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A note on determinantal representation of a Schröder–König-like simultaneous method for finding polynomial zeros

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ABSTRACT

Using Padé approximation, Sakurai, Torii and Sugiura derived in the paper (Sakurai et al., 1991) the generalized iterative method of order $n+2$ for finding all zeros of a polynomial, where n is the highest order of a polynomial derivative involved in the presented iterative formula. In this note we give the determinantal representation of this method and analyze procedures for its implementation and some computational aspects.

1. Introduction

The rediscoveries of the already known formulas are not seldom in scientific disciplines; undoubtedly, they appear most frequently in mathematics. A very illustrative example was given in [1], in which it was proved that six iteration functions of general form, derived in the period from 1946 until 1999 in various ways and expressed in different forms, are actually equivalent. And yet, they are equivalent to Schröder's family of the second kind [2] derived for rational functions in 1870 by Schröder (the paper translated in English by Stewart [3]) and later extended by König [4] in 1884 for analytic functions. This family, often known in the literature as Schröder–König's family, plays the main role in this paper.

As mentioned by Kalantari in [5, Chapter X], "... *different formulations of an iteration function ... imply that whatever is proved for one form also applies to the other forms. These different but equivalent formulations also allow the discovery of new properties that may not be evident from other formulation*". This Kalantari's remark and his fruitful formulation of the mentioned Schröder–König's family of iterative methods considered in a determinantal form in [5], have motivated us to give a determinantal representation of a powerful family of iterative methods for the simultaneous determination of polynomial zeros derived by Sakurai, Torii and Sugiura in [6]. This family was constructed by applying $[1/n-1]$-Padé approximant to the rational function

$$P(x)/\prod_{\substack{j=1\\ j\neq i}}^{m}(x-x_j),$$

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where $P(x)$ is a polynomial of degree m having only simple zeros and $x_1, \ldots, x_m$ are approximations to the zeros of P. For short, this family will be referred to as STS-family, after the authors initials.

Why a determinantal representation? Using a determinantal form and possible advantages of the equivalent formula of iteration functions cited above, Kalantari derived a lot of useful and beautiful properties of Schröder–König's family in his book [5]. Similarly to Kalantari's treatment of Schröder–König's family, our determinantal representation of STS-family produces beneficial properties. This affirmative expectation is based on the specific form of the determinant given in this note which implicitly defines STS-methods. Namely, this determinant is associated to a matrix which possesses the following characteristics:

(i) its descending diagonal form left to right is constant (property of a Toeplitz matrix);
(ii) all entries of a matrix above the first superdiagonal entries are equal to 0 (property of a lower Hessenberg matrix).

Specific properties of the mentioned matrices can lead to interesting relations if STS-family is represented in the determinantal form.

In this note we show that STS-family [6], derived by using Padé approximation, has a suitable determinantal representation which directly arises from Schröder–König's family. Therefore, one can expect that some advantages of Kalantari's study of Schröder–König's family in the determinantal form could also be valid for the determinantal representation of STS-family. Another convenient property is an easy generation of particular members of STS-family starting from the associated determinant.

In this note we use the notion of Padé approximation so that, for the readers' convenience, we first give the following definition.

Definition 1. Let $F(x)$ and $G(x)$ be mutually prime polynomials of degree at most M and N, respectively, and let $G(x_0) \neq 0$. Assume that Taylor series of an analytic function $f(z)$ at the point x_0 is given by

$$f(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \cdots .$$

If the rational function $R_{M,N}(x) = F(x)/G(x)$ satisfies

$$f(x)G(x) - F(x) = O\Big(\big(x - x_0\big)^{M+N+1}\Big),$$

then the rational function $R_{M,N}(x)$ is called $[M/N]$-Padé approximant for $f(x)$ at the point x_0.

Let P be a monic polynomial of degree m with simple zeros $\alpha_1, \ldots, \alpha_m$ and let $x_1, \ldots, x_m$ be reasonably close approximations to these zeros. The following rational function is of considerable importance in the construction of simultaneous methods

$$W_i(x) := \frac{P(x)}{\Pi_i(x)}, \quad \text{where } \Pi_i(x) = \prod_{\substack{j=1 \\ j\neq i}}^{m} (x - x_j), \quad (i \in \mathcal{I}_m), \tag{1}$$

see, e.g., [7,8]. We use the abbreviation $\mathcal{I}_m = \{1, \ldots, m\}$ to denote the index set.

Using the $[1/n-1]$ Padé approximant for the function $W_i(x)$ at the point x_i, Sakurai, Torii and Sugiura have derived in [6] the following family of simultaneous methods:

$$\left\{\begin{array}{l} \textbf{STS Algorithm } (\textit{Simultaneous formula by the Padé approximation – STS-family}). \\ \quad \textbf{For } k := 1 \textbf{ to } n \textbf{ do} \\ \quad\quad \textit{Step } (1)\ \textbf{Compute} \text{ the numerator } F(x) \text{ of the } [1/n-1] \text{ -Padé approximant} \\ \quad\quad\quad\quad \text{for } W_i(x) \text{ at } x_i. \\ \quad\quad \textit{Step } (2)\ \textbf{Solve} \text{ the linear equation } F(x) = 0 \text{ and } \textbf{set} \text{ this solution} \\ \quad\quad\quad\quad \text{as the next approximation } \hat{x}_i. \end{array}\right. \tag{2}$$

The above algorithm is named after the initials of the authors of [6].

For the sake of simplicity, in what follows we will often write

$$\sum_{j\neq i} a_j \equiv \sum_{\substack{j=1 \\ j\neq i}}^{m} a_j, \quad \text{and} \quad \prod_{j\neq i} b_j \equiv \prod_{\substack{j=1 \\ j\neq i}}^{m} b_j.$$

We also introduce the abbreviations

$$d_\lambda(x) = \frac{P^{(\lambda)}(x)}{P(x)}, \quad S_{\lambda,i}(x) = \sum_{\substack{j=1 \\ j\neq i}}^{m} \frac{1}{(x - x_j)^\lambda}, \quad A_\lambda(x) = \frac{f^{(\lambda)}(x)}{\lambda! f(x)} \quad (\lambda = 1, 2, \ldots),$$

where $(\cdot)^{(\lambda)}$ stands for the λth derivative. For demonstration, we present three methods arising from the STS Algorithm (2) by taking different values of n. For simplicity, in what follows we omit the iteration index and write x_i and $\hat{x}_i$ instead of $x_i^{(k)}$ and $x_i^{(k+1)}$, respectively, where k is the iteration index.

Example 1. For $n = 1$ we have the iterative method

$$\hat{x}_i = x_i - \frac{1}{\frac{P'(x_i)}{P(x_i)} - \sum_{j\neq i} \frac{1}{x_i - x_j}} \quad (i \in \mathcal{I}_m).$$

This is the well-known Ehrlich's method of third order [9].

Example 2. Let $n = 2$, then we have the fourth order iterative method, see [6]

$$\hat{x}_i = x_i - \frac{2\big[d_1(x_i) - S_{1,i}(x_i)\big]}{d_1(x_i)^2 - d_2(x_i) - S_{2,i}(x_i) + \big(d_1(x_i) - S_{1,i}(x_i)\big)^2} \quad (i \in \mathcal{I}_m).$$

This method can be obtained as a special cases from the fourth-order family presented in [10].

Example 3. To save space, we will suppress the dependency on x_i and write only d_λ and $S_{\lambda,i}$. For $n = 3$ one obtains the fifth order simultaneous method

$$\hat{x}_i = x_i - \frac{3\left(d_1^2 - d_2 - S_{2,i} + (d_1 - S_{1,i})^2\right)}{2\, d_1^3 - 3(d_1 - S_{1,i})\left(d_2 - d_1^2 + S_{2,i}\right) - 3\, d_1 d_2 + (d_1 - S_{1,i})^3 + d_3 - S_{3,i}} \quad (i \in \mathcal{I}_m).$$

Remark 1. The choice of initial approximations of polynomial zeros and the determination of their multiplicities, very important tasks in the implementation of polynomial root-finders, was considered in detail in the book [11] and the dissertation [12], as well as in the references cited there. A lot of results on geometry of polynomial zeros can be found in [13]. The choice of initial approximations that guarantees convergence of most frequently used simultaneous methods was considered in the book [11] and the recent results of Proinov and his coauthors in [14–16]. For further study, see also the papers [17–19]. Finally, a number of numerical examples, without and with corrections, were tested in many papers applying the methods presented in Examples 1–3. Because of the existence of vast results in the mentioned areas, we will not consider these tasks in this paper.

Remark 2. Let f be an analytic function with a simple zero α. In 1953 Householder [20] constructed the family of iterative methods

$$\hat{x}_i = \mathcal{K}_n(x_i) := x_i + n\left[\frac{\big(1/f(x)\big)^{(n-1)}}{\big(1/f(x)\big)^{(n)}}\right]_{x=x_i} \quad (n = 1, 2, \ldots) \tag{3}$$

of the order $n + 1$. Taking $f(x) = W_i(x) = P(x)/\Pi_i(x)$ in (3), Sakurai, Torii and Sugiura [6] derived STS Algorithm.

Remark 3. Using Lemma 5 stated in [6] regarding to the $[1/n - 1]$-Padé approximant for $W_i(x)$, it was proved in [6] that the order of convergence of the simultaneous method defined by STS Algorithm is $n + 2$.

Same as before, let f be an analytic function having a simple zero α. In 1946 Hamilton [21] derived the family of root-finding methods which can be represented in the form

$$\hat{x}_i = \mathcal{H}_n(x_i) := x_i - \frac{\delta_{n-1}[f; x_i]}{\delta_n[f; x_i]} \quad (n \geq 1), \tag{4}$$

where $\delta_n[f; x_i]$ is the functional determinant of order n defined by

$$\delta_0(x) = \delta_0[f; x] = 1,$$
$$\delta_n(x) = \delta_n[f; x] = \begin{vmatrix} A_1(x) & 1 & 0 & \cdots & 0 \\ A_2(x) & A_1(x) & 1 & \cdots & 0 \\ A_3(x) & A_2(x) & A_1(x) & \cdots & 0 \\ \vdots & & & & \\ A_n(x) & A_{n-1}(x) & A_{n-2}(x) & \ldots & A_1(x) \end{vmatrix}. \tag{5}$$

The determinantal representation was suggested by E. T. Whittacker, see [20, p. 24]. The convergence order of the iterative method (4) is $n + 1$ assuming that the zero α of f is simple.

2. Determinantal representation of STS Algorithm

In this paper we focus on to the determinantal representation of STS Algorithm. It is easy to observe that the polynomial $P(x)$ and the rational function $W_i(x)$ given by (1) have the same zeros. This means that we can substitute $f(x) \equiv P(x)$ with $W_i(x)$

in (4). Then the coefficients A_λ, appearing in the determinant $\delta_n[f; x]$ given by (5), can be replaced by their corresponding functional coefficients

$$B_{\lambda,i}(x) = \frac{W_i^{(\lambda)}(x)}{\lambda! W_i(x)} \quad (\lambda = 0, 1, 2, \ldots). \tag{6}$$

In this way we obtain the functional determinant:

$$\begin{aligned} \Delta_{0,i}(x) &= \Delta_{0,i}[P; x] = 1, \\ \Delta_{n,i}(x) &= \Delta_{n,i}[P; x] = \begin{vmatrix} B_{1,i}(x) & 1 & 0 & \cdots & 0 \\ B_{2,i}(x) & B_{1,i}(x) & 1 & \cdots & 0 \\ B_{3,i}(x) & B_{2,i}(x) & B_{1,i}(x) & \cdots & 0 \\ \vdots & & & & \\ B_{n,i}(x) & B_{n-1,i}(x) & B_{n-2,i}(x) & \ldots & B_{1,i}(x) \end{vmatrix}. \end{aligned} \tag{7}$$

To find all zeros of the polynomial P for each i, we set $x = x_i^{(k)}$ and construct the following family of iterative methods for simultaneous determination of all zeros of the polynomial P:

$$x_i^{(k+1)} = x_i^{(k)} - \frac{\Delta_{n-1,i}\big[P; x_i^{(k)}\big]}{\Delta_{n,i}\big[P; x_i^{(k)}\big]} \quad (n \geq 1,\ i \in \mathcal{I}_m,\ k = 0, 1, \ldots). \tag{8}$$

The determinant $\Delta_{n,i}$ is evaluated at the point x_i using the recurrent relation

$$\Delta_{0,i}(x_i) = 1, \quad \Delta_{n,i} = \sum_{r=1}^{n} (-1)^{r+1} B_{r,i}(x_i) \Delta_{n-r,i}(x_i) \tag{9}$$

which is obtained by expanding the determinant (9) along the first column. The evaluation of the coefficients $B_{r,i}$ is carried out by the recurrent relation (13) given later.

Now we show that the simultaneous methods (8) are equivalent to the simultaneous methods defined by the STS Algorithm (2) for a fixed n. First, let us note that the simultaneous methods (8), represented in the determinantal form, arise from Hamilton's method (4) by substituting $f(x) \equiv P(x)$ by $W_i(x) = P(x)/\Pi_i(x)$, while STS-methods, given by the STS Algorithm, are obtained from Householder's method (3) using the same substitution and $[1/n-1]$-Padé approximation, see Remark 3.

To prove the equivalency of the STS Algorithm (2) and (8), it is necessary and sufficient to prove that Householder's method (3) and Hamilton's method (4) are equivalent. We use the following lemma proved in [22] by induction.

Lemma 1. *The following relation is valid*

$$\left(\frac{1}{f(x)}\right)^{(n)} = \frac{n!\delta_n(x)}{(-1)^n f(x)} \quad (n = 1, 2, \ldots). \tag{10}$$

Using (10) and the iterative formulas (3) and (4), we find

$$\begin{aligned} \mathcal{K}_n(x_i) :&= x_i + n\left[\frac{\big(1/f(x)\big)^{(n-1)}}{\big(1/f(x)\big)^{(n)}}\right]_{x=x_i} = x_i + n\frac{(n-1)!\delta_{n-1}(x_i)}{(-1)^{n-1}f(x_i)} \cdot \frac{(-1)^n f(x_i)}{n!\delta_n(x_i)} \\ &= x_i - \frac{\delta_{n-1}(x_i)}{\delta_n(x_i)} =: \mathcal{H}_n(x_i). \end{aligned}$$

Therefore, Hamilton's family (4) and Householder's family (3) are equivalent.

It is worth noting that the methods (3) and (4) were known to the German mathematician E. Schröder many decades ago in a different but equivalent form, which has been mentioned at the beginning of this note. An extensive study of this method was given in the book *Polynomial Root-Finding and Polynomiography* [5]. Kalantari analyzed Schröder–König's method mainly in the determinantal form, which was one of the main motivations for writing this note, see remarks in Introduction. Therefore, the family (8) can be referred to as the family of simultaneous methods of Schröder–König's type, or shorter, the SK-like family. It is assumed that the priority and the original idea in the construction of STS-methods is attributed to the authors of the STS Algorithm [6].

To implementation of the methods (8) requires the determination of $B_{q,i}(x)$ defined by (6). Let $T(x) = P'(x)/P(x)$. Using the logarithmic derivative we find from (1)

$$B_{1,i}(x) = \frac{W_i'(x)}{W_i(x)} = \frac{P'(x)}{P(x)} - \sum_{j \neq i} \frac{1}{x - x_j} = T(x) - S_{1,i}(x),$$

wherefrom

$$W_i'(x) = W_i(x)\Big(T(x) - S_{1,i}(x)\Big). \tag{11}$$

Applying Leibniz' rule to the derivative of the product of two functions in (11), we find

$$\begin{aligned} W_i^{(q)}(x) &= \sum_{\lambda=0}^{q-1} \binom{q-1}{\lambda} W_i^{(q-\lambda-1)}(x)\Big(T(x) - S_{1,i}(x)\Big)^{(\lambda)} \\ &= \sum_{\lambda=0}^{q-1} \binom{q-1}{\lambda} W_i^{(q-\lambda-1)}(x)\Big(T^{(\lambda)}(x) + (-1)^{\lambda+1}\lambda! S_{\lambda+1,i}(x)\Big), \end{aligned} \tag{12}$$

where $T^{(0)}(x) \equiv T(x)$. By dividing both sides of (12) with $q!W_i(x)$, we obtain after short arrangement

$$B_{0,i}(x) = 1, \quad B_{q,i}(x) = \frac{W_i^{(q)}(x)}{q!W_i(x)} = \frac{1}{q}\sum_{\lambda=0}^{q-1} \frac{B_{q-\lambda-1,i}(x)}{\lambda!}\Big(T^{(\lambda)}(x) + (-1)^{\lambda+1}\lambda! S_{\lambda+1,i}(x)\Big). \tag{13}$$

As emphasized in [6], the order of convergence of the STS-family (2) can be accelerated using a hybrid method. The sums

$$S_{\lambda,i}(x_i) = \sum_{j\neq i} \frac{1}{(x_i - \underline{x}_j)^{\lambda}}, \tag{14}$$

appearing in the family of simultaneous methods (8), use the approximations $x_1, \ldots, x_m$. The accelerated convergence of the family (8) can be achieved by employing in (14) better approximations x_j^* to the zeros instead of just x_j (marked by _) in (14).

Generally speaking, since the family (8) of order $n+2$ deals with polynomial derivatives of order not higher than n, any method $x_j^* = \Phi(P, P', \ldots, P^{(r)}; x_j)$ of order $r+1$ $(r \le n)$ (that is, $|x_j^* - \alpha| = O(|x_j - \alpha|^{r+1})$) for finding a simple zero can be used instead of the approximation x_j without a loss of computational efficiency.

Let us define the SK-family with *corrective approximations* x_j^* by the iterative formula

$$\hat{x}_i = x_i - \frac{\Delta^*_{n-1,i}(x_i)}{\Delta^*_{n,i}(x_i)} \quad (i \in \mathcal{I}_m). \tag{15}$$

The star * in (15) indicates that corrective approximations x_j^* are employed in (14) instead of x_j (marked by _). In the absence of corrections (that is, $x_j^* = x_j$), for convenience we set $r = 0$. Then the following assertion, already proved in [6] for the presented hybrid method, is valid:

Theorem 1. *If initial approximations $x_1^{(0)}, \ldots, x_m^{(0)}$ are sufficiently close to the corresponding simple zeros $\alpha_1, \ldots, \alpha_m$ of the polynomial P, then the order of convergence of the accelerated SK-family (15) is $n+r+2$ $(r \le n)$.*

Example 4. For demonstration, we give a simple example of an accelerated method. Taking Newton's approximations $x_j^* = x_j - P(x_j)/P'(x_j)$ (note that there are no additional polynomial calculations) instead of x_j in the sum of Ehrlich's third order method (see Example 1), we obtain the iterative method

$$\hat{x}_i = x_i - \frac{1}{\frac{P'(x_i)}{P(x_i)} - \sum_{j\neq i} \frac{1}{x_i - x_j + P(x_j)/P'(x_j)}} \quad (i \in \mathcal{I}_m)$$

of the fourth order. This method is often known in the literature as Nourein's method [23].

3. Computational aspects

In order to implement the STS Algorithm (2), efficient methods for the computation of Padé approximants are needed, see [6] for suitable references. In particular, to obtain the $[1/n-1]$-Padeé approximant for the rational function $W_i(x) = P(x)/\Pi_i(x)$, an efficient method that requires the calculation of the Taylor development of $P(z)$ and $\Pi_i(x)$ at the point x_i up to the required order, was described in [24].

In the implementation of the iterative method (8) the determinants $\Delta_{n-1,i}$ and $\Delta_{n,i}$ are calculated using the recurrent relation (9). This relation needs the values of $B_{q,i}(x)$ given by (6). From (13) we see that the calculation of $B_{q,i}(x)$ requires the λth derivative of $T(x) = P'(x)/P(x)$, which is not a trivial task for a large λ. To resolve this task we apply Leibniz' rule for the product of the functions $P'(x)$ and $1/P(x)$:

$$T^{(\lambda)}(x) = \sum_{r=0}^{\lambda} \binom{\lambda}{r} \Big(P(x)\Big)^{(\lambda-r+1)} \left(\frac{1}{P(x)}\right)^{(r)}. \tag{16}$$

The problem of finding $T^{(\lambda)}(x)$ is now reduced to the evaluation of the rth derivative $\left(\frac{1}{P(x)}\right)^{(r)}$. To find the derivatives of higher order of reciprocal $1/P(x)$, we use the result stated by R. A. Leslie [25].

Let $\mathcal{D}^r f$ represent the rth derivative of the function $f(x)$ with $\mathcal{D}^0 f \equiv f$ and $Df \equiv f'$. Suppressing the independent variable x, Leslie [25] derived the following matrix relation that involves the derivatives of P and $1/P$:

$$\begin{bmatrix} P & 0 & 0 & 0 & \cdots & 0 \\ \mathcal{D}P & P & 0 & 0 & & 0 \\ \mathcal{D}^2 P & 2\mathcal{D}P & P & 0 & & 0 \\ \mathcal{D}^3 P & 3\mathcal{D}^2 P & 3\mathcal{D}P & P & & 0 \\ \vdots & & & & & \\ \mathcal{D}^r P & \binom{r}{1}\mathcal{D}^{r-1}P & \binom{r}{2}\mathcal{D}^{r-2}P & \binom{r}{3}\mathcal{D}^{r-3}P & \cdots & P \end{bmatrix} \begin{bmatrix} 1/P \\ \mathcal{D}[1/P] \\ \mathcal{D}^2[1/P] \\ \mathcal{D}^3[1/P] \\ \vdots \\ \mathcal{D}^r[1/P] \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{17}$$

Note that the coefficients in the first matrix are binomial coefficients of Pascal's triangle. To find $D^r[1/P]$ (the last element in the second matrix), it is necessary to calculate all previous derivatives $\mathcal{D}[1/P],\ \mathcal{D}^2[1/P], \ldots, \mathcal{D}^{r-1}[1/P]$, which means that a successive procedure has to be applied starting with $\mathcal{D}[1/P] = -P'/P^2$. Hence, the system of $r+1$ linear equations in $r+1$ unknowns, represented in the matrix form (17), reduces to the single equation

$$\sum_{\nu=0}^{r} \binom{r}{\nu} \mathcal{D}^{r-\nu}P \cdot \mathcal{D}^{\nu}[1/P] = 0,$$

assuming that the entries $\mathcal{D}[1/P],\ \mathcal{D}^2[1/P], \ldots, \mathcal{D}^{r-1}[1/P]$ are calculated in the previous steps. From the last equation we find

$$\mathcal{D}^r[1/P] = \left(\frac{1}{P}\right)^{(r)} = -\frac{1}{P}\Bigg[\mathcal{D}^r P \cdot \frac{1}{P} + \binom{r}{1}\mathcal{D}^{r-1}P \cdot \mathcal{D}[1/P] + \binom{r}{2}\mathcal{D}^{r-2}P \cdot \mathcal{D}^2[1/P] + \cdots + \binom{r}{r-1}\mathcal{D}P \cdot \mathcal{D}^{r-1}[1/P]\Bigg]. \tag{18}$$

Therefore, any iterative method from the SK-families (8) and (16) is realized by combining the presented relations (18), (16), (13), (9), and (8).

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