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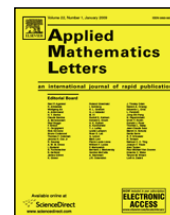
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Traub's accelerating generator of iterative root-finding methods

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ABSTRACT

An accelerating generator of iterative methods for finding multiple roots, based on Traub's differential–difference recurrence relation, is presented. It is proved that this generator yields an iteration function of order $r + 1$ starting from arbitrary iteration function of order r . In this way, it is possible to construct various iterative formulas of higher order for finding single roots of nonlinear equations and all simple or multiple roots of algebraic polynomials, simultaneously. For demonstration, two iterative methods of the fourth order in ordinary (real or complex) arithmetic and an iterative method in interval arithmetic are presented.

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1. Introduction

Fundamental and challenging results of Traub [1] on a general theory of iteration algorithms for the numerical solution of nonlinear equations were developed almost half a century ago. However, many contributions from Traub's 1964 book are still inspiring and are real. Recently, many worth variants on Traub's classic results were presented in [2]. In this paper, we also consider some of Traub's classic results from 1964. We restrict our study to Traub-like accelerating generator for iterative methods for finding simple or multiple roots of nonlinear equations $f(x) = 0$. In particular, we construct iterative methods for the simultaneous determination of polynomial roots in ordinary and interval arithmetic. All of these methods are produced by suitable accelerating generator of iteration functions. An iterative method of the order of convergence of $r + 1$ is generated from the previous method of order r using a special transformation. Such an accelerating generator was proposed in [3]. Here we presented another one based on Traub's recurrence relation [1].

Let α be the zero of a function f of multiplicity m . Following Traub's terminology [1], we will say that an iteration function φ is of order r and write $\varphi \in K_r$ if it defines an iterative method of order r . To generate the basic sequence of root-solvers, Traub [1] derived the following differential–difference recurrence relation

$$\varphi_{r+1}(x) = \varphi_r(x) - \frac{m}{r} u(x) \varphi_r'(x), \quad u(x) = \frac{f(x)}{f'(x)}, \quad (1)$$

where $\varphi_r(x)$ is a given iteration function which defines the iterative method of the order of convergence r . The recurrence relation (1) starts with Newton's methods $\varphi_2(x) = \mathcal{N}(x) = x - f(x)/f'(x)$ (for simple roots) and $\varphi_2(x) = \tilde{\mathcal{N}}(x) = x - mf(x)/f'(x)$ (for multiple roots). In the case of simple roots, the generated sequence

$$E_2 = \mathcal{N}(x) = x - u(x), \quad E_3 = E_2 - A_2(x)u(x)^2, \quad E_4 = E_3 - (2A_2(x)^2 - A_3(x))u(x)^2, \dots$$

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makes the well-known Schröder–König family $\mathbb{E} = \{E_2, E_3, E_4, \dots\}$ of the first kind, see [4,1], where $A_k(x) = f^{(k)}(x)/(k!f'(x))$.

The following natural question arises: *Is it possible to take an iteration function $\varphi_k \notin \mathbb{E}$ and still generate an iterative method of order $k + 1$?* The study of this question is the main goal of this paper; we show that the relation (1) can be used for generating iterative formulas starting not only from the mentioned Newton methods $\varphi_2(x)$ but from any iterative method of arbitrary order r (Section 2). In this way it is possible to construct various iterative formulas of higher order for finding single (simple or multiple) root of nonlinear equations (Section 3) and all simple or multiple roots of algebraic polynomials, simultaneously (Section 4). In Section 5, we derive a root-relation which is convenient for the construction of an iterative method for the simultaneous inclusion of simple or multiple roots of an algebraic polynomial. For simplicity, the abbreviation I.F. will henceforth be used for iteration function.

2. Traub's accelerating generator of iterative methods

We start from the well-known assertion on the order of convergence of iterative root-finding methods.

Theorem 1 (Traub [1, Theorem 2.2]). *Let φ be I.F. such that φ and its derivatives $\varphi', \dots, \varphi^{(r)}$ are continuous in the neighborhood of a zero α of a given function f . Then φ defines an iterative method of order r if and only if*

$$\varphi(\alpha) = \alpha, \quad \varphi'(\alpha) = \dots = \varphi^{(r-1)}(\alpha) = 0, \quad \varphi^{(r)}(\alpha) \neq 0. \quad (2)$$

The following theorem is concerned with the acceleration of iterative methods by using Traub's relation (1).

Theorem 2. *Let $\varphi_r(x)$ be an I.F. which defines the method $x_{k+1} = \varphi_r(x_k)$ ($k = 0, 1, \dots$) of order r for finding a simple or multiple zero of a given sufficiently many times differentiable function f . Then the iterative method*

$$x_{k+1} = \varphi_{r+1}(x_k) := \varphi_r(x_k) - \frac{m}{r} u(x_k) \varphi_r'(x_k), \quad (r \geq 2; k = 0, 1, \dots), \quad (3)$$

originated from (1), where m denotes the multiplicity of the above-mentioned zero, has the order of convergence $r + 1$.

Proof. For two real or complex numbers z and w we will write $z = O_M(w)$ if $|z| = O(|w|)$ (the same order of their moduli), where O represents the Landau symbol.

Let us introduce the error $\varepsilon = x - \alpha$. Since $\varphi_r \in K_r$, bearing in mind the relations (2) we find by Taylor's series

$$\varphi_r(x) = \alpha + \frac{1}{r!} \varphi_r^{(r)}(\alpha) \varepsilon^r + \frac{1}{(r+1)!} \varphi_r^{(r+1)}(\alpha) \varepsilon^{r+1} + O_M(\varepsilon^{r+2}), \quad (4)$$

and

$$\varphi_r'(x) = \frac{1}{(r-1)!} \varphi_r^{(r)}(\alpha) \varepsilon^{r-1} + \frac{1}{r!} \varphi_r^{(r+1)}(\alpha) \varepsilon^r + O_M(\varepsilon^{r+1}). \quad (5)$$

Let $f(x) = (x - \alpha)^m g(x)$, $g(\alpha) \neq 0$. Hence

$$u(x) = \frac{f(x)}{f'(x)} = \frac{\varepsilon}{m} - \frac{\varepsilon^2}{m^2} \frac{g'(x)}{g(x)} + O_M(\varepsilon^3). \quad (6)$$

By virtue of (4)–(6), we get

$$\varphi_{r+1}(x) = \varphi_r(x) - \frac{mu(x)}{r} \varphi_r'(x) = \alpha + \frac{1}{r!} \left(\frac{g'(x)}{g(x)} \cdot \frac{\varphi_r^{(r)}(\alpha)}{m} - \frac{\varphi_r^{(r+1)}(\alpha)}{r} \right) \varepsilon^{r+1} + O_M(\varepsilon^{r+2}).$$

Hence, $\varphi_{r+1}(x) - \alpha = O_M(\varepsilon^{r+1})$, which means that $\varphi_{r+1} \in K_{r+1}$. \square

In what follows, we will demonstrate three applications of Traub's accelerating generator (3) to derive some new iterative formulas in connection with Traub's inspired results.

3. Application 1: fourth-order method for a single root

Let $A_k(x) = f^{(k)}(x)/(k!f'(x))$ as above. The third-order Halley-like method for finding a multiple zero α of multiplicity m of a real or complex function f is defined by (see, e.g., [5,6])

$$H(x) = x - \frac{2u(x)}{(m+1)/m - 2u(x)A_2(x)}.$$

Let us note that $H \notin \mathbb{E}$. Finding $H'(x)$ and applying Traub's formula (1) in the form

$$H_4(x) = H(x) - \frac{mu(x)}{3}H'(x)$$

with $r = 3$, after short arrangement we obtain the fourth-order iterative method (omitting argument x of u , A_2 and A_3)

$$H_4(x) = x - \frac{mu(7 + 6m - m^2 - 12muA_2 + 12m^2u^2(A_2^2 - A_3))}{3(m + 1 - 2muA_2)^2}.$$

In the case of a simple zero ($m = 1$), the above iterative formula reduces to

$$H_4(x) = x - \frac{u(1 - uA_2 + u^2(A_2^2 - A_3))}{(1 - uA_2)^2}.$$

We can continue to generate higher-order methods using H_4 in (1), and so on, but these iterative formulas are rather cumbersome.

Remark 1. Higher-order methods derived in this paper have a structure of the form

$$\hat{x} = x - \frac{b_0 - b_1f(x) - b_2f(x)^2 - \dots - b_p f(x)^p}{1 - c_1f(x) - c_2f(x)^2 - \dots - c_q f(x)^q}.$$

If approximations x are reasonably close to the zero α , then $|f(x)|$ is small enough. The above polynomial form (in $f(x)$) of the numerator and denominator prevents negative effect of rounding errors. However, the disadvantage of higher-order iterative formulas comes from the use of derivatives of higher order, which increases the total computational costs of these fast but expensive methods. This means that one-point iterative methods of a very high order are not suitable for practical application.

4. Application 2: fourth-order simultaneous method

Let $f(x) = x^n + a_{n-1}x^{n-1} + \dots + a_1x + a_0$ be a monic polynomial (leading coefficient is 1) of degree n having real or complex roots $\alpha_1, \dots, \alpha_v$ ($v \leq n$) of multiplicities μ_1, \dots, μ_v , respectively, and let $I_v = \{1, \dots, v\}$ be the index set. Assume that x is an approximation to the root α_i which is improved iteratively, and let $x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_v$ be approximations to the remaining roots which are fixed during the iterative process. Consider the I.F.

$$M(x) = x - \frac{\mu_i}{\frac{1}{u(x)} - \sum_{j \in I_v \setminus \{i\}} \frac{\mu_j}{x - x_j}} \tag{7}$$

which defines, in fact, the modified Newton method of the form

$$\tilde{M}(x) = x - \frac{\mu_i f(x)}{f'(x) + \lambda f(x)}, \quad (\lambda \text{ is a real parameter}), \tag{8}$$

studied by numerous authors. The form (7) was analyzed by Maehly [7] for simple roots. It is known that the iteration function (8) defines a quadratically convergent method; see, e.g., [8]. Therefore, the iteration function $M(x)$ given by (7) also defines a quadratically convergent method.

For simplicity, introduce the abbreviation

$$S_{k,i}(x) = \sum_{j \in I_v \setminus \{i\}} \frac{\mu_j}{(x - x_j)^k} \quad (k = 1, 2).$$

Then

$$M'(x) = 1 + \frac{\mu_i \left(u(x)^2 S_{2,i}(x) + u(x) \frac{f''(x)}{f'(x)} - 1 \right)}{\left(1 - u(x) S_{1,i}(x) \right)^2}.$$

Let us apply Traub's accelerating formula (1) to the iteration function (7) taking $r = 2$, then we obtain

$$\begin{aligned} \widehat{M}(x) &:= M(x) - \frac{\mu_i u(x)}{2} M'(x) \\ &= x - \mu_i u(x) - \frac{\mu_i u(x) \left(1 - \mu_i + u(x) \mu_i \frac{f''(x)}{f'(x)} - u(x)^2 (S_{1,i}^2(x) - \mu_i S_{2,i}(x)) \right)}{2(1 - u(x) S_{1,i}(x))^2}. \end{aligned} \tag{9}$$

The I.F. $\widehat{M}(x)$ defines the third-order method assuming that only the approximation x to the root α_i is iterated. Obviously, the method (9) applied in this manner is inefficient and has little practical importance. For this reason, let us assume now that all approximations x_1, \dots, x_ν (with $x = x_i$) are improved simultaneously in the course of iterative process. Then the iterative formula (9) becomes

$$\hat{x}_i = \widehat{M}(x_i) = x_i - \mu_i u_i - \frac{\mu_i u_i \left(1 - \mu_i + u_i \mu_i \frac{f''(x_i)}{f'(x_i)} - u_i^2 (S_{1,i}^2 - \mu_i S_{2,i}) \right)}{2(1 - u_i S_{1,i})^2} \quad (i \in I_\nu), \tag{10}$$

where we introduce $u_i = u(x_i)$, $S_{k,i} = S_{k,i}(x_i)$ and \hat{x}_i is a subsequent approximation. The iterative method (10) can serve for the simultaneous determination of multiple roots of a polynomial. In what follows all quantities in the subsequent iteration will be denoted by the symbol $\widehat{}$.

As mentioned above, the I.F. $M(x)$ is of the second order if only one approximation is iterated in the iterative process. If all approximations are simultaneously improved, then the method defined by $\hat{x}_i = M(x_i)$ is the Ehrlich-like third-order method for multiple roots (see [9,10]). In a similar way, $\widehat{M}(x_i)$ defines the fourth-order method, which is the subject of the following theorem.

Theorem 3. Assume that approximations x_1, \dots, x_ν are sufficiently close to the roots $\alpha_1, \dots, \alpha_\nu$. Then the iterative method defined by (10) has the order of convergence four.

Proof. Let

$$T_{k,i} = \sum_{j \in I_\nu \setminus \{i\}} \frac{\mu_j}{(x_i - \alpha_j)^k} \quad (k = 1, 2).$$

Starting from the factorization $f(x) = \prod_{j=1}^\nu (x - \alpha_j)^{\mu_j}$, we find

$$\frac{d}{dx} \log(f(x)) = \frac{f'(x)}{f(x)} = \sum_{j=1}^\nu \frac{\mu_j}{x - \alpha_j}, \tag{11}$$

$$-\frac{d}{dx} \left(\frac{f'(x)}{f(x)} \right) = \frac{f'(x)^2 - f(x)f''(x)}{f(x)^2} = \sum_{j=1}^\nu \frac{\mu_j}{(x - \alpha_j)^2}. \tag{12}$$

Taking $x = x_i$ in (11) and (12), and introducing the error $\varepsilon_i = x_i - \alpha_i$, we obtain

$$\frac{1}{u_i} = \frac{\mu_i}{\varepsilon_i} + T_{1,i}, \quad \text{that is, } u_i = \frac{\varepsilon_i}{\mu_i + \varepsilon_i T_{1,i}}, \tag{13}$$

and (using (13))

$$\frac{f''(x_i)}{f'(x_i)} = \frac{1}{u_i} - \frac{\mu_i u_i}{\varepsilon_i^2} - u_i T_{2,i} = \frac{\mu_i + \varepsilon_i T_{1,i}}{\varepsilon_i} - \frac{\mu_i}{\varepsilon_i(\mu_i + \varepsilon_i T_{1,i})} - \frac{\varepsilon_i T_{2,i}}{\mu_i + \varepsilon_i T_{1,i}}. \tag{14}$$

Substituting (13) and (14) in (10), after extensive but elementary calculations we obtain

$$\widehat{M}(x_i) - \alpha_i = \frac{\varepsilon_i^3 \left(2\varepsilon_i(T_{1,i} - S_{1,i})^2 T_{1,i} + \mu_i(T_{1,i} - S_{1,i})(3T_{1,i} - S_{1,i}) + \mu_i^2(T_{2,i} - S_{2,i}) \right)}{2(\mu_i + \varepsilon_i T_{1,i})(\mu_i + \varepsilon_i(T_{1,i} - S_{1,i}))^2}. \tag{15}$$

Assume that $\varepsilon \in \{\varepsilon_1, \dots, \varepsilon_\nu\}$ is the error of the largest modulus but preserving the same order of moduli of all errors, that is, $|\varepsilon_j| = O(|\varepsilon|)$. Since

$$T_{1,i} - S_{1,i} = \sum_{j \in I_\nu \setminus \{i\}} \mu_j \left(\frac{1}{x_i - \alpha_j} - \frac{1}{x_i - \alpha_j} \right) = - \sum_{j \in I_\nu \setminus \{i\}} \frac{\mu_j \varepsilon_j}{(x_i - \alpha_j)(x_i - \alpha_j)} = O_M(\varepsilon),$$

and

$$T_{2,i} - S_{2,i} = \sum_{j \in I_\nu \setminus \{i\}} \mu_j \left(\frac{1}{(x_i - \alpha_j)^2} - \frac{1}{(x_i - \alpha_j)^2} \right) = - \sum_{j \in I_\nu \setminus \{i\}} \frac{\mu_j \varepsilon_j (2x_i - x_j - \alpha_j)}{(x_i - \alpha_j)^2 (x_i - \alpha_j)^2} = O_M(\varepsilon),$$

returning to (15) and bearing in mind that the denominator of (15) tends to $2\mu_i^3$ as $\varepsilon_i \rightarrow 0$, we find

$$\hat{\varepsilon}_i = \widehat{x}_i - \alpha_i = \widehat{M}(x_i) - \alpha_i = \varepsilon_i^3 O_M(\varepsilon) = O_M(\varepsilon^4).$$

This means that the order of convergence of the simultaneous method defined by (10) is four. \square

If all roots are simple ($\mu_1 = \dots = \mu_n = 1$), then the iterative formula (10) reduces to

$$\widehat{M}(x_i) = x_i - u_i - \frac{u_i^2 \left(\frac{f''(x_i)}{f'(x_i)} - u_i(S_{1,i}^2 - S_{2,i}) \right)}{2(1 - u_i S_{1,i})^2} \quad (i = 1, \dots, n),$$

where $S_{k,i} = \sum_{j \in I_n \setminus \{i\}} \frac{1}{(x_i - x_j)^k}$ ($k = 1, 2$).

Combining (3) and (9) we can construct iterative method of the fifth order for simultaneous finding simple or multiple roots of polynomials, which can be further accelerated using (3).

5. Application 3: inclusion method for polynomial roots

Substituting the sums $S_{1,i}$ and $S_{2,i}$ by the sums $T_{1,i}$ and $T_{2,i}$ (respectively) in (9), we obtain

$$M^*(x_i) = x_i - \mu_i u_i - \frac{\mu_i u_i \left(1 - \mu_i + u_i \mu_i \frac{f''(x_i)}{f'(x_i)} - u_i^2 (T_{1,i}^2 - \mu_i T_{2,i}) \right)}{2(1 - u_i T_{1,i})^2} \quad (i = 1, \dots, v). \tag{16}$$

Lemma 1. $M^*(x_i) = \alpha_i$.

The proof is straightforward by substituting (11) and (12) in (15).

In this section real or complex intervals are denoted in bold. Let $\widehat{\mathbf{X}}_i := \mathbf{M}(x_i)$ be a real or complex interval extension of $M^*(x_i)$ obtained by substituting the roots α_j ($j \neq i$) in the sums $T_{1,i}$ and $T_{2,i}$ on the right-hand side of (15) by (real or complex) intervals \mathbf{X}_j that contain these roots (that is, $\alpha_j \in \mathbf{X}_j$). It is assumed that x_i is the midpoint of the interval \mathbf{X}_i . More about interval extension can be found in the book [11].

According to the subset property and Lemma 1 it follows $\alpha_i = M^*(x_i) \in \widehat{\mathbf{X}}_i = \mathbf{M}(x_i)$. Define a new inclusion interval $\widehat{\mathbf{X}}_i$ by

$$\widehat{\mathbf{X}}_i := x_i - \mu_i u_i - \frac{\mu_i u_i \left(1 - \mu_i + u_i \mu_i \frac{f''(x_i)}{f'(x_i)} - u_i^2 (\mathbf{S}_{1,i}^2 - \mu_i \mathbf{S}_{2,i}) \right)}{2(1 - u_i \mathbf{S}_{1,i})^2} \quad (i = 1, \dots, v), \tag{17}$$

where

$$\mathbf{S}_{k,i} = \sum_{\substack{j=1 \\ j \neq i}}^v \mu_j \left(\frac{1}{x_i - \mathbf{X}_j} \right)^k \quad (k = 1, 2).$$

If the denominator of (17) does not contain the origin, then the iterative formula (17) defines an iterative interval method for the simultaneous inclusion of all multiple roots of a polynomial P providing $\alpha \in \mathbf{X}_i$ in each iterative step. Conditions for the convergence and the order of convergence of the interval method (17) will be considered in the forthcoming research.

6. Further improvements

The presented accelerating generator of Traub's type produces higher-order basic methods for finding simple and multiple roots of nonlinear equations. The basic method (10) in real or complex arithmetic and the method (17) in real or complex interval arithmetic can serve for further improvements by using suitable corrections which considerably accelerate the convergence speed of the basic methods without additional function evaluations. In this way their computational efficiency is significantly increased. Such an approach for simple zeros is presented in the papers [12,13], together with an extensive discussion of initial computationally verifiable conditions that guarantee the convergence of the methods presented in this paper, numerical examples and comparison of various methods of the similar type, including the basic methods (10) and (17) and their improvements. For this reason and the required limit of papers addressed to this journal, the reviews of computational aspects and convergence conditions are omitted.

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