Lecture Notes in Mathematics

Miodrag Petković

Point Estimation of Root Finding Methods

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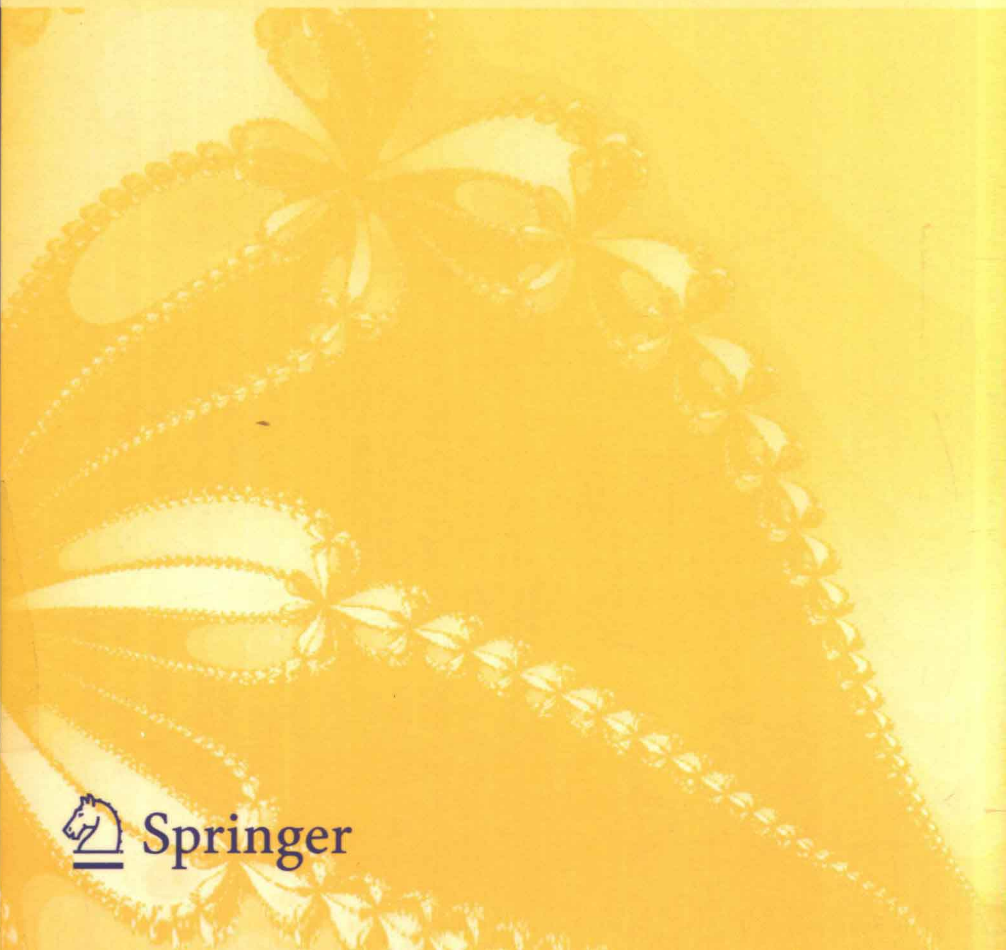

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To Ljiljana

Preface

The problem of solving nonlinear equations and systems of equations ranks among the most significant in the theory and practice, not only of applied mathematics but also of many branches of engineering sciences, physics, computer science, astronomy, finance, and so on. A glance at the bibliography and the list of great mathematicians who have worked on this topic points to a high level of contemporary interest. Although the rapid development of digital computers led to the effective implementation of many numerical methods, in practical realization, it is necessary to solve various problems such as computational efficiency based on the total central processor unit time, the construction of iterative methods which possess a fast convergence in the presence of multiplicity (or clusters) of a desired solution, the control of rounding errors, information about error bounds of obtained approximate solution, stating computationally verifiable initial conditions that ensure a safe convergence, etc. It is the solution of these challenging problems that was the principal motivation for the present study.

In this book, we are mainly concerned with the statement and study of initial conditions that provide the guaranteed convergence of an iterative method for solving equations of the form $f(z) = 0$. The traditional approach to this problem is mainly based on asymptotic convergence analysis using some strong hypotheses on differentiability and derivative bounds in a rather wide domain. This kind of conditions often involves some unknown parameters as constants, or even desired roots of equation in the estimation procedure. Such results are most frequently of theoretical importance and they provide only a qualitative description of the convergence property. The first results dealing with the computationally verifiable domain of convergence were obtained by Smale (1981), Smale (1986), Shub and Smale (1985), and Kim (1985). This approach, often referred to as "point estimation theory," treats convergence conditions and the domain of convergence in solving an equation $f(z) = 0$ using only the information of f at the initial point $z^{(0)}$.

In 1981, Smale introduced the concept of an *approximate zero* as an initial point which provides the safe convergence of Newton's method. Later, in 1986, he considered the convergence of Newton's method from data at a single point. X. Wang and Han (1989) and D. Wang and Zhao (1995) obtained some improved results. The study in this field was extended by Kim (1988) and Curry (1989) to some higher-order iterative methods including Euler's method and Halley's method, and by Chen (1989), who dealt with the general Newton-like quadratically convergent iterative algorithms. A short review of these results is given in the first part of Chap. 2. Wang–Zhao's improvement of Smale's convergence theorem and an interesting application to the Durand–Kerner method for the simultaneous determination of polynomial zeros are presented in the second part of Chap. 2.

The main aim of this book is to state such quantitative initial conditions for predicting the immediate appearance of the guaranteed and fast convergence of the considered numerical algorithm. Special attention is paid to the convergence analysis of iterative methods for the simultaneous determination of the zeros of algebraic polynomials. However, the problem of the choice of initial approximations which ensure a safe convergence is a very difficult one and it cannot be solved in a satisfactory way in general, not even in the case of simple functions, such as algebraic polynomials. In 1995, the author of this book and his contributors developed two procedures to state initial conditions for the safe convergence of simultaneous methods for finding polynomial zeros. The results were based on suitable localization theorems for polynomial zeros and the convergence of error sequences. Chapter 3 is devoted to initial conditions for the guaranteed convergence of most frequently used iterative methods for the simultaneous approximations of all simple zeros of algebraic polynomials. These conditions depend only on the coefficients of a given polynomial $P(z) = z^n + a_{n-1}z^{n-1} + \cdots + a_1 z + a_0$ of degree n and the vector of initial approximations $\boldsymbol{z}^{(0)} = \big(z_1^{(0)}, \ldots, z_n^{(0)}\big)$. In particular, some efficient a posteriori error bound methods that produce disks containing the sought zeros and require fewer numerical operations than the corresponding ordinary interval methods are considered in the last part of Chap. 3.

The new results presented in Chaps. 4 and 5 are concerned with the higher-order families of methods for the simultaneous determination of complex zeros. These methods are based on the iterative formula of Hansen–Patrick's type for finding a single zero. As in Chap. 3, we state computationally verifiable initial conditions that guarantee the convergence of the presented methods. Initial conditions ensuring convergence of the corresponding iterative methods for the inclusion of polynomial zeros are established in Chap. 5. Convergence behavior of the considered methods is illustrated by numerical examples.

I wish to thank Professor C. Carstensen of Humboldt University in Berlin. Our joint work (*Numer. Math.* 1995) had a stimulating impact on the development of the basic ideas for obtaining some results given in this book. I am grateful to Professor S. Smale, the founder of the point estimation theory, who drew my attention to his pioneering work. I am also thankful to my contributors and coauthors of joint papers Professor T. Sakurai of the

University of Tsukuba, Professor Đ. Herceg of the University of Novi Sad, Professor S. Ilić, Dr. L. Rančić, Dr. D. Milošević, and Professor D. Đorđević of the University of Niš for numerous important suggestions and valuable comments. What I especially wish to acknowledge is the assistance and exceptional efforts of Sonja Dix-Stojanović and Aleksandra Milošević who read the complete manuscript. Many small errors were eliminated in this manner.

My principal thanks, however, go to my wife Professor Ljiljana Petković for her never-failing support, encouragement, and permanent discussions during the preparation of the manuscript.

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Contents

Chapter 1
Basic Concepts

In this chapter, we give some basic concepts and properties, necessary in our investigation of convergence characteristics of root finding methods. Most of these methods are reviewed in Sect. 1.1, together with some historical notes and various principles for their construction. Section 1.2 contains several results concerning the localization of polynomial zeros. We restrict ourselves to inclusion disks in the complex plane that contain complex zeros of a given polynomial. In Sect. 1.3, we give the basic properties and operations of circular complex interval arithmetic, prerequisite to a careful analysis of the bounds of complex quantities that appear in our study and the construction of inclusion methods described in Sect. 5.3.

1.1 Simultaneous Methods for Finding Polynomial Zeros

The problem of determining the zeros of a given polynomial is one of the first nonlinear problems that mathematicians meet in their research and practice. Although this problem seems to be simple at first sight, a perfect algorithm for finding polynomial zeros has not been established yet, in spite of numerous algorithms developed during the last 40 years. Each numerical method possesses its own advantages and disadvantages, so that it is not easy to choose the "best" method for a given polynomial equation. Let us emphasize that the rapid development of computing machines implies that many algorithms, formerly of academic interest only, become feasible in practice.

Most algorithms calculate only one zero at a time. In cases when all zeros are needed, these algorithms usually work serially as follows: when a zero has been computed to sufficient accuracy, then the corresponding linear factor is removed from the polynomial by the Horner scheme and the process is applied again to determine a zero of the "deflated" polynomial whose degree is now lowered by one. This is the method of successive *deflations*. If a great accuracy of desired approximations to the zeros is required, the polynomial obtained

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after divisions by the previously calculated (inaccurate) linear factors may be falsified to an extent which makes the remaining approximate zeros erroneous. This is a flaw of the method of successive removal of linear factors. The next disadvantage appears in those situations where it is sufficient to find approximations with only a few significant digits. But, as mentioned above, the method of deflation requires approximations of great accuracy. Besides, this procedure cannot ensure that the zeros are determined in increasing order of magnitude (see Wilkinson [190]), which is an additional shortcoming of deflation.

The above difficulties can be overcome in many situations by approximating all zeros simultaneously. Various approaches to these procedures have been developed: the method of search and exclusion (Henrici [57, Sect. 6.11]), methods based on the fixed point relations (e.g., Börsch-Supan [9], [10], Ehrlich [33], X. Wang and Zheng [182], Gargantini [47], [48]), *qd* algorithm (Henrici [57, Sect. 7.6]), a globally convergent algorithm that is implemented interactively (Farmer and Loizou [39]), tridiagonal matrix method (Brugnano and Trigiante [12], Schmeisser [159]), companion matrix methods (Smith [168], Niu and Sakurai [93], Fiedler [40], Malek and Vaillancourt [86]), methods based on the application of root finders to a suitable function ([69], [124], [146], [156]), methods which use rational approximations (Carstensen and Sakurai [18], Sakurai et al. [157], [158]), and others (see, for instance, Wilf [189], Pasquini and Trigiante [103], Jankins and Traub [67], Farmer and Loizou [37], [38]). See also Pan's survey paper [101] and references cited therein.

Part I: Simultaneous Methods Based on Fixed Point Relations

In this book, we deal mainly with the simultaneous methods based on fixed point relations (FPR). Such an approach generates algorithms with very fast convergence in complex "point" arithmetic as well as in complex interval arithmetic using the following procedure.

Let $\zeta_1, \dots, \zeta_n$ be the zeros of a given monic (normalized, highest coefficient 1) polynomial $P(z) = z^n + a_{n-1}z^{n-1} + \cdots + a_1 z + a_0$ of degree n and let $z_1, \dots, z_n$ be their respective approximations. We consider two types of FPR

$$\zeta_i = F_1(z_1, \dots, z_{i-1}, z_i, \zeta_i, z_{i+1}, \dots, z_n), \tag{1.1}$$

$$\zeta_i = F_2(\zeta_1, \dots, \zeta_{i-1}, z_i, \zeta_{i+1}, \dots, \zeta_n), \tag{1.2}$$

where $i \in \boldsymbol{I}_n := \{1, \dots, n\}$. Now we give several FPR which have been the basis for the construction of the most frequently used iterative methods for the simultaneous determination of polynomial zeros in complex arithmetic and complex interval arithmetic. In the latter development, we will frequently use *Weierstrass' correction* $W_i(z_i) = P(z_i)/\prod_{j \neq i}(z_i - z_j)$ $(i \in \boldsymbol{I}_n)$. Sometimes, we will write W_i instead of $W_i(z_i)$. In addition to the references given behind the type of FPR, the derivation of these FPR may be found in the book [109] of M. Petković.

For brevity, we will sometimes write

$$\sum_{j\neq i} x_j \text{ instead of } \sum_{\substack{j=1\\ j\neq i}}^{n} x_j \quad \text{and} \quad \prod_{j\neq i} x_j \text{ instead of } \prod_{\substack{j=1\\ j\neq i}}^{n} x_j.$$

Example 1.1. ***The Weierstrass-like FPR*** [109]:

$$\zeta_i = z - \frac{P(z)}{\prod_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)} \quad (i \in \boldsymbol{I}_n). \tag{F_1}$$

Equation (F_1) follows from the factorization $P(z) = \prod_{j=1}^{n}(z-\zeta_j) = (z-\zeta_i)\prod_{\substack{j=1\\ j\neq i}}^{n}(z-\zeta_j)$.

Example 1.2. ***The Newton-like FPR*** [50], [106]:

$$\zeta_i = z - \frac{1}{\dfrac{P'(z)}{P(z)} - \sum_{\substack{j=1\\ j\neq i}}^{n}\dfrac{1}{z-\zeta_j}} \quad (i \in \boldsymbol{I}_n). \tag{F_2}$$

Applying the logarithmic derivative to $P(z) = \prod_{j=1}^{n}(z-\zeta_j)$, the identity

$$\frac{P'(z)}{P(z)} = \sum_{j=1}^{n}\frac{1}{z-\zeta_j} \tag{1.3}$$

is obtained. Finding $z-\zeta_i$ from (1.3), we get (F_2).

Example 1.3. ***The Börsch-Supan-like FPR*** [11], [107]:

$$\zeta_i = z - \frac{W_i}{1 + \sum_{\substack{j=1\\ j\neq i}}^{n}\dfrac{W_j}{\zeta_i - z_j}} \quad (i \in \boldsymbol{I}_n). \tag{F_3}$$

Lagrange's interpolation applied to the distinct points $z_1, \ldots, z_n$ ($\neq \zeta_i$, $i \in \boldsymbol{I}_n$) gives

$$P(z) = W_i \prod_{\substack{j=1 \\ j \neq i}}^{n} (z - z_j) + \prod_{j=1}^{n} (z - z_j) \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{W_j}{z - z_j} + 1 \right). \tag{1.4}$$

Taking $z = \zeta_i$ and solving the obtained equation in $\zeta_i - z_i$, from (1.4) we derive (F_3).

Example 1.4. ***The square root FPR*** [47], [106]:

$$\zeta_i = z - \frac{1}{\left[\dfrac{P'(z)^2 - P(z)P''(z)}{P(z)^2} - \displaystyle\sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{1}{(z - \zeta_j)^2} \right]^{1/2}} \quad (i \in \boldsymbol{I}_n). \tag{F_4}$$

Differentiation of the identity (1.3) yields

$$-\left(\frac{P'(z)}{P(z)} \right)' = \frac{P'(z)^2 - P(z)P''(z)}{P(z)^2} = \sum_{j=1}^{n} \frac{1}{(z - \zeta_j)^2}, \tag{1.5}$$

wherefrom we extract the term $(z - \zeta_i)^2$ and derive (F_4).

Example 1.5. ***The Halley-like FPR*** [109], [182]:

$$\zeta_i = z - \frac{1}{\dfrac{P'(z)}{P(z)} - \dfrac{P''(z)}{2P'(z)} - \dfrac{P(z)}{2P'(z)} \left[\left(\displaystyle\sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{1}{z - \zeta_j} \right)^2 + \displaystyle\sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{1}{(z - \zeta_j)^2} \right]}. \tag{F_5}$$

Equation (F_5) can be obtained by substituting the sums (1.3) and (1.5) in the relation

$$\frac{P''(z)}{P(z)} = \left(\frac{P'(z)}{P(z)} \right)^2 + \left(\frac{P'(z)}{P(z)} \right)'.$$

Actually, (F_5) is a special case of a general fixed point relation derived by X. Wang and Zheng [182] by the use of Bell's polynomials (see Comment (M_5)).

Substituting the exact zeros $\zeta_1, \ldots, \zeta_n$ by their respective approximations $z_1, \ldots, z_n$ and putting $z = z_i$, from (1.1) and (1.2), we obtain iterative schemes

$$\hat{z}_i = F_1(z_1, \ldots, z_n) \quad (i \in \boldsymbol{I}_n), \tag{1.6}$$

$$\hat{z}_i = F_2(z_1, \ldots, z_n) \quad (i \in \boldsymbol{I}_n), \tag{1.7}$$

in (ordinary) complex arithmetic, where $\hat{z}_i$ is a new approximation to the zero ζ_i. Another approach consisting of the substitution of the zeros on the right side of (1.1) and (1.2) by their inclusion disks enables the construction of interval methods in circular complex interval arithmetic (see Sects. 1.3 and 5.3).

For illustration, we list below the corresponding simultaneous iterative methods based on the FPR given in Examples 1.1–1.5 and having the form (1.6) or (1.7).

The Durand–Kerner's or Weierstrass' method [1], [30], [32], [72], [148], [187], order 2:

$$\hat{z}_i = z_i - W_i = z_i - \frac{P(z_i)}{\prod_{\substack{j=1 \\ j \neq i}}^{n} (z_i - z_j)} \quad (i \in \boldsymbol{I}_n). \tag{M_1}$$

The Ehrlich–Aberth's method [1], [31], [33], [85], order 3:

$$\hat{z}_i = z_i - \frac{1}{\dfrac{P'(z_i)}{P(z_i)} - \sum_{\substack{j=1 \\ j \neq i}}^{n} \dfrac{1}{z_i - z_j}} \quad (i \in \boldsymbol{I}_n). \tag{M_2}$$

The Börsch-Supan's method [10], [95], order 3:

$$\hat{z}_i = z_i - \frac{W_i}{1 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \dfrac{W_j}{z_i - z_j}} \quad (i \in \boldsymbol{I}_n). \tag{M_3}$$

Let us introduce $\delta_{k,i} = \dfrac{P^{(k)}(z_i)}{P(z_i)}$ $(k = 1, 2)$. Then

$$\delta_{1,i}^2 - \delta_{2,i} = \frac{P'(z_i)^2 - P(z_i)P''(z_i)}{P(z_i)^2}.$$

The square root method [47], [142], order 4:

$$\hat{z}_i = z_i - \frac{1}{\left[\delta_{1,i}^2 - \delta_{2,i} - \sum_{\substack{j=1 \\ j \neq i}}^{n} \dfrac{1}{(z_i - z_j)^2}\right]^{1/2}} \quad (i \in \boldsymbol{I}_n). \tag{M_4}$$

The Halley-like or Wang–Zheng's method [182], order 4:

$$\hat{z}_i = z_i - \frac{1}{f(z_i) - \dfrac{P(z_i)}{2P'(z_i)}\left[\left(\sum_{\substack{j=1 \\ j \neq i}}^{n} \dfrac{1}{z_i - z_j}\right)^2 + \sum_{\substack{j=1 \\ j \neq i}}^{n} \dfrac{1}{(z_i - z_j)^2}\right]} \quad (i \in \boldsymbol{I}_n), \tag{M_5}$$

where

$$f(z_i) = \frac{P'(z_i)}{P(z_i)} - \frac{P''(z_i)}{2P'(z_i)} \tag{1.8}$$

is the denominator of Halley's correction

$$H(z_i) = H_i = \frac{1}{f(z_i)}, \tag{1.9}$$

which appears in the well-known classical Halley's method [4], [45], [54]

$$\hat{z}_i = z_i - H(z_i) = z_i - \frac{1}{\dfrac{P'(z_i)}{P(z_i)} - \dfrac{P''(z_i)}{2P'(z_i)}}. \tag{1.10}$$

Comment (M_1). Formula (M_1) has been rediscovered several times (see Durand [32], Dochev [30], Börsch-Supan [9], Kerner [72], M. Prešić [147], S. B. Prešić [149]) and it has been derived in various ways. But we emphasize the little known fact that this formula was known seven decades ago. In his lecture on the session of König, Academy of Science, held on 17 December 1891, Weierstrass communicated a new constructive proof of the fundamental theorem of algebra (printed in [187]). In this proof, Weierstrass used the sequences of numerical entries $\{a_\nu^{(\lambda)}\}$ ($\nu = 1, \ldots, n,\ \lambda = 0, 1, 2, \ldots$) defined successively by (eq. (29) in Weierstrass' work [187])

$$\begin{cases} a'_\nu = a_\nu - \dfrac{P(a_\nu)}{\prod_\mu (a_\nu - a_\mu)} \\ a''_\nu = a'_\nu - \dfrac{P(a'_\nu)}{\prod_\mu (a'_\nu - a'_\mu)} \qquad (\nu = 1, \ldots, n,\ \mu \gtrless \nu), \\ a'''_\nu = a''_\nu - \dfrac{P(a''_\nu)}{\prod_\mu (a''_\nu - a''_\mu)} \\ \text{and so on} \end{cases} \tag{1.11}$$

where P is a polynomial of degree n with the zeros $x_1, \ldots, x_n$.

The proof of the quadratic convergence of the iterative method (M_1) is ascribed to Dochev [30], although his proof is not quite precise. The works [82], [148], [162] offer a more precise proof. But it seems that the quadratic convergence of the sequence (1.11) was known to Weierstrass. Namely, for the maximal absolute differences $\varepsilon^{(\lambda)} = \max\limits_{1 \le \nu \le n} |a_\nu^{(\lambda)} - x_\nu|$, he derived the following inequality (eq. (32) in [187])

$$\varepsilon^{(\lambda)} < \left(\varepsilon^{(0)}\right)^{2^\lambda} \quad (\lambda = 1, 2, \ldots),$$

which points to the quadratic convergence of the sequences $\{a_\nu^{(\lambda)}\}$.

Note that Weierstrass did not use (1.11) for the numerical calculation of polynomial zeros. Durand [32] and Dochev [30] were the first to apply the iterative formula (M_1) in practice for the simultaneous approximation of polynomial zeros.

In 1966, Kerner [72] proved that (M_1) is, in fact, Newton's method $\hat{z} = z - F'(z)^{-1}F(z)$ for solving nonlinear systems applied to the system of nonlinear equations (known as Viète's formulae)

$$(-1)^k \varphi_k(z_1, \dots, z_n) - a_k = 0, \quad (k = 1, \dots, n), \tag{1.12}$$

where φ_k denotes the kth elementary symmetric function:

$$\varphi_k = \sum_{1 \le j_1 \le \cdots j_k \le n} z_{j_1} z_{j_2} \cdots z_{j_k}.$$

Since Newton's method is quadratically convergent, it follows immediately that the iterative method (M_1) also has quadratic convergence.

The iterative method (M_1) shares with the Halley's method (1.10) the distinction of being the most frequently rediscovered method in the literature. From the fact that many authors dealt with the formula (M_1), the iterative method (M_1) is called Weierstrass', Durand–Kerner's, or Weierstrass–Dochev's method; other combinations also appear in literature.

According to a great number of numerical experiments, many authors have conjectured that the method (M_1) possesses a global convergence in practice for almost all starting vectors $\boldsymbol{z}^{(0)} = (z_1^{(0)}, \dots, z_n^{(0)})$, assuming that the components of $\boldsymbol{z}^{(0)}$ are disjoint. This was proved for $n = 2$ (see [52], [64]) and for the cubic polynomial $P(z) = z^3$ (Yamagishi [64]), but this is an open problem still for a general $n \ge 3$.

Let us note that the method (M_1) works well even for the case where the zeros of P are not necessarily distinct (see Fraigniaud [43], Miyakoda [89], Pasquini and Trigiante [103], Carstensen [15], Kyurkchiev [81], Yamamoto, Furakane, and Nogura [193], Kanno, Kyurkchiev, and Yamamoto [69], Yamamoto, Kanno, and Atanassova [194], etc.). For these excellent properties and great computational efficiency, this method is one of the most frequently used simultaneous methods for determining polynomial zeros (see [109, Chap. 6]).

Comment (M_2). Although the method (M_2) was first suggested by Maehly [85] in 1954 for a refinement of the Newton's method and used by Börsch-Supan [9] in finding a posteriori error bounds for the zeros of polynomials, it is more often referred to as the Ehrlich–Aberth's method. Ehrlich [33] proved the cubic convergence of this method and Aberth [1] gave important contribution in its practical realization. The method (M_2) can also be derived from the Halley's method (1.10) using the approximation (see (1.49))