On the generalization of secant method and the order of convergence.

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Abstract

In this paper we start generalizing the well known Secant and Müller methods by using higher degree polynomials. Although such generalization does already exist, we prove in an original and elegant way that the order of convergence p is limited by p = 2. The techniques used in this paper could also be helpful in other contexts. We also perform some numerical experiments to reinforce the theoretical results.

Key Words. Nonlinear equations, Secant Method, Müller method, order of convergence.

1 Introduction

Methods to solve nonlinear equations have been defined and studied profusely from antique times in history. It is not a surprise given its importance in addressing real problems where such equations appear. Still nowadays a wide range of research is carried out in relation with this subject.

Secant method is one of the first methods that is taught in undergraduate courses, and is simple both in its definition and in its application to solve certain equations. It is known to be a close relative to Newton method that does not use derivatives in its computations. This fact allows the application of the Secant method in occasions where the information about the derivative is not at hand. Therefore, it finds its field of application. Many studies have been carried out regarding conditions to ensure the convergence of the method, establishing an interval or ball of convergence, considering new variants with some gain in certain scenarios, etcetera. Recent publications show the current interest for deepening the knowledge about this prolific method, see for example [1, 2, 3, 4, 5].

Engineers are quite inclined to the application of Newton method in many scientific fields in order to deal with nonlinear equations. However, there are applications where it is more suitable to apply the secant method or any other method free of derivatives in its formulation. We can find in the literature many situations of this kind, as for example [6, 7, 8, 9, 10].

Secant method belongs to the group of methods where the convergence of the method is not guaranteed unless certain initial conditions are satisfied, normally requiring starting the iterations from an initial point close enough to a solution of the equation. Once it is assume that the method

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is convergent, it appears another concept that is nothing more than the order of convergence which somehow measures the speed at which the method converges. Studying the order of convergence is a one of the first researches carried out about a new method after its definition. In the case of Secant method, the order of convergence coincides with the golden ratio $\phi = \frac{1+\sqrt{5}}{2} \approx 1.6$. The higher the order the convergence the faster it is expected the convergence of the method. Under this assumption, it is normal to consider methods with higher order of convergence. Müller method appears as a generalization of Secant method in the sense that it is derived from cutting a quadratic polynomial with the x axis instead of a straight line as the Secant method does. Müller method attains approximately an order of convergence p = 1.83, larger than the golden ratio. It seems then, that this method would be superior, but it highly depends on the problem, on the initial conditions and so on. It could happen that a method converges and the other does not for example. Müller method gives a method capable to compute not only real roots of a given nonlinear equation, but also complex ones. In this sense Müller method outperforms over Secant method. Many articles have been also written about Müller method, see for example [11, 12]. In this article we generalize Secant and Müller methods by considering higher degree polynomials. A thorough study is carried out on these new methods and their convergence order. These method have been already considered in the literature previously, but a proof for their order of convergence is not easy to find. We give a new proof of the fact that the convergence orders of the generalized methods originate an increasing sequence with limit p = 2. Different but similar techniques have been used in order to obtain high order iterative methods free of derivatives, such us [13, 14]. The paper is organized as follows: Section 2 is devoted to remind the

classical Secant and Müller methods. In Section 3 we present new methods generated by considering higher order polynomials. In Section 4 we study the convergence order for these methods using a witty approach. In Section 5 we carry out some numerical test to check the performance of the presented methods. Finally, we give some conclusions in Section 6.

2 Classical Secant and Müller methods

We start by reminding the Secant method. In order to obtain an approximation of the solution of the equation f(x) = 0, where f is a continuous function, this method is derived as follows. Let us consider two initial points $(x_{n-1}, f(x_{n-1}))$ and $(x_n, f(x_n))$. Then, we construct the point-slope equation of the straight line that contains both of them,

$$f(x) = f(x_n) + \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}(x - x_n).$$

We force this straight line to intersect the x-axis, so $f(x_{n+1}) = 0$. In this case,

$$f(x_n) + \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}(x_{n+1} - x_n) = 0.$$

Solving for x_{n+1} we find,

$$x_{n+1} = x_n - \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} f(x_n), \quad n \ge 1,$$
(1)

which is the iteration of the Secant method. As it is well-known, the order of convergence of this method is given by the golden ratio, $\frac{1+\sqrt{5}}{2} \approx 1.62$.

We continue with Müller method. We depart in this case from three initial points $(x_{n-2}, f(x_{n-2}))$,

 $(x_{n-1}, f(x_{n-1}))$ y $(x_n, f(x_n))$. And, we build the parabola that pass through them,

$$p(x) = A(x - x_n)^2 + B(x - x_n) + C.$$
(2)

The coefficients of this equation are obtained by solving the following system of equations and using the definition of divided differences,

$$\begin{cases} p(x_{n-2}) = A(x_{n-2} - x_n)^2 + B(x_{n-2} - x_n) + C, \\ p(x_{n-1}) = A(x_{n-1} - x_n)^2 + B(x_{n-1} - x_n) + C, \\ p(x_n) = A(x_n - x_n)^2 + B(x_n - x_n) + C = C. \end{cases}$$

Its solution is given by,

 $A = f[x_{n-2}, x_n, x_{n-1}],$ $B = f[x_{n-1}, x_n] + f[x_{n-2}, x_n, x_{n-1}](x_n - x_{n-1}),$ $C = f(x_n).$

We force the expression (2) to intersect the x-axis, so $p(x_{n+1}) = 0$. It follows that the next iterate will be the solution of the equation,

$$A(x_{n+1} - x_n)^2 + B(x_{n+1} - x_n) + C = 0.$$

Solving the second degree polynomial equation we find,

$$x_{n+1} = x_n - \frac{2C}{B \pm \sqrt{B^2 - 4AC}},\tag{3}$$

which is the Muller's method algorithm. This expression is different from the most usual one for quadratic equations due to the fact that it is needed to avoid catastrophic cancellation. The sign at the denominator is chosen to make the denominator as large as possible with the aim of reducing the distance between x_n and x_{n+1} .

For this method, it is known that the order of convergence is approximately 1.84.

A clear question arises immediately at this point, and it is to analyze the behavior of the family of methods that appears if we raise the degree of the polynomials.

3 Higher order methods: secant polynomial methods

Let us consider k + 1 pairs of points

$$(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_k, f(x_k))$$

We construct the interpolation polynomial p_k that contains them and we force it to intersect the xaxis, so $p_k(x) = 0$. Solving this equation, we find k options for the next iteration x_{k+1} of the sequence that approximates the root of a given equation f(x) = 0. We choose the one which is closer to x_k . At this point, to continue with the method we take the last k + 1 points

$$(x_1, f(x_1)), (x_2, f(x_2)), (x_3, f(x_3)), \dots, (x_k, f(x_k)), (x_{k+1}, f(x_{k+1})).$$

and we proceed in the same way as we have done in the previous step, we construct the interpolation polynomial p_{k+1} that includes them and we intersect it with the x-axis. Hence, we get x_{k+2} for the next iteration, and so on and so forth. We repeat the process till we get a sufficiently good approximation of the root in case of convergence. It is not expected that this method is always convergent, since the simpler Secant method is not convergent. But in case of convergence, it is expected that the larger k the larger the convergence order of the method. And this is true as we will see in the next section. Notice that the polynomial equation is more or less easily solvable for third and fourth degrees, but special methods for polynomials must be used for higher degrees.

In Figure 1, we show an example for cubic polynomials of how this method works. We start with four points, $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$ and $(x_3, f(x_3))$, and two iterations of the explained method are performed.



Figure 1: Two iterations of the Cubic Secant method starting with four initial points

4 Convergence order for the secant polynomial methods

Before we analyze the order of convergence of this generalized methods seen in previous section, we prove some useful lemmas.

Lemma 1. For every $k \ge 2$, the equation $x^k - \dots - x - 1 = 0$ has a unique positive and real root in the interval (1, 2).

Proof. Let us consider the function $g(x) = x^k - \dots - x - 1$, for all $k \ge 2$. We know that,

• $g \in \mathcal{C}([1,2])$, because g is a polynomial function.

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- $g(1) \cdot g(2) < 0$ due to:
 - 1. $g(1) = 1^k \dots 1 1 = (1^k 1) 1 \dots 1 = -(k 1) = 1 k < 0,$

2.
$$g(2) = 2^k - \dots - 2 - 1 = 2^k - \sum_{i=0}^{k-1} 2^i = 2^k - \frac{1-2^k}{1-2} = 2^k + 1 - 2^k = 1 > 0.$$

Applying Bolzano's theorem it follows that there exists $x_0 \in (1,2)$ such that $g(x_0) = 0$. On one hand, the last result shows the existence of a real root in (1,2), and on the other hand, the real coefficients of q ordered by descending variable exponents are,

$$-1$$
 $(k-1)$ -1 -1 .

Since there is only a sign change in the sequence of coefficients for all $k \ge 2$, we can deduce that there is only a unique positive root of the polynomial, thanks to Descartes rule of signs. Therefore we can conclude that for every $k \ge 2$ the equation $x^k - \dots - x - 1 = 0$ has an unique positive and real root in the interval (1, 2).

In the following lemmas we prove that all the other roots of the polynomial g have modulus less than 1.

Lemma 2. Let us consider the equation $x^k - ... - x - 1 = 0$ for $k \ge 3$ an odd integer number. Then, there is not a value of $\alpha \in (-1, 0]$ such that $g(\alpha) = 0$.

Proof. Given $g(x) = x^k - \dots - x - 1$ for $k \ge 3$ odd, we can rewrite it as,

$$g(x) = x^{k-1}(x-1) - x^{k-3}(x+1) - \dots - x^2(x+1) - (x+1), \quad \forall x \in (-1,0].$$

On one hand, since $k \ge 3$ and odd, we have that $x^j > 0$ $\forall j = 2, 4, ..., k - 3, k - 1$. On the other hand, x - 1 < 0 y x + 1 > 0 because $x \in (-1, 0]$. Therefore, g(x) < 0 $\forall x \in (-1, 0]$. This implies, that there exists no $\alpha \in (-1, 0]$ satisfying $g(\alpha) = 0$.

Lemma 3. Let us consider the equation $x^k - ... - x - 1 = 0$ for $k \ge 2$ an even integer number. Then, there exists a unique $\alpha \in (-1,0)$ such that $g(\alpha) = 0$.

Proof. Let us consider $g(x) = x^k - \dots - x - 1$ for $k \ge 2$ even.

• Uniqueness. Since g is a polynomial function, $g \in \mathcal{C}([-1,0])$ and g is derivable in (-1,0). In fact,

$$g'(x) = kx^{k-1} - (k-1)x^{k-2} - \dots - 3x^2 - 2x - 1 = kx^{k-1} - \sum_{i=0}^{k-2} (i+1)x^i.$$
 (4)

We observe that,

$$\sum_{i=0}^{k-2} (i+1)x^i = 1 + 2x + 3x^2 + \dots + (k-1)x^{k-2}$$
(5)

is a aritmetico-geometric sequence, and then there is an easy way to get its sum. Multiplying (5) by x,

$$x \cdot \sum_{i=0}^{k-2} (i+1)x^i = x + 2x^2 + 3x^3 + \dots + (k-1)x^{k-1},$$
(6)

and substracting (5) and (6) we get,

$$\sum_{i=0}^{k-2} (i+1)x^i - x \cdot \sum_{i=0}^{k-2} (i+1)x^i = 1 + x + x^2 + x^3 + \dots + x^{k-2} - (k-1)x^{k-1}$$
$$= \sum_{i=0}^{k-2} x^i - (k-1)x^{k-1} = \frac{1 - x^{k-1}}{1 - x} - (k-1)x^{k-1}.$$

Our term of interest, $\sum_{i=0}^{k-2} (i+1)x^i$, becomes,

$$(1-x)\sum_{i=0}^{k-2}(i+1)x^{i} = \frac{1-x^{k-1}}{1-x} - (k-1)x^{k-1} \Leftrightarrow \sum_{i=0}^{k-2}(i+1)x^{i} = \frac{1-x^{k-1}}{(1-x)^{2}} - \frac{(k-1)x^{k-1}}{1-x}.$$
 (7)

Plugging (7) into (4) we obtain,

$$g'(x) = kx^{k-1} - \frac{1 - x^{k-1}}{(1-x)^2} + \frac{(k-1)x^{k-1}}{1-x} = \frac{kx^{k-1}(1-x)^2 - 1 + x^{k-1} + (k-1)x^{k-1}(1-x)}{(1-x)^2}.$$

Thus, it is easy to inferred that g'(x) < 0,

$$\begin{split} g'(x) < 0 & \Leftrightarrow \quad \frac{kx^{k-1}(1-x)^2 - 1 + x^{k-1} + (k-1)x^{k-1}(1-x)}{(1-x)^2} < 0 \\ & \Leftrightarrow \quad kx^{k-1}(1-x)^2 - 1 + x^{k-1} + (k-1)x^{k-1}(1-x) < 0 \\ & \Leftrightarrow \quad kx^{k-1} + kx^{k+1} - 2kx^k - 1 + x^{k-1} + (k-1)x^{k-1} - (k-1)x^k < 0 \\ & \Leftrightarrow \quad kx^{k+1} + (1-3k)x^k + 2kx^{k-1} - 1 < 0. \end{split}$$

Due to the fact that $x \in (-1, 0)$ and $k \ge 2$ even, we have,

$$x^{k+1} < 0 \Rightarrow kx^{k+1} < 0, \qquad x^k > 0 \Rightarrow (1-3k)x^k < 0, \qquad x^{k-1} < 0 \Rightarrow 2kx^{k-1} < 0.$$

Therefore, $kx^{k+1} + (1-3k)x^k + 2kx^{k-1} - 1 < 0$, and g'(x) < 0, what means, g(x) is strictly decreasing. This implies that in case of existence of a root of the equation $x^k - \dots - x - 1 = 0$, for $k \ge 2$ even, this root must be unique.

• Existence. We know that $g \in \mathcal{C}([-1,0])$ and $g(-1) \cdot g(0) < 0$ since,

$$g(-1) = (-1)^k - (-1)^{k-1} - \dots - 1^2 - 1 - 1 = (-1)^k - \sum_{i=0}^{k-1} (-1)^i = (-1)^k - \frac{1 - (-1)^k}{1 - (-1)} \stackrel{k \ge 2\text{par}}{=} 1 - \frac{1 - 1}{2} = 1 > 0,$$

$$g(0) = 0^k - \dots - 0 - 1 = -1 < 0.$$

Using Bolzano theorem, there exist at least a value $\alpha \in (-1, 0)$ such that $g(\alpha) = 0$.

Once we have proven existence and uniqueness, we can affirm that for all $k \ge 2$ even, there exists a unique $\alpha \in (-1,0)$ such that $g(\alpha) = 0$.

Before proving the next lemma, we give without proof a useful calculus result that can be found for example in [15, 16].

Theorem 1. (Cauchy theorem) Let us consider a polynomial $x^n - b_{n-1}x^{n-1} - ... - b_1x - b_0$ with a unique real root r and $b_i > 0$, $|b_i| \ge |a_i| \forall i = 0, 1, 2, ..., n$. Then, the roots of $x^n + a_{n-1}x^{n-1} + ... + a_1x + a_0$ are located inside the ball $|x| \le r$.

Lemma 4. Let us consider the polynomial equation $x^k - ... - x - 1 = 0$ for all integer number $k \ge 2$. Let us call α_k the unique real root in (1,2). Then, if α is another root of the equation, then $|\alpha| < 1$.

Proof. We define the polynomial,

$$p_k(x) = x^k + b_{k-1}x^{k-1} + b_{k-2}x^{k-2} + \dots + b_2x^2 + b_1x + b_0 = (x - \alpha_1)(x - \alpha_2) \cdots (x - \alpha_k).$$

According to the Cardano Vieta formulas for this polynomial we get,

$$b_j = (-1)^{k-j} S_{k-j}^k \quad \forall j = 0, 1, ..., k-1,$$
(8)

where

$$S_j^k := \sum_{i \in V_j^k} \alpha_{i_1} \alpha_{i_2} \cdots \alpha_{i_j},$$

with V_j^k standing for the set containing all possible j-tuples among k indexes without repetition. This means that $\binom{k}{j}$ is the number of addends. In our case, $p_k(x) = x^k - \dots - x - 1$ for all $k \ge 2$, and then $b_j = -1, j = 0, 1, 2, \dots, k - 1$.

We also consider the following polynomial,

$$q_{k-1}(x) = x^{k-1} + c_{k-2}x^{k-2} + \dots + c_2x^2 + c_1x + c_0 = (x - \alpha_1)(x - \alpha_2) \cdots (x - \alpha_{k-1}),$$
(9)

and we search for its Cardano Vieta formulas.

$$c_j = (-1)^{k-j-1} S_{k-j-1}^{k-1} \quad \forall j = 0, 1, ..., k-2.$$
(10)

Given now $b_j = (-1)^{k-j} S_{k-j}^k = -1$ for $j = 0, 1, 2, \dots, k-1$, we decompose S_{k-j}^k in two terms:

- One term comprising the sum of all products of roots including α_k , that is, $\alpha_k S_{k-j-1}^{k-1}$.
- Another term avoiding α_k , that is, S_{k-j}^{k-1} .

It follows that, $b_j = (-1)^{k-j} (\alpha_k S_{k-j-1}^{k-1} + S_{k-j}^{k-1}) = -1.$ By successive equivalences, we get,

$$\begin{split} (-1)^{k-j} (\alpha_k S_{k-j-1}^{k-1} + S_{k-j}^{k-1}) &= -1 \Leftrightarrow \frac{(-1)^{k-j} (\alpha_k S_{k-j-1}^{k-1} + S_{k-j}^{k-1})}{-1} = \frac{-1}{-1} \Leftrightarrow \\ \Leftrightarrow (-1)^{k-j-1} (\alpha_k S_{k-j-1}^{k-1} + S_{k-j}^{k-1}) &= 1 \Leftrightarrow (-1)^{k-j-1} \alpha_k S_{k-j-1}^{k-1} = 1 - (-1)^{k-j-1} S_{k-j}^{k-1} \Leftrightarrow \\ \Leftrightarrow (-1)^{k-j-1} S_{k-j-1}^{k-1} = \frac{1 + (-1)^{k-j} S_{k-j}^{k-1}}{\alpha_k}, \end{split}$$

and this allows us to define a recurrence equation for c_j ,

$$c_j = (-1)^{k-j-1} S_{k-j-1}^{k-1} = \frac{1 + (-1)^{k-j} S_{k-j}^{k-1}}{\alpha_k} \quad \forall j = 1, 2, ..., k-2,$$
(11)

and using the expression of c_j in (10), the equation (11) can be written,

$$c_j = \frac{1+c_{j-1}}{\alpha_k} \quad \forall j = 1, 2, ..., k-2.$$

Moreover, for j = 0, using (10), $c_0 = (-1)^{k-1} S_{k-1}^{k-1} = (-1)^{k-1} \cdot \alpha_1 \cdot \alpha_2 \cdots \alpha_{k-1}$.

Taking into account that $b_0 = -1$, by (8), we get,

$$(-1)^{k}S_{k}^{k} = -1 \Leftrightarrow (-1)^{k} \cdot \alpha_{1} \cdot \alpha_{2} \cdots \alpha_{k-1}\alpha_{k} = -1 \Leftrightarrow (-1)^{k} \cdot S_{k-1}^{k-1}\alpha_{k} = -1 \Leftrightarrow (-1)^{k-1}S_{k-1}^{k-1} = \frac{1}{\alpha_{k}}$$

Then, $c_0 = (-1)^{k-1} S_{k-1}^{k-1} = \frac{1}{\alpha_k}$.

We obtain the Cardano Vieta formulas for the polynomial (9),

$$\begin{cases} c_0 = \frac{1}{\alpha_k}, \\ c_j = \frac{1+c_{j-1}}{\alpha_k} & \forall j = 1, 2, ..., k-2. \end{cases}$$

We notice that these coefficients present noticeable properties,

- 1. $c_j > 0$, $\forall j = 0, 1, ..., k 2$. 2. $c_j < \frac{1}{\alpha_k - 1}$, $\forall j = 0, 1, ..., k - 2$.
- 3. c_j forms an increasing sequence $\forall j = 0, 1, ..., k 2 : c_{j+1} > c_j, \ \forall j = 0, 1, ..., k 2.$

Let us prove it by induction,

- First, we verify the properties for j = 0,
 - 1. Since $\alpha_k \in (1,2)$, then $c_0 = \frac{1}{\alpha_k} > 0$.
 - 2. $\alpha_k \in (1,2)$ implies $c_0 = \frac{1}{\alpha_k} < \frac{1}{\alpha_k 1}$.
 - 3. We now check that $c_1 > c_0$,

$$c_1 = \frac{1+c_0}{\alpha_k} = \frac{1}{\alpha_k} + \frac{c_0}{\alpha_k} = c_0 + \frac{c_0}{\alpha_k} > c_0$$
, because $\alpha_k \in (1,2)$ and $c_0 > 0$.

- By induction hypothesis we suppose the result true for $j \in \mathbb{N}$, that is,
 - 1. $c_j > 0$.
 - 2. $c_j < \frac{1}{\alpha_k 1}$.
 - 3. c_j is and increasing sequence, $c_{j+1} > c_j$.
- Let us prove it for j + 1,
 - 1. Since $\alpha_k \in (1,2)$ and $c_j > 0$ by the induction hypothesis, then $c_{j+1} = \frac{1+c_j}{\alpha_k} > 0$.
 - 2. Also, from $c_j < \frac{1}{\alpha_k 1}$ by induction hypothesis, we get,

$$c_{j+1} = \frac{c_j + 1}{\alpha_k} < \frac{\frac{1}{\alpha_k - 1} + 1}{\alpha_k} = \frac{1 + \alpha_k - 1}{\alpha_k (\alpha_k - 1)} = \frac{\alpha_k}{\alpha_k (\alpha_k - 1)} = \frac{1}{\alpha_k - 1}.$$

3. Finally, we prove that $c_{j+2} > c_{j+1}$,

$$c_{j+2} = \frac{c_{j+1}+1}{\alpha_k} > c_{j+1} \Leftrightarrow c_{j+1}+1 > c_{j+1}\alpha_k \Leftrightarrow 1 > c_{j+1}(\alpha_k-1) \Leftrightarrow \frac{1}{\alpha_k-1} > c_{j+1}.$$

And since the last inequality holds as we have just seen in the previous point, then $c_{j+2} > c_{j+1}$.

Now, we build a k degree polynomial which posseses $\alpha = 1$ as root, apart from the same roots as $p_k(x)$ except α_k , being α_k the unique root of $p_k(x)$ in (1, 2).

$$g_k(x) = (x-1)(x^{k-1} + c_{k-2}x^{k-2} + \dots + c_2x^2 + c_1x + c_0)$$

= $x^k + (c_{k-2} - 1)x^{k-1} + (c_{k-3} - c_{k-2})x^{k-2} + (c_{k-4} - c_{k-3})x^{k-3} + \dots - c_0$
= $x^k + (c_{k-2} - 1)x^{k-1} + \sum_{i=k-2}^{1} (c_{i-1} - c_i)x^i - c_0.$

In order to apply the Cauchy theorem, Theorem 1, we also define the following auxiliary polynomial,

$$\tilde{g}_k(x) = x^k - (1 + c_{k-2})x^{k-1} - \sum_{i=k-2}^{1} (c_i - c_{i-1})x^i - c_0.$$

It is easy to see that \tilde{g}_k has also $\alpha = 1$ as root. Moreover, its coefficients, except the leading coefficient, are all negative. In fact, these coefficients in decreasing order are,

$$1 - (1 + c_{k-2}) - (c_{k-2} - c_{k-3}) \quad \dots \quad -c_0, \text{ where}$$

• 1 > 0.

- $-(1+c_{k-2}) < 0$, since $c_{k-2} > 0$.
- $-(c_j c_{j-1}) < 0$, because $c_j > c_{j-1}, \forall j = 0, 1, ..., k-2$.
- $-c_0 < 0$, due to the fact that $c_j > 0$, $\forall j = 0, 1, ..., k 2$.

Again using Descartes rule, since there is only one change of signs in the sequence of the coefficients, $\tilde{g}_k(x)$ has a unique positive real root, and it is $\alpha = 1$.

Applying now Theorem 1, we get that for any other root α of $g_k(x)$ we have $|\alpha| \leq 1$. It just remain to see that the equality is not possible, and then $|\alpha| < 1$. Evaluating $p_k(x) = x^k - \dots - x - 1 = 0$ at $x = \alpha$ we get,

$$\alpha^k - \ldots - \alpha - 1 = 0 \Leftrightarrow \alpha^k - \sum_{i=0}^{k-1} \alpha^i = 0 \Leftrightarrow \alpha^k - \frac{1 - \alpha^k}{1 - \alpha} = 0 \Leftrightarrow \alpha^k - \alpha^{k+1} - 1 + \alpha^k = 0 \Leftrightarrow \alpha^k (2 - \alpha) = 1.$$

Taking absolute values, $|\alpha|^k |2 - \alpha| = 1$.

Let us suppose by reduction to absurdity that $|\alpha| = 1$. In this case, it must be satisfied that $|2 - \alpha| = 1$. Thus, $\alpha \in B((2,0), 1)$. Together with $|\alpha| \leq 1$, that is, $\alpha \in B((0,0), 1)$, means that $\alpha = 1$. However, this reaches an absurd since,

$$p_k(1) = 1^k - \dots - 1 - 1 = -(k-1) \neq 0.$$

From this observation we get that $|\alpha| < 1$.

The next result proves a key equation to prove the order of convergence for the secant polynomial method defined.

Proposition 1. Let us suppose that the secant polynomial method with polynomials of degree k is convergent for a given set of initial points towards a simple root α of a k+1 differentiable function f, that is, $f(\alpha) = 0, f'(\alpha) \neq 0$. The errors $e_n = \alpha - x_n$ committed by the iterations $x_n, n \in \mathbb{N}$ satisfy the following equation,

$$e_{n+1} = M_{k,n} e_n e_{n-1} e_{n-2} \cdots e_{n-k}, \tag{12}$$

where $M_{k,n}$ is a constant dependent on n and k. Moreover, if $e_{n+1} \neq 0$, then there exists,

$$m_k = \lim_{n \to \infty} M_k = \frac{-f^{(k+1)}(\alpha)}{f'(\alpha)(k+1)!}.$$
 (13)

Proof. Notice that equation (12) is already known for the secant method (k = 1) and for Müller method (k = 2).

Let us consider the interpolating polynomial $p_k(x)$ of degree k which passes through the points $\{(x_n, f(x_n)), (x_{n-1}, f(x_{n-1})), \ldots, (x_{n-k}, f(x_{n-k}))\}$. The next iteration of the method x_{n+1} is built by choosing the root of $p_k(x)$ closest to the previous iteration, that is,

- 1. $p_k(x_{n+1}) = 0$,
- 2. x_{n+1} is chosen such that $|x_{n+1} x_n| = \min_{s} |s x_n|$ with $p_k(s) = 0$.

On one hand, if $x_{n+1} = \alpha$, then $M_k = 0$ and equation (12) is trivially true.

On the other hand, if $x_{n+1} \neq \alpha$, by using the Lagrange mean value theorem, there exists τ_n between x_{n+1} and α such that $p'_k(\tau_n) = \frac{p_k(\alpha) - p_k(x_{n+1})}{\alpha - x_{n+1}}$. Due to the fact that $p_k(x_{n+1}) = 0$, we get $p'_k(\tau_n) = \frac{p_k(\alpha)}{\alpha - x_{n+1}}$, what amounts to,

$$e_{n+1} = \frac{p_k(\alpha)}{p'_k(\tau_n)}.$$
(14)

Let us now prove by induction on k that $p_k(\alpha) = -f[x_{n-k}, \ldots, x_n, \alpha]e_ne_{n-1} \ldots e_{n-k}$. The base case for k = 1 comes from the secant method in this way,

$$p_{1}(\alpha) = f(x_{n}) + f[x_{n}, x_{n-1}](\alpha - x_{n}) = \frac{f(x_{n}) - f(\alpha)}{\alpha - x_{n}}(\alpha - x_{n}) + f[x_{n}, x_{n-1}](\alpha - x_{n})$$
$$= (\alpha - x_{n})(\frac{-f[x_{n}, \alpha] + f[x_{n-1}, x_{n}]}{\alpha - x_{n-1}})(\alpha - x_{n-1}) = -f[x_{n-1}, x_{n}, \alpha]e_{n}e_{n-1}.$$

Let us suppose the result true for k, that is, $p_k(\alpha) = -f[x_{n-k}, \ldots, x_n, \alpha]e_ne_{n-1}\ldots e_{n-k}$, and let us prove it for k+1.

$$p_{k+1}(\alpha) = p_k(\alpha) + f[x_{n-k-1}, x_{n-k}, \dots, x_n](\alpha - x_{n-k}) \dots (\alpha - x_n)$$

$$= p_k(\alpha) + f[x_{n-k-1}, x_{n-k}, \dots, x_n]e_n \dots e_{n-k}$$

$$= -f[x_{n-k}, \dots, x_n, \alpha]e_n e_{n-1} \dots e_{n-k} + f[x_{n-k-1}, x_{n-k}, \dots, x_n]e_n \dots e_{n-k}$$

$$= \frac{f[x_{n-k-1}, x_{n-k}, \dots, x_n] - f[x_{n-k}, \dots, x_n, \alpha]}{(\alpha - x_{n-k-1})} (\alpha - x_{n-k-1})e_n \dots e_{n-k}$$

$$= -f[x_{n-k-1}, x_{n-k}, \dots, x_n, \alpha]e_n \dots e_{n-k}e_{n-k-1}.$$

And the proof by induction is done. By plugging this result into (14) we get,

$$e_{n+1} = \frac{p_k(\alpha)}{p'_k(\tau_n)} = \frac{p_{k-1}(\alpha)}{p'_k(\tau_n)} + \frac{f[x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, x_{n-k}]e_n e_{n-1} e_{n-2} \cdots e_{n-k+1}}{p'_k(\tau_n)}$$
(15)
$$= e_n e_{n-1} e_{n-2} \cdots e_{n-k+1} \cdot \frac{-f[x_n, \dots, x_{n-k+1}, \alpha]}{p'_k(\tau_n)} + \frac{f[x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, x_{n-k}]e_n e_{n-1} e_{n-2} \cdots e_{n-k+1}}{p'_k(\tau_n)}$$
$$= \frac{e_n e_{n-1} e_{n-2} \cdots e_{n-k+1}}{p'_k(\tau_n)} \left(-f[x_n, \dots, x_{n-k+1}, \alpha] + f[x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, x_{n-k}]\right).$$

By using the property of symmetry of the divided differences and their definition we reach from (15) to,

$$e_{n+1} = \frac{e_n e_{n-1} e_{n-2} \cdots e_{n-k+1}}{p'_k(\tau_n)} (\alpha - x_{n-k}) (-f[x_{n-k}, x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, \alpha])$$

$$= \frac{e_n e_{n-1} e_{n-2} \cdots e_{n-k+1} e_{n-k}}{p'_k(\tau_n)} (-f[x_{n-k}, x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, \alpha]) = M_{k,n} e_n e_{n-1} e_{n-2} \cdots e_{n-k+1} e_{n-k},$$

with

$$M_{k,n} = \frac{-f[x_{n-k}, x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, \alpha]}{p'_k(\tau_n)}.$$

By using again the properties of the divided differences, we get,

$$M_{k,n} = \frac{-f[x_{n-k}, x_n, x_{n-1}, x_{n-2}, \dots, x_{n-k+1}, \alpha]}{p'_k(\tau_n)} = \frac{-f^{(k+1)}(\psi_n)}{p'_k(\tau_n)(k+1)!},$$

where ψ_n is an intermediate point among $\{x_{n-k}, x_n, x_{n-1}, x_{n-2}, ..., x_{n-k+1}, \alpha\}$. Since $p_k(x) = f(x_n) + f[x_n, x_{n-1}](x - x_n) + ... + f[x_n, x_{n-1}, ..., x_{n-k}](x - x_n) \dots (x - x_{n-k-1})$, then,

$$p'_{k}(x) = f[x_{n}, x_{n-1}] + f[x_{n}, x_{n-1}, x_{n-2}](x - x_{n})(x - x_{n-1}) + \dots + .$$
(16)

Since τ_n is an intermediate point among $x_n, x_{n-1}, x_{n-2}, ..., x_{n-k+1}, x_{n-k}, \alpha$, taking limits,

$$lim_{n\to\infty}p'_k(\tau_n) = f[\alpha,\alpha] = f'(\alpha) \neq 0.$$

Thus, there exists the limit,

$$m_k = \lim_{n \to \infty} M_k = \frac{-f^{(k+1)}(\alpha)}{f'(\alpha)(k+1)!}.$$

Before addressing the main theorem proving the order of convergence of a secant polynomial method of degree k, we introduced also the following lemma.

Lemma 5. Let us consider for each polynomial $g_k(x) = x^k - x^{k-1} - \ldots - x - 1$ the unique real root α_k in the interval (1,2). Then, the sequence $(\alpha_k)_{k=1}^{\infty}$ is strictly increasing and it has limit equal to 2.

Proof. Evaluating $g_{k+1}(x)$ at α_k we get,

$$g_{k+1}(\alpha_k) = \alpha_k^{k+1} - \alpha_k^k - \alpha_k^{k-1} - \dots - \alpha_k - 1 = \alpha_k^{k+1} - 2\alpha_k^k + (\alpha_k^k - \alpha_k^{k-1} - \dots - \alpha_k - 1).$$

Since α_k is a root of $g_k(x)$ we have $\alpha_k^k - \alpha_k^{k-1} - \dots - \alpha_k - 1 = 0$. Thus, $p_{k+1}(\alpha_k) = \alpha_k^{k+1} - 2\alpha_k^k = \alpha_k^k(\alpha_k - 2)$. Taking into account that $\alpha_k \in (1, 2)$, then $p_{k+1}(\alpha_k) = \alpha_k^k(\alpha_k - 2) < 0$.

We already know because of Lemma 1 that α_{k+1} is the unique positive root of g_{k+1} , and it is placed in (1, 2). Moreover, $\lim_{k \to +\infty} p_{k+1}(x) = +\infty$ and $\alpha_k > 0$ with $p_{k+1}(\alpha_k) < 0$. Then, in order not to contradict Bolzano's theorem, it must be $\alpha_k < \alpha_{k+1}$.

Let us now see that $\lim_{k \to +\infty} \alpha_k = 2$. We have just proven that,

$$\alpha_1 < \alpha_2 < \ldots < \alpha_k < \alpha_{k+1} < \ldots,$$

and therefore we deal with a strictly increasing sequence contained in the interval [1,2], and consequently upper bounded by 2. This means that there exists $L = \lim_{k \to +\infty} \alpha_k \leq 2$. Let us suppose by reduction to absurdity that $L = \lim_{k \to +\infty} \alpha_k < 2$.

We compute $\lim_{k \to +\infty} g_k(L)$ where,

$$g_k(L) = L^k - \sum_{j=0}^{k-1} L^j = L^k - \frac{1-L^k}{1-L} = L^k - \frac{L^k-1}{L-1} = \frac{L^{k+1}-L^k-L^k+1}{L-1} = \frac{L^{k+1}-2L^k+1}{L-1},$$

and thus,

$$\lim_{k \to +\infty} g_k(L) = \lim_{k \to +\infty} \frac{L^{k+1} - 2L^k + 1}{L - 1} = \lim_{k \to +\infty} \frac{L^k(L - 2) + 1}{L - 1} = -\infty < 0.$$

It follows that $\exists k_0 \geq 2 : p_{k_0}(L) < 0$. By Lemma 1 g_{k_0} has a unique positive root α_{k_0} located in (1,2). As $p_{k_0}(L) < 0$, it must be $L < \alpha_{k_0}$, what gives a contradiction since the sequence of α_k is strictly increasing and $\alpha_k \leq L \forall k$. Thus, $L = \lim_{k \to +\infty} \alpha_k = 2$.

Theorem 2. Let us suppose that the secant polynomial method with polynomials of degree k is convergent for a given set of initial points towards a simple root α of a k + 1 differentiable function f, that is, $f(\alpha) = 0, f'(\alpha) \neq 0$. Then, the order of convergence of the method is at least α_k .

Proof. From Proposition 1, we obtain

$$e_{n+1}(m_k)^{\frac{1}{k}} = e_n(m_k)^{\frac{1}{k}} \cdot e_{n-1}(m_k)^{\frac{1}{k}} \cdot e_{n-2}(m_k)^{\frac{1}{k}} \cdots e_{n-k}(m_k)^{\frac{1}{k}} \cdot \frac{M_k}{m_k}.$$

Actually, we deduce

$$ln\left(e_{n+1}(m_{k})^{\frac{1}{k}}\right) = ln\left(e_{n}(m_{k})^{\frac{1}{k}} \cdot e_{n-1}(m_{k})^{\frac{1}{k}} \cdot e_{n-2}(m_{k})^{\frac{1}{k}} \cdots e_{n-k}(m_{k})^{\frac{1}{k}} \cdot \frac{M_{k}}{m_{k}}\right) = \\ = ln\left(e_{n}(m_{k})^{\frac{1}{k}}\right) + ln\left(e_{n-1}(m_{k})^{\frac{1}{k}}\right) + ln\left(e_{n-2}(m_{k})^{\frac{1}{k}}\right) + \dots + \\ + ln\left(e_{n-k}(m_{k})^{\frac{1}{k}}\right) + ln\left(\frac{M_{k}}{m_{k}}\right).$$
(17)

Calling $F_i = ln(e_i(m_k)^{\frac{1}{k}})$, where i = n, n - 1, n - 2, ..., n - k, the expression (17) can be rewritten

as

$$F_{n+1} = F_n + F_{n-1} + F_{n-2} + \dots + F_{n-k} + \ln\left(\frac{M_k}{m_k}\right)$$

It is a linear and complete difference equation with constant coefficients.

As we are dealing with the order of convergence, we will work with limits, so we calculate $\lim_{n\to\infty} ln\left(\frac{M_k}{M}\right)$,

$$\begin{split} \lim_{n \to \infty} \ln\left(\frac{M_k}{M}\right) &= \lim_{n \to \infty} [\ln(M_k) - \ln(m_k)] = \lim_{n \to \infty} [\ln(M_k)] - \lim_{n \to \infty} [\ln(m_k)] \\ &= \ln\left(\lim_{n \to \infty} M_k\right) - \ln(m_k) = \ln(m_k) - \ln(m_k) = 0. \end{split}$$

Thus, we can consider the linear and homogeneous difference equation with constant coefficients $F_{n+1} = F_n + F_{n-1} + F_{n-2} + \ldots + F_{n-k}$. Its characteristic equation is $x^{k+1} - x^k - x^{k-1} - x^{k-2} - \ldots - x - 1 = 0$, whose positive roots provide us the order of convergence.

Using Lemma 1, we know that its unique positive root α_{k+1} is in the interval (1,2). In the meantime, Lemma 4 ensures that any other root verifies that it is strictly smaller than 1 in absolute value. Therefore, the order of convergence becomes at most 2.

Remark 1. A strategy for increasing the approximation order for higher order polynomials of the family introduced in this article is to initiate the method by choosing adequately the starting points, taking profit of the previous methods of lower order of approximation. That is, the first two points are chosen as close as possible to the existing root, the next iterate is then obtained by applying Secant method, which gives three starting points, and then Müller method can be considered to give another point, after this step the cubic method is used, and so on and so forth to reach the desired polynomial degree, see [17].

5 Numerical experiments

In this section we carry out some simple numerical experiments to reinforce the theoretical results, and see if the methods perform as expected. Our first experiments deals with the function $f_1(x) = x \sin(x^3 + 7)$, which presents a simple root at x = 0. We apply the cubic secant method, and the results can be seen in Table 1. We have used variable precision arithmetic with 200 digits. We give the initial starting points and the numerical convergence order attained. The iterations were run until two consecutive iterates were closer than 10^{-150} in absolute value. For example, for the cubic secant method the iteration was started with the points -1, -0.5, 0.5, 1 and the attained order of convergence was 1.929 which corresponds with the root of the polynomial $g_4(x) = x^4 - x^3 - x^2 - x - 1$ in the interval (1, 2), just as pointed out by Theorem 2.

Method	Initial Points	Number of iterations	Error	Order p
Cubic	[-1, -0.5, 0.5, 1]	10	$4.9553 \cdot 10^{-187}$	1.929

Table 1: Results obtained approximating the root x = 0 of the function $f_1(x) = x \sin(x^3 + 7)$ with an error smaller than 10^{-150} between successive iterations.

Since these methods are based on high degree polynomials, it is expected that they work fine for functions with a chiefly similar polynomial form, and this is what we try to show with our next experiment. We consider the function $f_3(x) = x^3 - 5x^2 - 10x - 30 + 0.02 \cos(x)$, and we run the generalized secant methods: secant, Müller, cubic, and quartic secant methods respectively. We want to approximate the root of $f_2(x)$ close to x = 7. The results can be observed in Table 2. In order to compute the convergence order in this experiment we have taken as exact root the previously approximated root with a much higher precision. Again, the results obtained are consistent with the developed theory.

Method	Initial Points	Iterations	Error	Order p	CPU time
Secant	[5, 100]	15	$1.680 \cdot 10^{-58}$	1.618	0.891
Müller	[5, 10, 100]	11	$2.800 \cdot 10^{-57}$	1.833	1.047
Cubic	[-5, 5, 8, 12]	6	$4.445 \cdot 10^{-70}$	1.908	1.203
Quartic	[-10, -7, -5, 5, 7]	6	$2.196 \cdot 10^{-92}$	1.965	2.828

Table 2: Results obtained by approximating the root close to x = 7 of the function $f_2(x) = x^3 - 5x^2 - 10x - 30 + 0.02 \cos(x)$ with an error smaller than 10^{-50} between successive iterations.

Since polynomials of degree 5 or higher are not algebraically solvable, the implementation of the family of methods in Proposition 1 would require the approximation of roots of such polynomials by using specialized methods for polynomials, and this in turn would increase significantly the overall computational cost. This computational cost could be reduced by refining the methods via the strategy explained in Remark 1.

6 Conclusions

A complete study on the order of convergence of the family of methods that arise from the secant and Müller methods by considering higher degree polynomials have been carried out. Rigorous proofs of the main results have been derived, observing that the methods give a sequence of orders of convergence which is strictly increasing and with limit 2. To obtain the theoretical results about the boundedness of the absolute value of the complex roots of a polynomial we have used an interesting new approach based on Cardano-Vieta's formulas and the Cauchy theorem. Finally, some numerical results have been shown indicating that the numerical results reinforce the proven theoretical results.

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