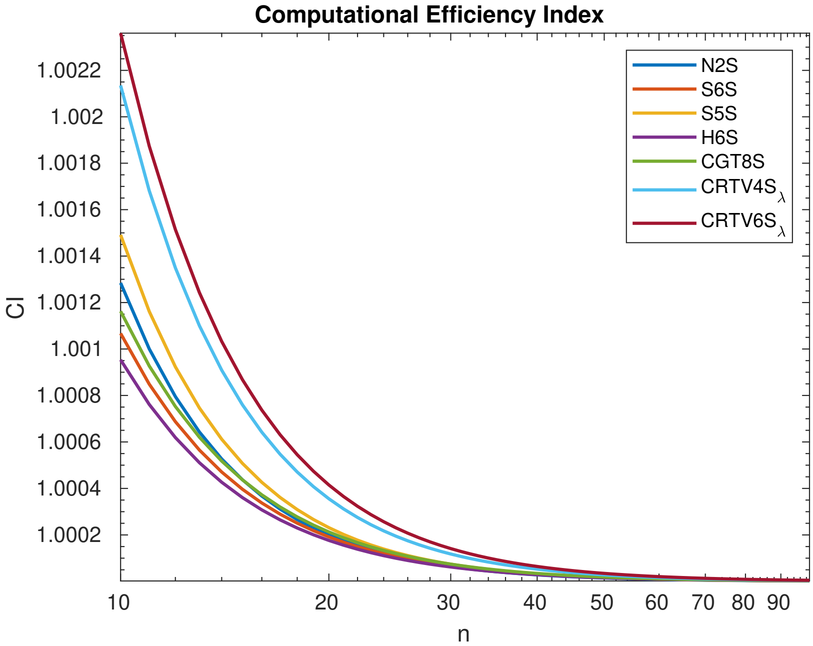

Figure 2: CEI for $n = 10$ to 100 (logarithmic scale)

4.2 Comparison with some specific high-order methods

We compare the efficiency of the new class of methods with N2S, S6S, S5S, H6S y CGT8S in Tables 1 and 2.

Since all the methods of the $CRTV4S_\lambda$ family have the same efficiency, we proceed to unify their analysis. The same as with those of the $CRTV6S_\lambda$ family.

Figures 1 and 2, from Tables 1 and 2, clearly show that the class of methods CRTV Hyperfamily (2), including CRTV4S$_\lambda$ and CRTV6S$_\lambda$, significantly outperforms in terms of computational efficiency and effectiveness the others. This corroborates the analysis presented on Maximally Efficient Methods in Subsection 4.1.

5 Numerical Results

We compare in the same problem the iterative methods $N2S$, $S6S$, and $CGT8S$ with the members of CRTV6S$_\lambda$ Family whose second step is the new extension to systems of Ostrowski, Chun, KLAM$_5$ and KLAM$_2$, taking the values $\lambda \in \{-4, 0, -5, 2\}$ in (12), which we denote as CRTV6S$_{-4}$, CRTV6S$_0$, CRTV6S$_{-5}$, and CRTV6S$_2$, respectively. The maximum number of iterations considered is 50 and the stopping criterion is $\left\|x^{(k+1)} - x^{(k)}\right\| < 10^{-600}$ or $\left\|F(x^{(k+1)})\right\| < 10^{-600}$. Each calculation was performed using Matlab R2022b with variable precision arithmetic with a mantissa of 2000 digits to minimize rounding errors.

We must take into account that the Approximate Computational Order of Convergence (ACOC),

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

as numerical approximation of the theoretical order of an iterative method. In addition, we show the Computational Effort, computed by equation (8).

Table 3: ***System size=500***

Method	*CPUTime*	*Iter*	$\left\|x^{(k+1)}-x^{(k)}\right\|$	$\left\|F(x^{(k+1)})\right\|$	*ACOC*
N2S	51.42	7	2.01×10^{-380}	9.06×10^{-762}	2.00
S6S	170.95	3	1.98×10^{-168}	8.89×10^{-1013}	6.00
CGT8S	64.94	3	0	0	-
$CRTV6S_{-4}$	32.63	3	1.75×10^{-178}	1.54×10^{-1074}	6.00
$CRTV6S_{-5}$	33.16	3	1.78×10^{-178}	1.75×10^{-1074}	6.00
$CRTV6S_0$	30.87	3	1.79×10^{-178}	1.75×10^{-1074}	6.00
$CRTV6S_2$	34.58	3	1.78×10^{-178}	1.76×10^{-1074}	6.00

Table 4: ***Effort's Comparison (System Size 500)***

Method	***Effort*** $(\times10^6)$	***vs N2S***	***vs*** $CRTV6S_\lambda$
N2S	*295*	*100 %*	*231 %*
S6S	*258*	*87 %*	*201 %*
CGT8S	*260*	*88 %*	*203 %*
$CRTV6S_\lambda$	*128*	*43 %*	*100 %*

Problem.

Consider the system of nonlinear equations of size 500:

$$e^{-x_i} - \sum_{j=1, j\neq i}^{m} x_j = 0, \quad i = 1, 2, \ldots, 500.$$

Here, with the initial aproximation $x^{(0)} = \left(\frac{1}{1000}, \cdots, \frac{1}{1000}\right)^T$ to obtain

$$\xi = (0.00200000399735\ldots, 0.00200000399735\ldots, \cdots\cdots, 0.00200000399735\ldots)^T.$$

The methods of the CRTV6S$_\lambda$ family preserve the theoretical order in very large systems. They can also compete with methods of equal or higher order, as shown in Tables 1 and 2.

Now let us stop at the computational effort. It is not difficult to notice the superiority of the methods of CRTV, as we can see in Table 3. The CRTV6S$_\lambda$ family, which is a particular case, makes much better use of the computational effort compared to the others.

Taking this criterion into account, if we take the CRTV6S$_\lambda$ family as a reference, all the methods, including N2S, need more than twice the computational effort, in all the numerical tests.

Therefore, the methods of the CRTV Hyperfamily constitute a substantial improvement over Newton's method, not only because of the order of convergence or because they require fewer iterations, but also they manage to exceed the same tolerance but with little more than 40% of the computational effort than that used by Newton's method. It also achieves this with half the effort of the other 6th and 8th order methods.

6 Conclusions

In this manuscript we have defined LOE, LEC and Maximal Efficiency in Pth-order and minimum number of steps to reach an arbitrary Pth-order. We conclude that a necessary and sufficient condition for a method to be maximally efficient Pth-order is that it be LEC with minimum number of steps .

The class of optimal fourth-order maximally efficient methods outperforms any requiring two Jacobian evaluations up to the twelfth-order. So the sixth-order maximally efficient class is better up the twenty-first-order 2JP methods.

The CRTV4S$_\lambda$ family is optimal according to the Cordero-Torregrosa conjecture with convergence or order four and includes new and more efficient extensions to the vectorial case of the Ostrowski, Chun and KLAM$_5$ methods than those known up to now. We have shown that the CRTV6S$_\lambda$ family of maximally efficient sixth-order methods is superior in efficiency and numerical performance to highly efficient methods found in the literature, including eighth-order methods. In addition to requiring less than half the computational effort than that used by the other methods, as can be seen in the numerical performance.

This work constitutes the basis of the theory on maximally efficient methods and least-eval-cost, which is intended to be a criterion that allows the construction of better methods.

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