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MULTIPOINT METHODS FOR THE DETERMINATION OF MULTIPLE ZEROS OF A POLYNOMIAL

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Abstract. Simultaneous methods for finding multiple zeros of a polynomial are considered. The proposed class of methods has a multipoint character and does not require a knowledge of the multiplicity order of the sought zeros, which is the main and favorable feature of these methods. To avoid division by zero in the case of the same approximations, the differences $z_i - z_j$ in iterative formulas use the approximation z_i from the mth iteration and the approximations z_j $(j \neq i)$ from the $(m-1)$th iteration. The convergence analysis of the most frequently used simultaneous methods in multipoint mode is given. It is shown that the iterative methods with corrections are not efficient since their order of convergence is considerably reduced.

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1. Introduction

Let

$$P(z) = z^n + a_1 z^{n-1} + \cdots + a_n$$

be a polynomial with simple zeros $\zeta_1, \ldots, \zeta_n$ and the corresponding approximations $z_1^{(m)}, \ldots, z_n^{(m)}$ of these zeros in mth iteration, $m = 0, 1, 2, \ldots$. A typical method for an iterative improvement of these approximations is defined by

$$(1)\quad z_i^{(m+1)} = z_i^{(m)} - \frac{P(z_i^{(m)})}{\prod\limits_{j \neq i} (z_i^{(m)} - z_j^{(m)})} \quad (i \in I_n := \{1, \ldots, n\};\ m = 0, 1, \ldots)$$

and it is known as Weierstrass' method. In practice this method has good behavior even in the cases when ζ_i are not necessarily distinct zeros although the convergence is linear.

In the recent paper [5] Kanno, Kjurkchiev i Yamamoto have shown how the Weierstrass method can be used for simultaneous finding of all multiple zeros

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when their multiplicities are not known. The authors have proposed a variant of this method which has a multipoint character. In order to avoid division by zero in the case of the same approximations, in the denominator of formula (1), the approximation z_i from mth iteration and approximation z_j $(j \neq i)$ from the $(m-1)$th step are used, that is, the modified formula has the form

$$(2) \qquad z_i^{(m+1)} = z_i^{(m)} - \frac{P(z_i^{(m)})}{\prod_{j\neq i}(z_i^{(m)} - z_j^{(m-1)})} \quad (i \in I_n;\ m = 1,2,\ldots).$$

In the sequel we consider a possibility of the application of the multiponit modifications of some well known methods for the simultaneous determination of simple or multiple zeros of a polynomial. Particular attention is paid to a theoretical analysis of the R-order of convergence of the modified methods.

Let $\varepsilon_i^{(m)} = z_i^{(m)} - \zeta_i$ $(i \in I_n)$ denote the error of approximation in the mth iteration in the realization of a multipoint method which generates a sequence $\{z_i^{(m)}\}$ of approximations to the zeros $\zeta_1, \ldots, \zeta_n$. For a wide class of iterative methods for the simultaneous finding of polynomial zeros, the following relations can be derived

$$(3) \qquad \varepsilon_i^{(m+1)} = \alpha_i \left(\varepsilon_i^{(m)}\right)^p \sum_{\substack{j=1\\ j\neq i}}^{n} \beta_{ij} \left(\varepsilon_j^{(m-1)}\right)^q \quad (i \in I_n),$$

where α_i and β_{ij} are complex constants, and $p, q \geq 1$ are integers.

Apart from standard notation, for two complex numbers w_1 and w_2 whose magnitudes are of the same order we will write $w_1 = O_M(w_2)$.

2. Convergence order of multipoint methods

We are going to prove the following assertion:

Theorem 1. *Let $\zeta_1, \ldots, \zeta_n$ be the zeros of a polynomial P, and starting approximations $z_1^{(0)}, \ldots, z_n^{(0)}$ have been determined so that they are sufficiently close to these zeros. Then the multipoint algorithm for which the relations (3) hold, is locally convergent with the R-order of convergence at least η_A, where η_A is the unique positive root of the equation*

$$(4) \qquad \eta^2 - p\eta - q = 0.$$

Proof. According to the conditions of the theorem we can find positive constants A and B such that $|\alpha_i| \leq A$ and $|\beta_{ij}| \leq B$. If in each iterative step m we define an absolute error $e_m = \|\mathbf{z}^{(m)} - \zeta\|_\infty$, then from (3) we get

$$(5) \qquad e_{m+1} \leq C e_m^p e_{m-1}^q, \quad C = (n-1)AB.$$

In view of the choice of starting values we can adopt $e_0 < 1$. Then from (5) it follows that the sequence $\{e_m\}$ tends to zero.

Let $e_0 = O(E)$, where $0 < E < 1$, and let η_A be the convergence order of the sequence $\{e_m\}$, i.e. $e_{m+1} = O\left(e_m^{\eta_A}\right)$. Then

$$e_m = O\left(E^{\eta_A^m}\right), \quad e_{m-1} = O\left(E^{\eta_A^{m-1}}\right).$$

From (5) we get

$$e_{m+1} = O\left(e_m^p \cdot e_{m-1}^q\right) = O\left(E^{p\eta_A^m + q\eta_A^{m-1}}\right).$$

On the basis of the last relation and the fact that $e_{m+1} = O\left(E^{\eta_A^{m+1}}\right)$, by comparing the exponents, we find

$$\eta_A^2 = p\eta_A + q.$$

Whence follows that $\eta_A > 0$ satisfies the equation (3). □

3. Some examples

In this section we consider the convergence rate of the most frequently used iterative methods with and without corrections. For the sake of simplicity, the approximations $z_j^{(m-1)}$ of the zeros $\zeta_1, \ldots, \zeta_n$ from the iterative step $m - 1$ will be denoted by z_j^*, and the approximations $z_i^{(m)}$ by z_i. According to this notation we introduce the errors $\varepsilon_i = z_i - \zeta_i$ and $\varepsilon_j^* = z_j^* - \zeta_j$. A new approximation $z_i^{(m+1)}$ will be denoted by $\hat{z}_i$, and the corresponding error by $\hat{\varepsilon}_i = \hat{z}_i - \zeta_i$.

MULTIPOINT WEIERSTRASS-LIKE METHOD

As already pointed in Introduction, this method was considered in [5]. The following asymptotic relation of the form (3) can be derived

$$\hat{\varepsilon}_i \sim \varepsilon_i \sum_{j \neq i} O_M(\varepsilon_j^*),$$

that is, $p = 1, q = 1$. By Theorem 1, from the equation $\eta^2 - \eta - 1 = 0$ we find that the R-order of convergence of the Weierstrass-like method (2) is at least $\eta_A = (1 + \sqrt{5})/2 \approx 1.618$.

MULTIPOINT MAEHLY-LIKE METHOD

Taking the approximations z_j^* from the preceding step instead of the approximations z_j in the Maehly method ([1], [2],[4],[6])

$$\hat{z}_i = z_i - \cfrac{1}{\cfrac{P'(z_i)}{P(z_i)} - \displaystyle\sum_{j \neq i} \cfrac{1}{z_i - z_j}} \quad (i \in I_n),$$

we get the multipoint Maehly-like method

$$\hat{z}_i = z_i - \frac{1}{\dfrac{P'(z_i)}{P(z_i)} - \sum_{j \neq i} \dfrac{1}{z_i - z_j^*}} \quad (i \in I_n). \tag{6}$$

Applying the logarithmic differentiation we find $\dfrac{P'(z_i)}{P(z_i)} = \sum_{j=1}^{n} \dfrac{1}{z_i - \zeta_i}$, so that from (6) there follows

$$\begin{aligned}
\hat{\varepsilon}_i &= \varepsilon_i - \frac{1}{\dfrac{1}{\varepsilon_i} + \sum_{j \neq i} \dfrac{1}{z_i - \zeta_j} - \sum_{j \neq i} \dfrac{1}{z_i - z_j^*}} \\
&= \varepsilon_i - \frac{\varepsilon_i}{1 + \varepsilon_i \sum_{j \neq i} \dfrac{\zeta_j - z_j^*}{(z_i - \zeta_j)(z_i - z_j^*)}} = -\frac{\varepsilon_i^2 \sum_{j \neq i} A_{ij} \varepsilon_j^*}{1 - \varepsilon_i \sum_{j \neq i} A_{ij} \varepsilon_j^*},
\end{aligned}$$

where $A_{ij} = \dfrac{1}{(z_i - \zeta_j)(z_i - z_j^*)}$. Therefore

$$\hat{\varepsilon}_i = O_M(\varepsilon_i^2) \sum_{j \neq i} O_M(\varepsilon_j^*),$$

whence, by solving the equation $\eta^2 - 2\eta - 1 = 0$ $(p = 2, q = 1)$, we find that the R-order of convergence of the multipoint method (6) is at least $\eta_A = 1 + \sqrt{2} \approx 2.414$.

MULTIPOINT BÖRSCH-SUPAN-LIKE METHOD

Replacing z_j by z_j^* in the Börsch-Supan iterative formula [2]

$$\hat{z}_i = z_i - \frac{W_i}{1 + \sum_{j \neq i} \dfrac{W_j}{z_i - z_j}} \quad (i \in I_n),$$

we come to the multipoint Börsch-Supan-like method

$$\hat{z}_i = z_i - \frac{W_i^*}{1 + \sum_{j \neq i} \dfrac{W_j^*}{z_i - z_j^*}} \quad (i \in I_n), \tag{7}$$

where

$$W_i^* = \frac{P(z_i)}{\prod\limits_{j\neq i}(z_i - z_j^*)}, \quad W_j^* = \frac{P(z_j^*)}{\prod\limits_{k\neq j}(z_j^* - z_k^*)}$$

are Weierstrass-like corrections with $z_k^* = z_i$ if $k = i$.

In order to determine the convergence rate of (7), we use the fixed point relation

$$\zeta_i = z_i - \frac{W_i^*}{1 + \sum\limits_{j\neq i} \dfrac{W_j^*}{\zeta_i - z_j^*}} \quad (i \in I_n). \tag{8}$$

Subtracting (8) from (7), we obtain

$$\hat{\varepsilon}_i = \frac{W_i^*}{1 + \sum\limits_{j\neq i} \dfrac{W_j^*}{\zeta_i - z_j^*}} - \frac{W_i^*}{1 + \sum\limits_{j\neq i} \dfrac{W_j^*}{z_i - z_j^*}} = -\varepsilon_i \frac{W_i^*}{c_i} \sum_{j\neq i} d_{ij} W_j^*,$$

where

$$c_i = \Big(1 + \sum_{j\neq i} \frac{W_j^*}{\zeta_i - z_j^*}\Big)\Big(1 + \sum_{j\neq i} \frac{W_j^*}{z_i - z_j^*}\Big), \quad d_{ij} = \frac{1}{(\zeta_i - z_j^*)(z_i - z_j^*)}.$$

Considering that $W_i^* = O_M(\varepsilon_i)$ and $W_j^* = O_M(\varepsilon_j^*)$, $(j \neq i)$, we come to the relation

$$\hat{\varepsilon}_i = -\frac{\varepsilon_i W_i^*}{c_i} \sum_{j\neq i} O_M(\varepsilon_j^*) = O_M(\varepsilon_i^2) \sum_{j\neq i} O_M(\varepsilon_j^*), \quad \text{that is, } p = 2,\ q = 1.$$

Solving the equation $\eta^2 - 2\eta - 1 = 0$ we find that the R-order of convergence of the multipoint Börsch-Supan-like method (7) is at least $1 + \sqrt{2} \approx 2.414$.

MULTIPOINT HALLEY-LIKE METHOD

If we define the sums

$$S_{\lambda,i} = \sum_{\substack{j=1\\ j\neq i}}^{n} \frac{1}{(z_i - z_j^*)^\lambda} \quad (i \in I_n;\ \lambda = 1, 2),$$

$$\Sigma_{1,i} = \sum_{\substack{j=1\\ j\neq i}}^{n} \frac{1}{z_i - \zeta_j} \quad (i \in I_n),$$

the abbreviations

$$a_{ij} = (z_i - \zeta_j)(z_i - z_j^*), \quad b_{ij} = 2z_i - z_j^* - \zeta_j$$

and the function

$$f(z)=\frac{P'(z)}{P(z)}-\frac{P''(z)}{2P'(z)},$$

then the simultaneous Halley-like method has the form of ([10], [12])

$$\hat{z}_i=z_i-\frac{1}{f(z_i)-\dfrac{P(z_i)}{2P'(z_i)}\Big[S_{1,i}^2+S_{2,i}\Big]}\quad (i\in I_n), \tag{9}$$

or

$$\hat{z}_i=z_i-\frac{\dfrac{2P'(z_i)}{P(z_i)}}{\Big[\dfrac{P'(z_i)}{P(z_i)}\Big]^2+\dfrac{P'(z_i)^2-P''(z_i)P(z_i)}{P(z_i)^2}-S_{1,i}^2-S_{2,i}}\quad (i\in I_n). \tag{10}$$

The method has been given this name because the function f in the denominator of the formula (9) appears in the well-known third order Halley's iterative formula

$$\hat{z}=z-\frac{1}{f(z)}=\frac{1}{\dfrac{P'(z)}{P(z)}-\dfrac{P''(z)}{2P'(z)}}$$

for determination of a simple zero of the polynomial P.

We will show that the multipoint Halley-like method (9) belongs to a class of methods for which the relation (3) holds, which means that Theorem 1 can be applied to this method. For this purpose we use the identities

$$\frac{P'(z)}{P(z)}=\sum_{j=1}^{n}\frac{1}{z-\zeta_j} \tag{11}$$

and

$$\frac{P'(z)^2-P''(z)P(z)}{P(z)^2}=\sum_{j=1}^{n}\frac{1}{(z-\zeta_j)^2}, \tag{12}$$

which can be easily derived by means of the logarithmic differentiation.

At first, from (11) we have

$$\frac{2P'(z_i)}{P(z_i)}=2\Big(\frac{1}{z_i-\zeta_i}+\sum_{j\neq i}\frac{1}{z_i-\zeta_j}\Big)=2\Big(\frac{1}{\varepsilon_i}+\Sigma_{1,i}\Big)$$

and

$$\begin{aligned}\Big(\frac{P'(z_i)}{P(z_i)}\Big)^2-S_{1,i}^2 &= \left(\sum_{j=1}^{n}\frac{1}{z_i-\zeta_j}\right)^2-\left(\sum_{j\neq i}\frac{1}{z_i-z_j^*}\right)^2\\ &= \Big(\frac{1}{\varepsilon_i}-\sum_{j\neq i}\frac{\varepsilon_j^*}{a_{ij}}\Big)\Big(\frac{1}{\varepsilon_i}+S_{1,i}+\Sigma_{1,i}\Big).\end{aligned}$$

By means of the identity (12) we find

$$\begin{aligned}\frac{P'(z_i)^2 - P''(z_i)P(z_i)}{P(z_i)^2} - S_{2,i} &= \sum_{j=1}^{n} \frac{1}{(z_i - \zeta_j)^2} - \sum_{j\neq i} \frac{1}{(z_i - z_j^*)^2} \\ &= \frac{1}{\varepsilon_i^2} - \sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}.\end{aligned}$$

Using the last two relations, from (10) we get

$$\hat{z}_i - \zeta_i = z_i - \zeta_i - \frac{2\Big(\dfrac{1}{\varepsilon_i} + \Sigma_{1,i}\Big)}{\Big(\dfrac{1}{\varepsilon_i} - \displaystyle\sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}}\Big)\Big(\dfrac{1}{\varepsilon_i} + S_{1,i} + \Sigma_{1,i}\Big) + \dfrac{1}{\varepsilon_i^2} - \displaystyle\sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}},$$

that is,

$$\hat{\varepsilon}_i = \varepsilon_i - \frac{2\varepsilon_i\big(1 + \varepsilon_i \Sigma_{1,i}\big)}{\Big(1 - \varepsilon_i \displaystyle\sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}}\Big)(1 + \varepsilon_i S_{1,i} + \varepsilon_i \Sigma_{1,i}\Big) + 1 - \varepsilon_i^2 \displaystyle\sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}}.$$

After bringing to the same denominator, we obtain

$$\text{(13)}\quad \hat{\varepsilon}_i = \frac{\varepsilon_i^2}{G_{ij}}\Big\{S_{1,i} - \Sigma_{1,i} - \sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}} - \varepsilon_i\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}} + \sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}\Big]\Big\},$$

where

$$G_{ij} = 2 + \varepsilon_i\Big(S_{1,i} + \Sigma_{1,i} - \sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}}\Big) - \varepsilon_i^2\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}} + \sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}\Big].$$

Since

$$S_{1,i} - \Sigma_{1,i} - \sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}} = \sum_{j\neq i}\Big(\frac{1}{z_i - z_j^*} - \frac{1}{z_i - \zeta_j} - \frac{z_j^* - \zeta_j}{(z_i - z_j^*)(z_i - \zeta_j)}\Big) = 0,$$

from (13) there follows

$$\hat{\varepsilon}_i = -\frac{\varepsilon_i^3}{G_{ij}}\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i} \frac{\varepsilon_j^*}{a_{ij}} + \sum_{j\neq i} \frac{b_{ij}\varepsilon_j^*}{a_{ij}^2}\Big],$$

or in the form

$$\hat{\varepsilon}_i = \varepsilon_i^3 \sum_{j\neq i} c_{ij}\varepsilon_j^*, \quad \text{where} \quad c_{ij} = -\frac{a_{ij}\big(S_{1,i} + \Sigma_{1,i})\big) + b_{ij}}{a_{ij}^2 G_{ij}}. \tag{14}$$

Note that $G_{ij} \to 2$ when $\varepsilon \to 0$, so that the relation (14) has the form (3) where $p = 3$, $q = 1$. Thus, we can directly apply Theorem 1. The lower bound of the R-order or convergence of the multipoint Halley-like method (9) is the unique positive root of the equation $\eta^2 - 3\eta - 1 = 0$, that is, $\eta_A = (3 + \sqrt{13})/2 \approx 3.303$.

MULTIPOINT MAEHLY-LIKE METHOD WITH NEWTON'S CORRECTION

If we introduce Newton's correction $N_j^* = P(z_j^*)/P'(z_j^*)$ in the multipoint Maehly-like method (6), we get the method

$$\hat{z}_i = z_i - \frac{1}{\dfrac{P'(z_i)}{P(z_i)} - \displaystyle\sum_{j\neq i} \frac{1}{z_i + N_j^* - z_j^*}} \qquad (i \in I_n)$$

(c.f. [7], [9]). Whence there follows

$$\begin{aligned}
\hat{\varepsilon}_i &= \varepsilon_i - \frac{1}{\dfrac{1}{\varepsilon_i} + \displaystyle\sum_{j\neq i}\left(\frac{1}{z_i - \zeta_i} - \frac{1}{z_i + N_j^* - z_j^*}\right)} \\
&= \varepsilon_i - \frac{\varepsilon_i}{1 + \varepsilon_i \displaystyle\sum_{j\neq i} \frac{N_j^* - z_j^* + \zeta_j}{(z_i - \zeta_j)(z_i + N_j^* - z_j^*)}} \\
&= \frac{\varepsilon_i^2}{1 + \tau_i} \sum_{j\neq i} \frac{N_j^* - \varepsilon_j^*}{l_{ij}},
\end{aligned}$$

where we have put

$$l_{ij} = (z_i - \zeta_j)(z_i + N_j^* - z_j^*) \quad \text{and} \quad \tau_i = \sum_{j\neq i} \frac{N_j^* - \varepsilon_j^*}{a_{ij}}.$$

Considering that $N_j^* - \varepsilon_j^* = O_M({\varepsilon_j^*}^2)$, we find

$$\hat{\varepsilon}_i = O_M(\varepsilon_i^2) \sum_{j\neq i} O_M({\varepsilon_j^*}^2).$$

On the basis of (3), from the last relation we have $p = 2$ and $q = 2$ so that the lower bound of the R-order of convergence can be obtained as a solution of the equation $\eta^2 - 2\eta - 2 = 0$, i.e. $\eta_A = 1 + \sqrt{3} \approx 2.732$.

MULTIPOINT BÖRSCH-SUPAN-LIKE METHOD WITH WEIERSTRASS' CORRECTION

Multipoint Börsch-Supan-like method with the Weierstrass correction reads

$$\hat{z}_i = z_i - \frac{W_i^*}{1 + \sum_{j \neq i} \frac{W_j^*}{z_i - W_i^* - z_j^*}} \quad (i \in I_n).$$

This accelerated method is obtained from (8) putting $\zeta_i := z_i - W_i^*$ (see [3], [8]). By using the fixed point relation (8) we have

$$\begin{aligned} \hat{\varepsilon}_i &= \frac{W_i^*}{1 + \sum_{j \neq i} \frac{W_j^*}{\zeta_i - z_j^*}} - \frac{W_i^*}{1 + \sum_{j \neq i} \frac{W_j^*}{z_i - W_i - z_j^*}} \\ &= \frac{W_i^*}{s_i} \sum_{j \neq i} b_{ij} W_j^* (\zeta_i - z_j^* - z_i + W_i^* + z_j^*) \\ &= \frac{W_i^*}{s_i} \sum_{j \neq i} t_{ij} W_j^* (W_i^* - \varepsilon_i), \end{aligned}$$

where

$$\begin{aligned} s_i &= \sum_{j \neq i} t_{ij} W_j^* (W_i^* - \varepsilon_i) \Big(1 + \sum_{j \neq i} \frac{W_j^*}{z_i - W_i^* - z_j^*}\Big), \\ t_{ij} &= \frac{1}{(\zeta_i - z_j^*)(z_i - W_i - z_j^*)}. \end{aligned}$$

The Weierstrass-like correction is $W_i^* = P(z_i) / \prod_{j \neq i} (z_i - z_j^*)$ and after developing into a series it can be brought to the form of

$$W_i^* = \varepsilon_i \Big(1 + \sum_{j \neq i} \frac{\varepsilon_j^*}{z_i - \zeta_i} + \cdots \Big).$$

Therefore, $W_i^* - \varepsilon_i = \varepsilon_i \sum_{j \neq i} O_M(\varepsilon_j^*)$, which leads to the relation

$$\hat{\varepsilon}_i = O_M(\varepsilon_i^2) \sum_{j \neq i} O_M(\varepsilon_j^{*^2}).$$

Whence, by comparing with the relation (3), we see that $p = 2$, $q = 2$, and, the lower bound of the R-order of convergence is the solution of the equation $\eta^2 - 2\eta - 2 = 0$, i.e. $\eta_A = 1 + \sqrt{3} \approx 2.732$.

MULTIPOINT HALLEY-LIKE METHOD WITH NEWTON'S CORRECTION

Let the sum $\Sigma_{1,i}$ and the function f be defined as in the multipoint Halley-like method (9). We introduce the sum

$$S_{\lambda,i} = \sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{1}{(z_i + N_j^* - z_j^*)^\lambda} \quad (i \in I_n;\ \lambda = 1,2),$$

and the abbreviations

$$r_{ij} = (z_i - \zeta_j)(z_i + N_j^* - z_j^*), \quad q_{ij} = 2z_i + N_j^* - z_j^* - \zeta_j.$$

Then the multipoint simultaneous Halley-like method with Newton's correction has the form

$$\hat{z}_i = z_i - \frac{1}{f(z_i) - \dfrac{P(z_i)}{2P'(z_i)}\Big[S_{1,i}^2 + S_{2,i}\Big]} \quad (i \in I_n), \tag{15}$$

or

$$\hat{z}_i = z_i - \frac{\dfrac{2P'(z_i)}{P(z_i)}}{\Big[\dfrac{P'(z_i)}{P(z_i)}\Big]^2 + \dfrac{P'(z_i)^2 - P''(z_i)P(z_i)}{P(z_i)^2} - S_{1,i}^2 - S_{2,i}} \tag{16}$$

(see [11]).

From the identity (11) we have

$$\frac{2P'(z_i)}{P(z_i)} = 2\Big(\frac{1}{z_i - \zeta_i} + \sum_{j\neq i} \frac{1}{z_i - \zeta_j}\Big) = 2\Big(\frac{1}{\varepsilon_i} + \Sigma_{1,i}\Big).$$

Then

$$\begin{aligned} \Big(\frac{P'(z_i)}{P(z_i)}\Big)^2 - S_{1,i}^2 &= \Bigg(\sum_{j=1}^{n} \frac{1}{z_i - \zeta_j}\Bigg)^2 - \Bigg(\sum_{j\neq i} \frac{1}{z_i + N_j^* - z_j^*}\Bigg)^2 \\ &= \Big(\frac{1}{\varepsilon_i} - \sum_{j\neq i} \frac{\varepsilon_j^* - N_j^*}{a_{ij}}\Big)\Big(\frac{1}{\varepsilon_i} + S_{1,i} + \Sigma_{1,i}\Big). \end{aligned}$$

By virtue of the identity (12) we find

$$\begin{aligned} \frac{P'(z_i)^2 - P''(z_i)P(z_i)}{P(z_i)^2} - S_{2,i} &= \sum_{j=1}^{n} \frac{1}{(z_i - \zeta_j)^2} - \sum_{j\neq i} \frac{1}{(z_i + N_j^* - z_j^*)^2} \\ &= \frac{1}{\varepsilon_i^2} - \sum_{j\neq i} \frac{q_{ij}(\varepsilon_j^* - N_j^*)}{r_{ij}^2}. \end{aligned}$$

Using the last two relations and setting $e_j^* = \varepsilon_j^* - N_j^*$, from (16) we obtain

$$\hat{z}_i - \zeta_i = z_i - \zeta_i - \frac{2\Big(\dfrac{1}{\varepsilon_i} + \Sigma_{1,i}\Big)}{\Big(\dfrac{1}{\varepsilon_i} - \sum_{j\neq i}\dfrac{e_j^*}{r_{ij}}\Big)\Big(\dfrac{1}{\varepsilon_i} + S_{1,i} + \Sigma_{1,i}\Big) + \dfrac{1}{\varepsilon_i^2} - \sum_{j\neq i}\dfrac{q_{ij}e_j^*}{r_{ij}^2}},$$

that is,

$$\hat{\varepsilon}_i = \varepsilon_i - \frac{2\varepsilon_i\big(1 + \varepsilon_i\Sigma_{1,i}\big)}{\Big(1 - \varepsilon_i\sum_{j\neq i}\dfrac{e_j^*}{r_{ij}}\Big)(1 + \varepsilon_i S_{1,i} + \varepsilon_i\Sigma_{1,i}\Big) + 1 - \varepsilon_i^2\sum_{j\neq i}\dfrac{q_{ij}e_j^*}{r_{ij}^2}}.$$

After bringing to the same denominator, we get

$$\hat{\varepsilon}_i = \frac{\varepsilon_i^2}{G_{ij}}\Big\{S_{1,i} - \Sigma_{1,i} - \sum_{j\neq i}\frac{e_j^*}{r_{ij}} - \varepsilon_i\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i}\frac{e_j^*}{r_{ij}} + \sum_{j\neq i}\frac{q_{ij}e_j^*}{r_{ij}^2}\Big]\Big\}, \tag{17}$$

where

$$G_{ij} = 2 + \varepsilon_i\Big(S_{1,i} + \Sigma_{1,i} - \sum_{j\neq i}\frac{e_j^*}{a_{ij}}\Big) - \varepsilon_i^2\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i}\frac{e_j^*}{a_{ij}} + \sum_{j\neq i}\frac{b_{ij}e_j^*}{a_{ij}^2}\Big].$$

Since

$$S_{1,i} - \Sigma_{1,i} - \sum_{j\neq i}\frac{e_j^*}{r_{ij}} = \sum_{j\neq i}\Big(\frac{1}{z_i + N_j^* - z_j^*} - \frac{1}{z_i - \zeta_j} - \frac{e_j^*}{(z_i + N_j^* - z_j^*)(z_i - \zeta_j)}\Big) = 0,$$

from (17) there follows

$$\hat{\varepsilon}_i = -\frac{\varepsilon_i^3}{G_{ij}}\Big[\big(S_{1,i} + \Sigma_{1,i}\big)\sum_{j\neq i}\frac{e_j^*}{r_{ij}} + \sum_{j\neq i}\frac{q_{ij}e_j^*}{r_{ij}^2}\Big],$$

or, since $e_j^* = \varepsilon_j^* - N_j^* = O_M(\varepsilon_j^{*^2})$,

$$\hat{\varepsilon}_i = \varepsilon_i^3\sum_{j\neq i}O_M(\varepsilon_j^{*^2}).$$

Since $G_{ij} \to 2$ when $\varepsilon \to 0$, by comparing the last relation and (3) we find $p = 3$ and $q = 2$. Therefore, R-order of convergence of the multipoint Halley-like method with Newton's correction is the unique positive root of the equation $\eta^2 - 3\eta - 2 = 0$, that is, $\eta_A = (3 + \sqrt{17})/2 \approx 3.562$.

In the end we give in the table a review of lower bounds of the convergence rate of all the methods considered in this paper, parameters p and q, as well as the convergence orders of basic methods (in brackets).

Multipoint method	p	q	Convergence order
Weierstrass'	1	1	1.618 (2)
Maehly's	2	1	2.414 (3)
Börsch-Supan's	2	1	2.414 (3)
Halley's	3	1	3.303 (4)
Maehly's, with Newton's correction	2	2	2.732 (4)
Börsch-Supan's, with Weiestrass's correction	2	2	2.732 (4)
Halley's, with Newton's correction	3	2	3.562 (5)

From the above table we see that multipoint methods without corrections slightly lose convergence rate, while multipoint methods with correction are not of practical importance because their convergence order drastically decreases. For instance, convergence order of the Maehly method with Newton's correction is 4, while for its multipoint version is only 2.732. The same holds for the multipoint Börsch-Supan method with Weierstrass' correction. The convergence order of the Halley method with Newton's correction is 5, and this order falls to approximately 3.562 in the case of multipoint version.

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SPECIAL MESHES AND HIGHER–ORDER SCHEMES FOR SINGULARLY PERTURBED BOUNDARY VALUE PROBLEMS

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Abstract. Bakhvalov (B) and Shishkin (S) meshes are used very often to discretize singular perturbation problems. The smoother B meshes are more complicated than the piecewise equidistant S meshes, but their considerably better accuracy usually outweighs this. In this paper, we point out that the real advantage of S meshes comes to light when constructing higher–order discretizations. We show this by considering an almost third–order finite–difference scheme for a semilinear problem with two small parameters.

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1. Introduction

Let us consider the following singularly perturbed boundary value problem:

$$(1)\quad -\varepsilon^2 u'' - \mu u' + c(x,u) = 0, \quad x \in X = [0,1], \quad u(0) = U_0, \quad u(1) = U_1,$$

where

$$(2)\qquad 0 < \varepsilon << 1, \quad \mu = \varepsilon^{1+p}, \quad p \geq \frac{1}{2},$$

c is a sufficiently smooth function and U_0 and U_1 are real numbers. For $x \in X$ and $u \in \mathbb{R}$, we also assume

$$(3)\qquad c_u(x,u) > m^2 > 0, \quad m > 0.$$

This problem is used as a suitable problem to illustrate our point that the only advantage of the Shishkin [13], or S, meshes over the Bakhvalov [2], or B, meshes is that higher–order discretizations are much simpler on S meshes, since too complicated nonequidistant schemes can be avoided. Problem (1) is not artificially constructed for this purpose: it also models transport phenomena arising in chemistry or biology, [3]. It belongs to the class of singularly perturbed boundary value problems with two small parameters, which have been analyzed

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asymptotically in [9] and numerically in [15], [16], and most recently in two dimensions in [5]. On numerical methods for singular perturbation problems in general, one can find in two 1996 books, [8] and [12], and on S and B meshes in particular, in [14], [17], [10], [11], [18], and [6], for instance.

Space limitations prevent us from presenting here some generalizations; they will appear elsewhere. One of them is straightforward, viz. replacing the $-\mu u'$-term in (1) with $-\mu b(x)u'$. Another, the inclusion of the case $0 < p < \frac{1}{2}$, requires some modifications of the numerical method. It is also possible to construct a similar scheme for the case $p = 0$ and to prove its stability, but the proof of ε-uniform convergence is still open.

2. The discretizations

Let X^h denote any mesh with the points $0 = x_0 < x_1 < \cdots < x_N = 1$. Problem (1) requires a mesh which is dense near both $x = 0$ and $x = 1$. This is because the unique solution, u_ε, of (1) has in general two exponential boundary layers at the endpoints of X. Moreover, the following estimates hold for $x \in X$ and $k = 0, 1, 2, \dots$, see [15] and [16]:

$$|u_\varepsilon^{(k)}| \le M[1 + \varepsilon^{-k} v_0(x) + \varepsilon^{-k} v_1(x)], \tag{4}$$

where $v_t(x) = \exp(-m|x-t|/\varepsilon)$, $t = 0, 1$, and M is used throughout the paper as a generic constant which is independent of both ε and N.

For simplicity, let N be even and let both B and S meshes be symmetric with respect to $x_{N/2} = \frac{1}{2}$. The meshes are described below on $[0, \frac{1}{2}]$. A B mesh introduced in [14] is used in this paper as a comparison to the standard S mesh. It is generated by $x_i = \lambda(i/N)$, where

$$\lambda(t) = \begin{cases} \varphi(t) := \varepsilon \frac{t}{q-t} & \text{if } t \in [0, \alpha], \\ \tau(t) := \varphi'(\alpha)(t-\alpha) + \varphi(\alpha) & \text{if } t \in [\alpha, \frac{1}{2}], \end{cases}$$

with $0 < \alpha < q < \frac{1}{2}$ and α solving the equation $\tau(\alpha) = \frac{1}{2}$.

The S mesh is piecewise equidistant. It is formed by using a fine mesh on the interval $[0, \sigma := a\varepsilon \ln N]$ and a coarse mesh on $[\sigma, \frac{1}{2}]$ (it is assumed that $a > 0$ and $\sigma < \frac{1}{2}$). Let the index J be defined by $x_J = \sigma$ and let $N \le MJ$.

Let $h_i = x_i - x_{i-1}$, $i = 1, 2, \dots, N$, and let $w^h = [w_1, w_2, \dots, w_{N-1}]^T$ be the vector corresponding to a mesh function on $X^h \setminus \{0, 1\}$. We formally set $w_0 := U_0$ and $w_N := U_1$.

The following nonequidistant central scheme can be used on both meshes:

$$T_C w_i = -\varepsilon^2 D_C'' w_i - \mu D_C' w_i + c_i, \quad i = 1, 2, \dots, N-1,$$

with

$$D_C'' w_i = \frac{2}{h_i + h_{i+1}} \left(\frac{w_{i-1} - w_i}{h_i} + \frac{w_{i+1} - w_i}{h_{i+1}} \right),$$

$$D'_C w_i = \frac{1}{h_i + h_{i+1}} \left[\frac{h_{i+1}}{h_i}(w_i - w_{i-1}) + \frac{h_i}{h_{i+1}}(w_{i+1} - w_i) \right],$$

and $c_i = c(x_i, w_i)$.

We would also like to use an equidistant four–point third–order scheme, D'' to approximate u''. Let h denote the mesh step and let $s = (3-\sqrt{15})/6 \approx -.145$. Then,

$$D''w_i = h^{-2}[(1-s)w_{i-1} + (3s-2)w_i + (1-3s)w_{i+1} + sw_{i+2}], \tag{5}$$

is a $O(h^3)$ scheme for $u''(x_i + sh)$. It is interesting to compare this scheme to that in [4], which is also a four–point third–order scheme for u'' and even makes use of the same quantity s. However, the latter, which is optimal in the sense of minimizing the truncation error, uses special nonequidistant points and therefore cannot be applied here. It is too complicated to construct a nonequidistant generalization of (5). Besides, that can be done in several different ways and it is hard to tell in advance which one will produce the most suitable scheme, cf. [17]. Because of all those complications, (5) will be used here only on a portion of the fine parts of the S mesh. It will be combined with two other third–order schemes,

$$D'w_i = (12h)^{-1}[(6s-5)w_{i-1} - 3(2s+1)w_i - 3(2s-3)w_{i+1} + (6s-1)w_{i+2}]$$

and

$$Dw_i = \frac{1}{12}w_{i-1} + \left(\frac{5}{6} - s\right) w_i + \left(\frac{1}{12} + s\right) w_{i+1},$$

to give the following discretization scheme:

$$Tw_i = -\varepsilon^2 D''w_i - \mu D'w_i + c(x_i + sh, Dw_i).$$

Then, T and T_C are used to form a hybrid scheme T_H,

$$T_H w_i = \begin{cases} Tw_i \text{ for } 1 \le i \le J-2, \\ T_C w_i \text{ for } J-1 \le i \le N/2, \\ \text{symmetrical scheme w.r.t. } x_{N/2} = \frac{1}{2} \text{ for } N/2+1 \le i \le N-1. \end{cases}$$

Thus, we are going to consider two discretizations of problem (1), both of the form

$$Rw_i = 0, \quad i = 1, 2, \ldots, N-1, \tag{6}$$

where either $R \equiv T_C$ or $R \equiv T_H$. This is an $(N-1) \times (N-1)$ nonlinear system. Our numerical results will show that the special meshes stabilize T_C, which is not surprising having the result in [1] in mind. On the B mesh, we can expect second–order ε–uniform accuracy, whereas on the S mesh, the second order is diminished by logarithmic factors. As for T_H, it is analyzed in the next section.

3. The error estimate for T_H

The key assumption in the following analysis of the scheme T_H is

$$\varepsilon \le MN^{-1}(\ln N)^{3/2}. \tag{7}$$

Even though this is certainly a theoretical restriction, it is practically quite acceptable, since the relationship between ε and N is usually such that no mesh point lies inside the layer when the mesh is equidistant. This can be expressed by the inequality

$$\varepsilon \ln \frac{1}{\varepsilon} \le MN^{-1},$$

which implies (7).

Let F be an $(N-1) \times (N-1)$ matrix denoting the Fréchet derivative of the operator T_H on the S mesh, $F = T'_H(w^h)$ for an arbitrary vector w^h. Let also $\|w^h\| = \max_{1 \le i \le N-1} |w_i|$ and let the corresponding subordinate matrix norm be denoted in the same way. Moreover, let N_0 denote a sufficiently large positive integer independent of ε. Then we can prove the following stability result which is crucial for our main result.

Theorem 1. *Let (2), (3), and (7) hold and let $N \ge N_0$. Then F is a nonsingular matrix and $\|F^{-1}\| \le M$. Thus, the discrete problem (6) with $R \equiv T_H$ on the S mesh has a unique solution.*

Proof. This is a nonstandard stability proof, since $F = [f_{ij}]$ is not an L–matrix, nor can we fully apply to F Lorenz's standard decomposition (SD), [7]. We consider several cases.

1. $p \ge 1$. In this case, the nonzero elements of F are $f_{ii} > 0$, $f_{i,i\pm1} \le 0$, $i = 1, 2, \ldots, N-1$, (setting formally $f_{10} = f_{N-1,N} = 0$), and because of the four–point scheme D'', $f_{i,i+2} > 0$, $i = 1, 2, \ldots, J-2$, and symmetrically $f_{i,i-2} > 0$, $i = N-J+2, \ldots, N-1$. By looking at the coefficients of the schemes D'' and D''_C which dominate the elements of F, we can prove that

$$4f_{i,i+2}f_{i+1,i+1} \le f_{i,i+1}f_{i+1,i+2}, \quad i = 1, 2, \ldots, J-2.$$

The last $J-2$ rows of F satisfy an analogous inequality. This is equivalent to Lorenz's SD and implies that F is an inverse–monotone matrix. Then $\|F^{-1}\| \le m^{-2}$ follows easily.

2. $\frac{1}{2} \le p < 1$. We cannot prove now that F is inverse monotone, since the signs of the F–elements resulting from T_C are not fixed any longer. Instead, we decompose F appropriately, $F = A + B$. The scheme $-\mu D'_C w_i$, $i = K, \ldots, N-K$, is separated from the rest of the discretization to form B and $A = F - B$. Here K is either J or $J+1$.

2.a $\varepsilon^{p-1} \le MN$. In this case we choose $K = J+1$, since $f_{JJ} > 0$ and $f_{J,J\pm1} \le 0$.

It holds that $||B|| \le M\mu N$.

2.b $\varepsilon^{1-p} \le M/N$. Now $K = J$ and

$$||B|| \le M\varepsilon^p \frac{N}{\ln N} \le M \frac{1}{N^{p/(1-p)}} \cdot \frac{N}{\ln N} \le M \frac{1}{\ln N}.$$

The last inequality holds because of $p/(1-p) \ge 1$.

In both subcases 2.a and 2.b, A is inverse monotone by SD and satisfies $||A^{-1}|| \le m^{-2}$. Also, note that because of (7) and $N \ge N_0$, $||B||$ can be made sufficiently small so that $||A^{-1}|| ||B|| \le M < 1$. Then we use

$$||F^{-1}|| = ||(I + A^{-1}B)^{-1}A^{-1}|| \le \frac{||A^{-1}||}{1 - ||A^{-1}B||} \le M$$

to conclude the proof. □

Let $u_\varepsilon^h = [u_\varepsilon(x_1), u_\varepsilon(x_2), \ldots, u_\varepsilon(x_{N-1})]^T$. In the next theorem, we prove an ε–uniform error estimate for T_H.

Theorem 2. *Let (2), (3), and (7) hold and let $N \ge N_0$. Then,*

$$||w^h - u_\varepsilon^h|| \le M \left(\frac{\ln N}{N}\right)^3,$$

where w^h is the solution of the system (6) with $R \equiv T_H$ on the S mesh with $am \ge 4$.

Proof. Using (4) and a fairly standard technique on the S mesh (see the relevant references mentioned in the introduction), we can prove the consistency error estimate

$$||T_H u_\varepsilon^h|| \le M \left[\frac{\varepsilon^2}{N} + \left(\frac{\ln N}{N}\right)^3\right] \le M \left(\frac{\ln N}{N}\right)^3,$$

where the last inequality follows from (7). Then Theorem 1 completes the proof. Note that the above term ε^2/N results from $T_C u_\varepsilon^h(x_J)$. □

4. Numerical results

Let us consider the following enzyme kinetics problem from [3],

$$\text{(8)} \qquad Pu := -\varepsilon^2 u'' - \varepsilon^{3/2} u' + \frac{u}{1+u} = 0, \quad u(0) = u(1) = 1.$$

This problem satisfies (2) with $p = \frac{1}{2}$ and (3) holds only locally. Since the constant functions 1 and 0 are respectively the upper and lower solutions of (8), only the values $u \in [0, 1]$ are of interest and then $c_u \geq \frac{1}{4}$, so that any $m \in (0, \frac{1}{2})$ can be used. The exact solution of problem (8) is not known but it behaves like

$$y_\varepsilon(x) = e^{-x/\varepsilon\sqrt{2}} + e^{(x-1)/\varepsilon\sqrt{2}}.$$

In order to run our numerical experiments more easily, we changed the differential equation in (8) to $Pu = f(x)$, where $f(x) = Py_\varepsilon(x)$. This means that we can take y_ε for the solution of the modified problem, since y_ε practically satisfies the boundary conditions.

In addition to $p = \frac{1}{2}$, we have tested other values of p and the results are similar, even for the theoretically unsafe values of $p \in (0, \frac{1}{2})$.

The table below shows a comparison between T_H and T_C. T_H is used on the S mesh with $J = .45N$ and $a = 8.2$, so that $am \geq 4$. The B mesh uses $q = .45$. Err stands for the maximum pointwise error and Ord is the numerically calculated order of convergence. All the methods represented in the table are uniform in ε, since the results are the same for $\varepsilon = 10^{-k}$, $k = 6, 8, 10, 12$. It may be disappointing that Ord for T_H is considerably less than 3, but the results are still significantly better than those obtained by T_C, even on the B mesh. We can conclude from the results for T_C on the S mesh that the reason for the lower Ord is not the scheme but the S mesh itself. Nevertheless, it is obvious that the use of S mesh pays off when it is combined with a higher–order scheme.

Err and Ord for T_H and T_C

N	T_H on S mesh		T_C on B mesh		T_C on S mesh	
	Err	Ord	Err	Ord	Err	Ord
100	2.8E–5	—	5.2E–5	—	8.9E–4	—
200	6.3E–6	2.2	1.2E–5	2.1	3.1E–4	1.5
400	1.3E–6	2.3	3.0E–6	2.0	1.0E–4	1.6
800	2.4E–7	2.4	7.5E–7	2.0	3.3E–5	1.6
1600	4.2E–8	2.5	1.9E–7	2.0	1.0E–5	1.7

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