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On a class of higher order methods for simultaneous rootfinding of generalized polynomials

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Summary. Using the argument principle higher order methods for simultaneous computation of all zeros of generalized polynomials (like algebraic, trigonometric and exponential polynomials or exponential sums) are derived. The methods can also be derived following the continuation principle from [3]. Thereby, the unified approach of [7] is enlarged to arbitrary order N. The local convergence as well as a-priori and a-posteriori error estimates for these methods are treated on a general level. Numerical examples are included.

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1. Introduction

Let f be holomorphic in an open set D of the complex plane $\mathbb{C}$ having exactly n simple zeros $\xi_1, \ldots, \xi_n$. For simultaneous computation of these zeros, let $x_1, \ldots, x_n \in D$ be given simple approximants, sufficiently close to the zeros of f.

Following the continuation process from [3], assume that there exists a holomorphic function Q: $D \to \mathbb{C}$ having exactly the simple zeros $x_1, \ldots, x_n$ in D. In the particular cases of algebraic, trigonometric and exponential polynomials Q is easily obtained explicitly. In general, Q can be defined as the remainder of the interpolation of f using a n-dimensional Chebyshev space U and the knodes $x_1, \ldots, x_n$.

Provided the function Q is known, for $N \geqq 2$, one step of our *method* (M_N), as derived in Sect. 2, reads $(x_1, \ldots, x_n) \mapsto (\hat{x}_1, \ldots, \hat{x}_n)$, where

$$(1) \qquad (M_N): \quad \hat{x}_j := x_j + \sum_{\nu=1}^{N-1} \frac{(-1)^\nu}{\nu} \cdot \operatorname*{Res}_{z=x_j} \left(\frac{f(z) - Q(z)}{Q(z)} \right)^\nu \quad j \in \{1, \ldots, n\} .$$

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For instance, one step of method (M_2), (M_3), (M_4) explicitly reads

(M_2): $\hat{x}_j := x_j - f_0$

(M_3): $\hat{x}_j := x_j - 2f_0 + f_0 f_1 - f_0^2 q_2$

(M_4): $\hat{x}_j := x_j - 3f_0 + 3f_0 f_1 - f_0 f_1^2 + 3f_0^2 f_1 q_2 - f_0^2 f_2 - 3f_0^2 q_2 + f_0^3 q_3 - 2f_0^3 q_2^2$,

respectively, where, suppressing the index $j \in \{1, \ldots, n\}$,

$$f_k := \frac{f^{(k)}(x_j)}{k!Q'(x_j)}, \qquad q_k := \frac{Q^{(k)}(x_j)}{k!Q'(x_j)}$$

for $k = 0, 1, 2, \ldots$ and $j = 1, \ldots, n$. We mention that the higher order methods (M_N) can be easily obtained by formal algebraic computations with power series of f and Q.

In Sect. 3, it is proved that (M_N) is locally convergent with Q-order N. Moreover, in each component, the convergence is superlinear.

It will be shown in Sect. 4 that (M_2) is method (M) from [7]. Moreover, (M_N) is a natural generalization of the continuation process in [3] of order N which was firstly considered for algebraic polynomials in [5]. For $n = 1$, the so-called Euler-methods are obtained.

In Sect. 5, a-priori and a-posteriori error estimates are derived based on Rouché's theorem following [4]. Finally, Sect. 6 presents some illustrating numerical examples.

2. Lagrangian interpolation and method (M_N)

Recall that $f \in H(D)$, i.e. f is holomorphic in an open set D of the complex plane $\mathbb{C}$, and f has the simple zeros $\xi_1, \ldots, \xi_n$. Let $x_1, \ldots, x_n \in D$ be given approximants, sufficiently close to the zeros of f. In particular, we assume that $x_1, \ldots, x_n$ are pairwise distinct.

In addition let $U \subseteq H(D)$ be a n-dimensional complex Chebyshev-space. Then, there exists a unique interpolant $p := [U, x]pf \in U$ such that the remainder

$$r := [U, x]rf := f - [U, x]pf \in H(D) \tag{2}$$

vanishes in $x_1, \ldots, x_n$. Hence $Q(x) := r$ satisfies the assumptions of Sect. 1. The restriction to a complex Chebyshev-space is only for convenience of notation and can be relaxed; cf. Remark (iii) below.

Of course, choosing any base $b_1, \ldots, b_n$ of U, $[U, x]pf$ can be computed solving a certain linear equation, i.e.

$$[U, x]pf = (b_1, \ldots, b_n) \cdot (b_j(x_k)|_{j=1,\ldots,n}^{k=1,\ldots,n})^{-1} \cdot \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix}.$$

Frequently, we take the so-called *dual basis* $d_1 := d_1(x), \ldots, d_n := d_n(x)$, depending on $x = (x_1, \ldots, x_n)$ with

$$d_k(x_j) = \delta_{j,k} \quad j, k \in \{1, \ldots, n\},$$

where $\delta_{j,k} = 1, 0$ if $j = k$, $j \neq k$, respectively, is Kronecker's δ. Consequently,

(3) $$[U, \boldsymbol{x}]pf = \sum_{\nu=1}^{n} f(x_\nu) \cdot d_\nu(\boldsymbol{x}) .$$

It is not hard to see that

$$\begin{pmatrix} d_1(\boldsymbol{x}) \\ \vdots \\ d_n(\boldsymbol{x}) \end{pmatrix} = (b_j(x_k)|_{j=1,\ldots,n}^{k=1,\ldots,n})^{-1} \cdot \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}.$$

Thus, $d_1(\boldsymbol{x}), \ldots, d_n(\boldsymbol{x})$ is analytic in $\boldsymbol{x}$, provided the components $x_1, \ldots, x_n \in D$ of $\boldsymbol{x}$ are pairwise distinct.

To derive method (M_N), it is essential to assume that there exist nonoverlapping discs $D_1, \ldots, D_n$ and $B_1, \ldots, B_n$, respectively, lying compactly in D with

$$(\xi_1, \ldots, \xi_n) \in B := B_1 \times \ldots \times B_n \subseteq D_1 \times \ldots \times D_n$$

such that for any $\boldsymbol{x} \in B$

(4) $$\eta := \left\| \frac{[U, \boldsymbol{x}]pf}{[U, \boldsymbol{x}]rf} \right\|_{\infty, \partial D_1 \cup \ldots \cup \partial D_n} < 1 .$$

Here, $\|\cdot\|_{\infty,S}$ denotes the supremum-norm on a set $S \subseteq D$ and it is assumed that the denominator is nonzero on $\partial D_1 \cup \ldots \cup \partial D_n$.

The following lemma shows that these assumptions can always be satisfied for nonoverlapping $D_1, \ldots, D_n$, taking B_j as a sufficiently small neighbourhood of the zero $\xi_j \in D_j$ of f.

Lemma 1. *Let $D_1, \ldots, D_n$ be open discs in D, having a positive distance from each other and from ∂D, with $\xi_j \in D_j$ for any $j \in \{1, \ldots, n\}$. Then, there exist open discs $B_1 \subseteq D_1, \ldots, B_n \subseteq D_n$ satisfying* (4). *Moreover, there exists a constant $C > 0$ such that for any $\boldsymbol{x} \in B$*

(5) $$\left\| \frac{[U, \boldsymbol{x}]pf}{[U, \boldsymbol{x}]rf} \right\|_{\infty, \partial D_1 \cup \ldots \cup \partial D_n} \leqq C \cdot \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu| .$$

Proof. Since f is nonzero in $D \setminus \{\xi_1, \ldots, \xi_n\}$,

$$m_1 := \min\{|f(z)| \,|z \in \partial D_1 \cup \ldots \cup \partial D_n\} > 0 .$$

Because the discs $D_1, \ldots, D_n$ have a positive distance from each other and from ∂D,

$$M_2 := \sup\{\|d_j(z)\|_{\infty, \partial D_\nu} |z \in D_1 \times \ldots \times D_n, j, \nu \in \{1, \ldots, n\}\} < \infty .$$

On the other hand, since $f(\xi_j) = 0$, the mean value theorem gives

$$|f(x_j)| \leqq M_3 \cdot |\xi_j - x_j|, \qquad M_3 := \|f'\|_{\infty, D_1 \cup \ldots \cup D_n} .$$

Altogether, for $z \in \partial D_j$,

$$|[U, \boldsymbol{x}]\, pf(z)| \leqq \sum_{\nu=1}^{n} |f(x_\nu)| \cdot |d_\nu(\boldsymbol{x})(z)| \leqq n \cdot M_2 \cdot M_3 \cdot \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu|$$

while

$$|[U,x]\,rf(z)| \geqq |f(z)| - |[U,x]\,pf(z)| \geqq m_1 - n \cdot M_2 \cdot M_3 \cdot \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu| .$$

Choosing, e.g., $B_1, \ldots, B_n \subset D$ to be the discs having the centers $\xi_1, \ldots, \xi_n$ and the radii less than or equal to r such that

$$1/2 \cdot m_1 > r \cdot n \cdot M_2 \cdot M_3$$

leads to

$$\left\| \frac{[U,x]\,pf}{[U,x]\,rf} \right\|_{\infty,\partial D_j} \leqq \frac{n \cdot M_2 \cdot M_3}{n \cdot M_2 \cdot M_3 \cdot r} \cdot \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu|$$

$$\leqq 1/r \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu| < 1, \qquad x \in B . \quad \square$$

Remarks. (i) Lemma 1 shows that η, defined in (4), tends to zero if $(x_\nu | \nu \in \{1, \ldots, n\})$ tends to $(\xi_\nu | \nu \in \{1, \ldots, n\})$. Therefore, it is no essential restriction to assume that η is sufficiently small.

(ii) Due to Rouché's theorem (see, e.g., [2]), (4) implies that D_j contains one zero of r, namely x_j, as well as one zero of f, $j \in \{1, \ldots, n\}$. Since there are only n zeros of f in D, f and r have *exactly* one zero in D_j, $j \in \{1, \ldots, n\}$.

(iii) For convenience of notation, Lemma 1 is formulated only in the complex case whereas it applies for real Chebyshev systems as well. Provided f as well as the elements of U are real valued analytic functions they may be continuated to an open set D containing the real zeros. Choosing $B_1, \ldots, B_n$ as real intervals, the proof of Lemma 1 remains true. Note that in this case $x \in \mathbb{R}^n$ implies $\hat{x} \in \mathbb{R}^n$.

In the sequel, this argument applies as well so that the complex case carries over to the real one. $\square$

The method (M_N) is based on the following theorem which gives a series representation of the exact zeros. Taking the first $N - 1$ terms in Eq. (6) gives the new approximant $\hat{x}_j$, cf. (1).

Theorem 1. *Let the discs* $B_1, \ldots, B_n$, $D_1, \ldots, D_n$, $B_j \subseteq D_j$, *satisfy* (4). *Then, for any* $x \in B$

$$\xi_j - x_j = \sum_{\nu=1}^{\infty} \frac{(-1)^\nu}{\nu} \cdot \operatorname*{Res}_{z=x_j} \left(\frac{[U,x]\,pf(z)}{[U,x]\,rf(z)} \right)^\nu . \tag{6}$$

Proof. The residue theorem (see, e.g., [2]), applied to f and $r := [U,x]\,rf$, proves

$$\xi_j = \frac{1}{2\pi i} \int_{\partial D_j} z \cdot \frac{f'(z)}{f(z)}\, dz \tag{7}$$

$$x_j = \frac{1}{2\pi i} \int_{\partial D_j} z \cdot \frac{r'(z)}{r(z)}\, dz . \tag{8}$$

Therefore and by partial integration,

$$\xi_j - x_i = \frac{1}{2\pi i}\int_{\partial D_j} z\cdot\left(\frac{f'(z)}{f(z)} - \frac{r'(z)}{r(z)}\right)dz$$

$$= -\frac{1}{2\pi i}\int_{\partial D_j} \log\frac{f(z)}{r(z)}\,dz$$

$$= -\frac{1}{2\pi i}\int_{\partial D_j} \log\left(1 + \frac{p(z)}{r(z)}\right)dz\,.$$

Note that (4) guarantees that the principal value of $\log(1 + p/r)$ is holomorphic in a neighbourhood of ∂D_j and can be developed into a power series, whence

$$\xi_j - x_j = -\frac{1}{2\pi i}\int_{\partial D_j}\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu}\left(\frac{p(z)}{r(z)}\right)^{\nu}dz$$

$$= \sum_{\nu=1}^{\infty}\frac{(-1)^{\nu}}{\nu}\cdot\frac{1}{2\pi i}\int_{\partial D_j}\left(\frac{p(z)}{r(z)}\right)^{\nu}dz\,.$$

Due to the residue theorem (see, e.g., [2]), this implies (6). □

3. Convergence

It is proved that method (M_N) is locally well-defined and of convergence order N. Moreover, method (M_N) is Q-superlinearly convergent in each component, see (10).

We remark that if D is a disc then $\operatorname{rad} D$ and $\operatorname{mid} D$ denote the radius and midpoint of D, respectively.

Theorem 2. *Under the assumptions of Lemma* 1, *let* $\operatorname{mid} B_j = \xi_j$ *and*

(9) $$\operatorname{rad} D_j\cdot\frac{\eta^N}{N(1-\eta)} < \operatorname{rad} B_j,\quad j\in\{1,\ldots,n\}\,.$$

Then, method (M_N) is feasible, i.e. for any $x\in B$, $\hat{x}$ as defined in (1) *also lies in B. Method (M_N) is locally convergent having Q-order N. In addition, there exists a constant $C>0$ such that for any $x\in B$*

(10) $$|\xi_j - \hat{x}_j| \leqq C^N\cdot|\xi_j - x_j|\cdot\max_{\nu=1,\ldots,n}|\xi_\nu - x_\nu|^{N-1},\quad j = 1,\ldots,n\,.$$

Proof. From (1), Theorem 1 and the related considerations,

$$|\xi_j - \hat{x}_j| \leqq \sum_{\nu=N}^{\infty}\frac{1}{2\pi\nu}\left|\int_{\partial D_j}\left(\frac{p(z)}{r(z)}\right)^{\nu}dz\right|\,.$$

To verify $\hat{x}\in B$, note that, using (4),

(11) $$|\xi_j - \hat{x}_j| \leqq \sum_{\nu=N}^{\infty}\frac{\operatorname{rad} D_j}{\nu}\eta^{\nu} < \operatorname{rad} D_j\frac{\eta^N}{N(1-\eta)} < \operatorname{rad} B_j\,,$$

by (9). To prove (10), let

$$a := f(x_j)\cdot d_j(x), \qquad h := [U, x]\, pf - a$$

and note that h/r is holomorphic in D_j, while, in general, a/r has a pole in x_j. Since $p = a + h$,

$$\int_{\partial D_j} \left(\frac{p(z)}{r(z)}\right)^{\nu} dz = \int_{\partial D_j} \left(\frac{a(z)}{r(z)} + \frac{h(z)}{r(z)}\right)^{\nu} dz$$

$$= \sum_{\mu=0}^{\nu} \binom{\nu}{\mu} \int_{\partial D_j} (a(z)/r(z))^{\mu}\cdot(h(z)/r(z))^{\nu-\mu}\, dz\,.$$

Due to the residue theorem, in the last sum, the summand for $\mu = 0$ is zero. Therefore,

$$\left|\int_{\partial D_j} \left(\frac{p(z)}{r(z)}\right)^{\nu} dz\right| \leqq \sum_{\mu=1}^{\nu} \binom{\nu}{\mu} \int_{\partial D_j} |a(z)/r(z)|^{\mu}\cdot|h(z)/r(z)|^{\nu-\mu}\,|dz|\,.$$

As in the proof of Lemma 1 we estimate

$$\|a/r\|_{\infty,\partial D_j} \leqq C_1\cdot|\xi_j - x_j|$$

$$\|h/r\|_{\infty,\partial D_j} \leqq C_2\cdot \max_{\nu=1,\ldots,n} |\xi_\nu - x_\nu|\,,$$

where C_1, C_2 depend only on $D_1, \ldots, D_n$, $B_1, \ldots, B_n$, f and U. This proves (10). □

Remark. If $f \in H(D)$ has n distinct zeros in D and $U \subseteq H(D)$ is a n-dimensional complex Chebyshev-space the assumptions of Lemma 1 can always be satisfied. Thus, by Theorem 2, there exist neighbourhoods $B_1, \ldots, B_n$ of the zeros of f such that choosing initial values in $B_1 \times \ldots \times B_n$ method (M_N) generates a sequence of approximants converging towards $(\xi_1, \ldots, \xi_n)$ having the order of convergence at least N, i.e. method (M_N) is locally convergent of order N.

4. Continuation process, unified method, Euler methods

This section discusses three relations to other methods. Firstly, the continuation method of [3] is sketched which gives method (M_N) using the Taylor method of N-th order for solving a certain initial value problem.

Secondly, it is proved that (M_2) is method (M) in the unified approach of [7] which is Newton-Raphson's method for a certain system of nonlinear equations.

Finally, the case $n = 1$, U being the space of constant functions, is considered which gives the sometimes called Euler-methods; in particular, (M_2) is Newton-Raphson's method for a single equation.

4.1 Continuation process

Following [3], let f and Q as in the first section and consider the homotopy

(12) $$H: [0, 1] \times D \to \mathbb{C}, \qquad (t, z) \mapsto (1 - t)\cdot Q(z) + t\cdot f(z)\,.$$

By assumption (4), using $p = f - Q$, $r = Q$, there holds

$$|H(t, z) - Q(z)| = |t| \cdot |f(z) - Q(z)| < |Q(z)|$$

for all $z \in \partial D_j$, $t \in [0, 1]$. Hence, by Rouché's theorem, for any $t \in [0, 1]$ there exists one and only one zero $z_j(t)$ of $H(t, \cdot)$ in D_j. Then, the identity $t \mapsto H(t, z_j(t)) = 0$ can be differentiated leading to the system of n ordinary differential equations

$$\dot{z}_j(t) = \frac{Q(z_j(t)) - f(z_j(t))}{(1-t)\cdot Q'(z_j(t)) + t\cdot f'(z_j(t))}, \quad j = 1, \ldots, n. \tag{13}$$

Since $z_j(0) = x_j$ is the given initial value and $z_j(1) = \xi_j$ has to be computed, any method for the numerical treatment of ordinary differential equations may be applied to obtain better approximants for the zeros of f.

By application of Taylor-approximants of $(N-1)$-th order $x_j^{(C)}$ is obtained from

$$\xi_j = z_j(1) \approx x_j^{(C)} := z_j(0) + \sum_{\nu=1}^{N-1} \frac{z_j^{(\nu)}}{\nu!}(0), \quad j = 1, \ldots, n.$$

As seen in the following lemma, this yields method (M_N).

Lemma 2. $x_j^{(C)} = \hat{x}_j, j = 1, \ldots, n.$

Proof. By (13) and the residue theorem,

$$\dot{z}_j(t) = \frac{1}{2\pi i} \int_{\partial D_j} \frac{Q(z) - f(z)}{(1-t)\cdot Q(z) + t\cdot f(z)}\, dz,$$

since the denominator has exactly the zero $z = z_j(t)$ in D_j. Therefore, for any $\nu \geqq 1$,

$$z_j^{(\nu)}(t) = \frac{(-1)^\nu(\nu-1)!}{2\pi i} \int_{\partial D_j} \left(\frac{f(z) - Q(z)}{(1-t)\cdot Q(z) + t\cdot f(z)}\right)^\nu dz.$$

For $t = 0$, $z_j(0) = x_j$, the residue theorem gives

$$\frac{z_j(t)^{(\nu)}(0)}{\nu!} = \frac{(-1)^\nu}{\nu} \cdot \operatorname*{Res}_{z=x_j} \left(\frac{f-Q}{Q}\right)^\nu$$

which proves the lemma (cf. (1)). □

In [3], [9] and [7] only (M_2) is considered and convergence is proved only for particular cases. We stress that Theorem 2 gives convergence for all methods simultaneously and also for all methods of higher order N.

4.2 Unified approach

The unified approach [7] is Newton-Raphson's method applied to

$$F: B_1 \times \ldots \times B_n \to U, z \mapsto \sum_{\nu=1}^{n} f(z_\nu)\cdot d_\nu(z),$$

where $d_1, \ldots, d_n$ belongs to the dual base as introduced in Sect. 2. Assuming that the inverse exists, one step of Newton-Raphson's method reads

$$x^{(NR)} := x - DF(x)^{-1}[F(x)]$$

and yields method (M) from [7].

As seen in the following lemma, (M_2) is [7, method (M)].

Lemma 3. *If* $N = 2$ *then* $x^{(NR)} = \hat{x}$.

Proof. Differentiation of $d_\nu(x)(x_j) = \delta_{\nu,j}$ with respect to x_μ, ν, μ, $j \in \{1, \ldots, n\}$, gives

$$\left(\frac{\partial}{\partial x_\mu} d_\nu(x)\right)(x_j) = -\delta_{j,\mu} \cdot d_\nu(x)'(x_j) . \tag{14}$$

The new approximant $x^{(NR)} = x + y$ in Newton-Raphson's method is defined by

$$DF(x)[y] + F(x) = 0 \in U \tag{15}$$

with the (Frechét-) derivative $DF(x)[y]$ of F at x evaluated at y. Using (14) and

$$DF(x)[y] = \sum_{j=1}^{n} y_j f'(x_j) d_j(x)$$
$$+ \sum_{j=1}^{n} \sum_{\nu=1}^{n} \sum_{\mu=1}^{n} y_j f(x_\nu) \left(\frac{\partial}{\partial x_j} d_\nu(x)\right)(x_\mu) d_\mu(x) \in U .$$

(15) is equivalent to

$$0 = f(x_j) + f'(x_j) \cdot y_j - \sum_{\nu=1}^{n} f(x_\nu) \cdot y_j \cdot d_\nu(x)'(x_j) \quad j \in \{1, \ldots, n\} .$$

Because of (2) and (3) this is

$$0 = f(x_j) + y_j \cdot Q'(x_j)$$

concluding the proof. □

The lemma shows that the unified approach [7] is included in the considerations of this note and that (M_2) converges quadratically. Moreover, by Theorem 2, we proved superconvergence in each component.

We finally remark that our notation of method (M) is slightly different from the original notation in [7]. There, some finite dimensional function space V, including f, is endowed with some normalizing linear functional $l \in V'$. In this note, we consider $U := \operatorname{Ker} l$.

4.3 Relation to the Euler-method

If $n = 1$ and U is the space of constant functions on D, then $[U, x]\, pf(z) = f(x_1)$ and hence

$$\hat{x}_1 = x_1 + \sum_{\nu=1}^{N-1} \frac{(-1)^\nu}{\nu} \cdot \operatorname*{Res}_{z=x_1} \left(\frac{f(x_1)}{f(z) - f(x_1)}\right)^\nu . \tag{16}$$

On the other hand, $[U, x]rf(z) = f(z) - f(x_1)$ has a simple zero (see Remark (ii) in Sect. 2) at $z = x_1$. Therefore, $f'(x_1) \neq 0$ and there exists an open disc V with $x_1 \in V$ such that f is injective in a neighbourhood of V. For the inverse function $g: f(V) \to V$ we have the integral formula

$$g(w) = \frac{1}{2\pi i} \int_{\partial V} \frac{z f'(z)}{f(z) - w} \, dz , \tag{17}$$

which follows directly from the residue theorem. Then, the *Euler-method* of order N is the Taylor development of the root (cf. [10, Sect. 14]) and reads $x_1 \mapsto x_1^{(E)}$, where

$$x_1^{(E)} := \sum_{\nu=0}^{N-1} \frac{g^{(\nu)}(f(x_1))}{\nu!} (-f(x_1))^\nu . \tag{18}$$

Lemma 4. *If* $n = 1$ *then* $x_1^{(E)} = \hat{x}_1$.

Proof. Differentiating (17) ν times with respect to w gives for $\nu \geqq 1$

$$\begin{aligned} g^{(\nu)}(w) &= \frac{\nu!}{2\pi i} \int_{\partial V} \frac{z f'(z)}{(f(z) - w)^{\nu+1}} \, dz \\ &= \frac{(\nu - 1)!}{2\pi i} \int_{\partial V} \frac{1}{(f(z) - w)^\nu} \, dz . \end{aligned}$$

By $w = f(x_1)$ and application of the residue theorem, we prove that the right hand sides of (16) and (18) are equal. □

5. Error estimates

In this section, we prove a-posteriori and a-priori error estimates giving upper bounds both for $x_j - \xi_j$ and $\hat{x}_j - \xi_j, j \in \{1, \ldots, n\}$, in terms of the data $x_1, \ldots, x_n$ and $f(x_1), \ldots, f(x_n)$, using the technique from [4].

Let D_j be a disc with center x_j and radius R_j lying compactly in D such that D_j contains exactly one zero, namely x_j, of $Q = [U, x] rf$, $j \in \{1, \ldots, n\}$. Define meromorphic functions $l_1, \ldots, l_n$ on D by

$$l_j(z) := \frac{d_j(x)(z)}{[U, x] rf(z)}, \quad j \in \{1, \ldots, n\} . \tag{19}$$

Each l_j is holomorphic in a neighbourhood of $\bar{D}_1 \cup \ldots \cup \bar{D}_n$ save for a simple pole at $z = x_j$. Thus, there exists a constant $m_j > 0$ such that

$$|l_j(z)| \leqq \frac{m_j}{|z - x_j|} \qquad \text{for } z \in D_1 \cup \ldots \cup D_n \text{ and } j \in \{1, \ldots, n\} . \tag{20}$$

Fix $j \in \{1, \ldots, n\}$ and let

$$\begin{aligned} \varepsilon_j &:= \min\{|x_j - x_k| \mid k \neq j\} , \\ \delta_j &:= \frac{m_j}{\varepsilon_j} \cdot |f(x_j)| , \\ \sigma_j &:= \sum_{\substack{k=1 \\ k \neq j}}^{n} \frac{m_k |f(x_k)|}{|x_j - x_k|} . \end{aligned}$$

If $\sqrt{\delta_j} + \sqrt{\sigma_j} < 1$ then define

$$\underline{R}_j := \tfrac{1}{2}\varepsilon_j \cdot (1 + \delta_j - \sigma_j - \sqrt{(1 + \delta_j - \sigma_j)^2 - 4\delta_j}) > 0$$

$$\underline{R}_j^{(N)} := \varepsilon_j \cdot \sqrt{\delta_j} \cdot \frac{(\sqrt{\delta_j} + \sqrt{\sigma_j})^{2N-1}}{N(1 - (\sqrt{\delta_j} + \sqrt{\sigma_j})^2)} \quad (N = 2, 3, \ldots).$$

Theorem 3. *If $\sqrt{\delta_j} + \sqrt{\sigma_j} < 1$ and $\underline{R}_j < R_j$ then the disc with center x_j and radius $\underline{R}_j$ contains exactly one zero ξ_j.*

If, in addition,

$$\frac{\varepsilon_j \sqrt{\delta_j}}{\sqrt{\delta_j} + \sqrt{\sigma_j}} < R_j$$

then the disc with center $\hat{x}_j$, which is the new approximant after one step of method (M_N) using the initial values $\boldsymbol{x}$, and radius $\underline{R}_j^{(N)}$ contains exactly one zero ξ_j.

Proof. For $z \in D_j$, $0 < |z - x_j| = r < R_j \leqq \varepsilon_j$, there holds

$$\left|\frac{[U, \boldsymbol{x}]\, pf(z)}{[U, \boldsymbol{x}]\, rf(z)}\right| = \left|\sum_{k=1}^{n} l_k(z) f(x_k)\right|$$

$$\leqq \frac{m_j}{r}|f(x_j)| + \sum_{\substack{k=1 \\ k \neq j}}^{n} \frac{m_k}{|x_k - x_j| - r}|f(x_k)|$$

$$\leqq \frac{\delta_j \varepsilon_j}{r} + \frac{\sigma_j}{1 - r/\varepsilon_j} =: \varphi(r).$$

If $\varphi(r) < 1$ then Rouché's theorem states that f and Q have the same number of zeros in the disc with center x_j and radius r. To ensure $\varphi(r) < 1$, consider the condition $\sqrt{\delta_j} + \sqrt{\sigma_j} < 1$ which is equivalent to $(1 + \delta_j - \sigma_j)^2 - 4\delta_j > 0$. Therefore, some computations show that $\varphi(r) < 1$ holds for $r \in (\underline{r}, \bar{r})$, where

$$\underline{r} := \frac{\varepsilon_j}{2} \cdot (1 + \delta_j - \sigma_j - \sqrt{(1 + \delta_j - \sigma_j)^2 - 4\delta_j}),$$

$$\bar{r} := \frac{\varepsilon_j}{2} \cdot (1 + \delta_j - \sigma_j + \sqrt{(1 + \delta_j - \sigma_j)^2 - 4\delta_j}).$$

If we let r tend to $\underline{r}$, we get the first assertion.

Using the inequality (11) in the proof of Theorem 2 with the disc D_j having the center x_j and the radius r and with $\eta \leqq \varphi(r)$ there follows, analogously,

$$|\xi_j - \hat{x}_j| \leqq \frac{r(\varphi(r))^N}{N(1 - \varphi(r))}. \tag{21}$$

Some calculations show that the convex function φ has in the interval $(\underline{r}, \bar{r})$ a minimum value of

$$\varphi\left(\frac{\varepsilon_j \sqrt{\delta_j}}{\sqrt{\delta_j} + \sqrt{\sigma_j}}\right) = (\sqrt{\delta_j} + \sqrt{\sigma_j})^2 < 1 = \varphi(\underline{r}) = \varphi(\bar{r}).$$

Substituting this value in (21) concludes the proof. □

Remarks. (i) For algebraic polynomials Theorem 3 is due to Börsch-Supan [4]. In this case $m_j = 1$ and numerical examples show good estimation of the exact errors.

(ii) In general, the estimation of m_j may be labourous. An example for trigonometric polynomials is given below in Lemma 5 where m_j may become large so that the estimates of Theorem 3 may be very large.

6. Applications, examples

This section discusses the particular cases of algebraic, trigonometric, exponential polynomials and exponential sums in Subsects. 1, 2, 3 and 4, respectively. Some numerical examples are presented.

6.1 Algebraic polynomials

Let f be a monic algebraic polynomial of degree n having the simple zeros $\xi_1, \ldots, \xi_n \in D = \mathbb{C}$. Let U denote the space of algebraic polynomials of degree less than or equal to $n-1$. Then, the remainder of Lagrange interpolation w.r.t U and the nodes $x_1, \ldots, x_n$, which approximate $\xi_1, \ldots, \xi_n$, is well-known, namely

$$Q(z) := [u, x]\, rf = (z - x_1) \cdot \ldots \cdot (z - x_n)\,.$$

With the abbreviation $W_j := f(x_j)/\prod_{k=1, i \neq j}^{n} (x_j - x_k)$, one step of method (M_2), (M_3), (M_4) reads (using the expressions of Sect. 1 and some additional computations)

$$(M_2): \quad \hat{x}_j := x_j - W_j$$

$$(M_3): \quad \hat{x}_j := x_j - W_j \cdot \left(1 - \sum_{k=1, k \neq j}^{n} \frac{W_k}{x_j - x_k}\right)$$

$$(M_4): \quad \hat{x}_j := x_j - W_j \cdot \left(1 - \sum_{k=1, k \neq j}^{n} \frac{W_k}{x_j - x_k} + \left(\sum_{k=1, k \neq j}^{n} \frac{W_k}{x_j - x_k}\right)^2\right)$$
$$+ W_j^2 \sum_{k=1, k \neq j}^{n} \frac{W_k}{(x_j - x_k)^2}\,.$$

Note that the required derivatives of f are computed using the interpolation representation

$$f(z) = Q(z) \cdot \left\{1 + \sum_{j=1}^{n} \frac{W_j}{z - x_j}\right\}.$$

We mention that (M_2) is Durand-Kerner's method, [1, 5–8, 11] while (M_3) is closely related to the third order method of Mahley, Ehrlich, Aberth [1, 11], i.e.

$$\hat{x}_j := x_j - \frac{W_j}{1 + \sum_{k=1, k \neq j}^{n} \frac{W_k}{x_j - x_k}},$$

and (M_4) is related to the Nourein type fourth order method [11]

$$\hat{x}_j := x_j - \frac{W_j}{1 + \sum_{k=1, k \neq j}^{n} \frac{W_k}{x_j - W_j - x_k}} .$$

These relations are seen by developing the last two methods (using the geometric series) and neglecting higher order terms in $W := \max_{k=1,\dots,n} |W_k|$ (of order 3, 4, ... and 4, 5, ..., respectively).

We finally notice that the slightly different methods [7, (4.2)] and [7, (4.3)] can be treated analogously.

6.2 Trigonometric polynomials

Let $y, \xi_1, \dots, \xi_{2n} \in [-\pi, +\pi)$ be pairwise distinct and let the real trigonometric polynomial

(22) $$f(t) = b_0 + \sum_{j=1}^{n} (a_j \cdot \sin(jt) + b_j \cdot \cos(jt))$$

of degree n, denoted by $f \in \mathscr{T}_n$ have the simple zeros $\xi_1, \dots, \xi_{2n}$. Let $x_1, \dots, x_{2n} \in [-\pi, +\pi)$ be distinct approximants for the zeros $\xi_1, \dots, \xi_{2n}$ not equal to y. Define

(23) $$d_j(t) := \frac{1}{c_j} \cdot \sin\left(\frac{t-y}{2}\right) \cdot \prod_{k=1, k \neq j}^{2n} \sin\left(\frac{t-x_k}{2}\right),$$

$$c_j := \sin\left(\frac{x_j - y}{2}\right) \cdot \prod_{k=1, k \neq j}^{2n} \sin\left(\frac{x_j - x_k}{2}\right).$$

Then, some (omitted) calculations show that $d_1, \dots, d_{2n}$ is a dual basis, dual with respect to $\boldsymbol{x}$, of

$$U := \{h \in \mathscr{T}_n | h(y) = 0\} .$$

Consequently,

$$r := [U, \boldsymbol{x}] rf := f - [U, \boldsymbol{x}] pf$$

equals $Q(t)$ as defined by

(24) $$Q(t) = \frac{1}{c} \cdot \prod_{j=1}^{2n} \sin \frac{t - x_j}{2}, \qquad c := \frac{\prod_{j=1}^{2n} \sin\left(\frac{y - x_j}{2}\right)}{f(y)} .$$

(For a proof notice that $h := r - Q \in \mathscr{T}_n$ has $2n + 1$ zeros, namely $y, x_1, \dots, x_{2n}$. Since $\mathscr{T}_n$ is a Chebyshev-space over $[-\pi, +\pi)$ this implies $h = 0$, i.e. $Q = r$.)

Therefore, method (M_N) is convergent of order N by Theorem 2. Using the formulas of the first section and

$$f_0 := \frac{2c \cdot f(x_i)}{\prod_{k=1, k \neq j}^{2n} \sin\left(\frac{x_j - x_k}{2}\right)}$$

$$f_1 := \frac{2c \cdot f'(x_i)}{\prod_{k=1,k \neq j}^{2n} \sin\left(\frac{x_j - x_k}{2}\right)}$$

$$f_2 := \frac{c \cdot f''(x_i)}{\prod_{k=1,k \neq j}^{2n} \sin\left(\frac{x_j - x_k}{2}\right)}$$

$$q_2 := 1/2 \sum_{k=1,k \neq j}^{2n} \cot\left(\frac{x_j - x_k}{2}\right)$$

$$q_3 := 1/4\left(1/2 \cdot \sum_{k=1,k \neq j}^{2n} \sum_{l=1,k \neq l \neq j}^{2n} \cot\left(\frac{x_j - x_k}{2}\right) \cdot \cot\left(\frac{x_j - x_l}{2}\right) - (n - 1/3)\right)$$

the methods (M_2), (M_3) and (M_4) are explicitly determined. Method (M_2) is known from [3] where the second order of convergence is proved explicitly. We stress that our general results give a convergence proof of higher order methods as well.

Example. Let $f(t) = \prod_{j=1}^{4} \sin \frac{t - \xi_j}{2}$ with $\xi_1 = -1.7$, $\xi_2 = 0.3$, $\xi_3 = 0.5$, $\xi_4 = 1.7$. As in [3, (3.2)] we consider the initial values $x_1^{(0)} = -1.5$, $x_2^{(0)} = 0$, $x_3^{(0)} = 0.7$, $x_4^{(0)} = 1.4$, $y = 1$. Table 1 gives the absolute errors of the approximants $x_1^{(v)}, \ldots, x_4^{(v)}$ in step v using method (M_2), (M_3) and (M_4) respectively. (As in the following examples, the numerical calculations were done on a personal computer with 18 decimal digits.) □

We continue with an application of the error estimates of the previous section. Since the dual basis $d_1, \ldots, d_n$ as well as the remainder Q is given in (23) and (24), we focus on the estimation of m_j in (20). D_j is the disc with center x_j and radius R_j, $j \in \{1, \ldots, n\}$. Then, l_j as defined in (19) reads

$$l_j(z) = \frac{c}{c_j} \cdot \frac{\sin\left(\frac{z - y}{2}\right)}{\sin\left(\frac{z - x_j}{2}\right)}.$$

Recall that $y, x_1, \ldots, x_{2n} \in [-\pi, \pi)$ are distinct such that for sufficiently small radii $R_1, \ldots, R_{2n}$

$$\varepsilon := \pi - \frac{1}{2} \max_{j,k=1,\ldots,2n} (|x_j - x_k| + R_k)$$

is positive.

Lemma 5. *If $\varepsilon > 0$ then* (20) *holds with m_j given by*

$$m_j = \frac{2|c| \cdot (\pi - \varepsilon)}{|c_j| \cdot \sin(\varepsilon)} \cdot \max_{k=1,\ldots,2n} \cosh(R_k/2). \tag{25}$$

Table 1. Examples for trigonometric polynomials

ν	Method (M_2)			
	$\|x_1^{(\nu)} - \xi_1\|$	$\|x_2^{(\nu)} - \xi_2\|$	$\|x_3^{(\nu)} - \xi_3\|$	$\|x_4^{(\nu)} - \xi_4\|$
1	$9.62\ 10^{-2}$	$1.68\ 10^{-1}$	$1.20\ 10^{-1}$	$1.53\ 10^{-1}$
2	$2.38\ 10^{-2}$	$6.31\ 10^{-2}$	$5.20\ 10^{-2}$	$4.10\ 10^{-2}$
3	$1.83\ 10^{-3}$	$1.31\ 10^{-2}$	$1.23\ 10^{-2}$	$3.31\ 10^{-3}$
4	$1.89\ 10^{-5}$	$8.23\ 10^{-4}$	$8.11\ 10^{-4}$	$3.34\ 10^{-5}$
5	$8.59\ 10^{-9}$	$3.70\ 10^{-6}$	$3.69\ 10^{-6}$	$1.36\ 10^{-8}$
6	$1.66\ 10^{-14}$	$7.59\ 10^{-11}$	$7.59\ 10^{-11}$	$2.28\ 10^{-14}$
7	0	$2.71\ 10^{-20}$	$5.42\ 10^{-20}$	0
ν	Method (M_3)			
	$\|x_1^{(\nu)} - \xi_1\|$	$\|x_2^{(\nu)} - \xi_2\|$	$\|x_3^{(\nu)} - \xi_3\|$	$\|x_4^{(\nu)} - \xi_4\|$
1	$4.77\ 10^{-2}$	$1.03\ 10^{-1}$	$8.10\ 10^{-2}$	$8.06\ 10^{-2}$
2	$1.02\ 10^{-3}$	$1.21\ 10^{-2}$	$1.17\ 10^{-2}$	$1.92\ 10^{-3}$
3	$7.82\ 10^{-8}$	$7.51\ 10^{-5}$	$7.51\ 10^{-5}$	$1.34\ 10^{-7}$
4	$1.21\ 10^{-16}$	$2.37\ 10^{-11}$	$2.37\ 10^{-11}$	$1.56\ 10^{-16}$
5	0	0	0	0
ν	Method (M_4)			
	$\|x_1^{(\nu)} - \xi_1\|$	$\|x_2^{(\nu)} - \xi_2\|$	$\|x_3^{(\nu)} - \xi_3\|$	$\|x_4^{(\nu)} - \xi_4\|$
1	$2.42\ 10^{-2}$	$6.87\ 10^{-2}$	$5.89\ 10^{-2}$	$4.32\ 10^{-2}$
2	$1.81\ 10^{-5}$	$2.34\ 10^{-3}$	$2.33\ 10^{-3}$	$3.48\ 10^{-5}$
3	$3.74\ 10^{-14}$	$1.96\ 10^{-8}$	$1.96\ 10^{-8}$	$4.94\ 10^{-14}$
4	0	0	0	0

Proof. Using $\sin|z| \leqq |\sin z| \leqq \cosh \operatorname{Im}(z)$, $z \in \mathbb{C}$, we firstly achieve for $z \in D_k$

$$\left|\sin\left(\frac{z-y}{2}\right)\right| \leqq \cosh(R_k/2), \quad k \in \{1, \ldots, n\}.$$

By definition of ε, we have for $z \in D_k$

$$|z - x_j|/2 \leqq |x_k - x_j|/2 + R_k/2 \leqq \pi - \varepsilon$$

and therefore

$$\left|\sin\left(\frac{z-x_j}{2}\right)\right| \geqq \sin\left|\frac{z-x_j}{2}\right| \geqq \frac{\sin\varepsilon}{\pi-\varepsilon} \cdot \frac{|z-x_j|}{2}.$$

Altogether, (20) holds with m_j given in (25). □

6.3 Exponential polynomials

Let f be a real exponential polynomial of degree n, i.e. $\mathbb{K} = \mathbb{R}$ and

$$f(t) = \sum_{k=-n}^{n} a_k \cdot \exp(kt), \quad t, a_{-n}, \ldots, a_n, \in \mathbb{R}.$$

Let f have the $m = 2n$ simple real zeros $\xi_1 < \xi_2 < \ldots < \xi_m$. As mentioned in [3] and [7] the exponential polynomial f can also be written in the form (22) where *sin* and *cos* has to be replaced by *sinh* and *cosh*, respectively.

Thus we may repeat the previous subsection replacing all trigonometric functions by their corresponding hyperbolic functions (up to some signs in second derivatives) to apply method (M_N).

Thus, the convergence order for method (M_N) is N, which is proved explicitly in [9] for $N = 2, 3$.

6.4 Exponential sums

Let $\lambda_1, \ldots, \lambda_{n+1}$ be real and distinct and consider an exponential sum $f \in V$,

$$V := \left\{ \sum_{j=1}^{n+1} b_j \cdot \exp(\lambda_j \cdot t) | b_j \in \mathbb{R} \right\},$$

having n simple and real zeros $\xi_1, \ldots, \xi_n$. Choosing some n-dimensional subspace U method (M_N) (as defined above) is locally convergent of order N. Method (M_2) is due to Frommer [7] where the following example is considered.

Table 2. Examples for exponential sums

v	Method (M_2)			
	$\lvert x_1^{(v)} - \xi_1\rvert$	$\lvert x_2^{(v)} - \xi_2\rvert$	$\lvert x_3^{(v)} - \xi_3\rvert$	$\lvert x_4^{(v)} - \xi_4\rvert$
1	$8.63\ 10^{-1}$	$9.34\ 10^{-1}$	$8.21\ 10^{-1}$	$3.48\ 10^{-1}$
2	$5.99\ 10^{-1}$	$7.70\ 10^{-1}$	$4.21\ 10^{-1}$	$6.27\ 10^{-3}$
3	$2.64\ 10^{-1}$	$4.25\ 10^{-1}$	$1.39\ 10^{-2}$	$7.89\ 10^{-4}$
4	$5.14\ 10^{-2}$	$7.12\ 10^{-2}$	$1.52\ 10^{-3}$	$1.48\ 10^{-5}$
5	$1.76\ 10^{-3}$	$2.14\ 10^{-3}$	$2.39\ 10^{-5}$	$2.89\ 10^{-8}$
6	$1.81\ 10^{-6}$	$2.23\ 10^{-6}$	$9.95\ 10^{-9}$	$1.95\ 10^{-12}$
7	$1.92\ 10^{-12}$	$2.35\ 10^{-12}$	$4.48\ 10^{-15}$	$4.34\ 10^{-19}$
8	$3.17\ 10^{-17}$	$5.20\ 10^{-18}$	$1.20\ 10^{-18}$	$2.17\ 10^{-19}$
v	Method (M_3)			
	$\lvert x_1^{(v)} - \xi_1\rvert$	$\lvert x_2^{(v)} - \xi_2\rvert$	$\lvert x_3^{(v)} - \xi_3\rvert$	$\lvert x_4^{(v)} - \xi_4\rvert$
1	$7.48\ 10^{-1}$	$8.71\ 10^{-1}$	$6.59\ 10^{-1}$	$1.12\ 10^{-1}$
2	$2.62\ 10^{-1}$	$4.27\ 10^{-1}$	$4.07\ 10^{-3}$	$1.56\ 10^{-3}$
3	$1.34\ 10^{-2}$	$1.52\ 10^{-2}$	$5.33\ 10^{-5}$	$5.23\ 10^{-7}$
4	$1.43\ 10^{-6}$	$1.45\ 10^{-6}$	$4.78\ 10^{-10}$	$1.12\ 10^{-13}$
5	$3.25\ 10^{-17}$	$6.83\ 10^{-18}$	$1.16\ 10^{-18}$	$3.25\ 10^{-19}$
v	Method (M_4)			
	$\lvert x_1^{(v)} - \xi_1\rvert$	$\lvert x_2^{(v)} - \xi_2\rvert$	$\lvert x_3^{(v)} - \xi_3\rvert$	$\lvert x_4^{(v)} - \xi_4\rvert$
1	$6.52\ 10^{-1}$	$8.10\ 10^{-1}$	$5.15\ 10^{-1}$	$1.12\ 10^{-2}$
2	$9.79\ 10^{-2}$	$1.54\ 10^{-1}$	$1.94\ 10^{-2}$	$2.81\ 10^{-5}$
3	$9.67\ 10^{-5}$	$9.34\ 10^{-5}$	$3.84\ 10^{-6}$	$1.76\ 10^{-13}$
4	$7.81\ 10^{-17}$	$5.29\ 10^{-17}$	$1.38\ 10^{-18}$	0

Example. Let $n = 4$, $\lambda_1 = -2$, $\lambda_2 = -0.5$, $\lambda_3 = 0$, $\lambda_4 = 0.7$ and $\lambda_5 = 2$. The coefficients of f were determined such that $b_5 = 1$ and f has the zeros $\xi_1 = -4$, $\xi_2 = -2$, $\xi_3 = 0$ and $\xi_4 = 2$. Let

$$U := \left\{ \sum_{j=1}^{5} b_j \cdot \exp(\lambda_j \cdot t) | b_j \in \mathbb{R}, b_5 = 0 \right\},$$

With the initial values $x_1^{(0)} = -5$, $x_2^{(0)} = -1$, $x_3^{(0)} = 1$, $x_4^{(0)} = 3$ Table 2 shows the absolute errors of method (M_N) for $N = 2, 3, 4$. From this, the convergence order $N = 2, 3, 4$ of method (M_N) can be observed. Note that the methods converge although the initial approximations were chosen far from the zeros of f to illustrate the wide domain of convergence of method (M_N). □

Remark. Note that, in contrast to the previous examples, the remainder $[U, x]\, rf$ is not known a-priori. It is known from [12] that a factorization of f as in the previous examples is not always possible. Consequently, the interpolant $[U, x]\, pf$ has to be determined numerically by solving a linear system of equations of dimension n. This requires $O(n^3)$ operations while the computation of an additional derivative of f and Q at any approximant $x_1, \ldots, x_n$ only needs $O(n^2)$ arithmetic operations.

Since the application of method (M_N) for higher order $N = 2, 3, 4, \ldots$ causes only solving one linear system of equations in each step this dominates the computational costs $O(n^3) + NO(n^2)$ for one step of (M_N). Thus, provided $N \ll n$, method (M_N) becomes more efficient for increasing $N = 2, 3, 4, \ldots$ such that higher order methods of the considered class (M_N) become of interest.

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