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THE LINK BETWEEN SCHRÖDER'S ITERATION METHODS OF THE FIRST AND SECOND KIND[1]

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Abstract. Schröder's methods of the first and second kind for solving a nonlinear equation $f(x) = 0$, originally derived in 1870, are of great importance in the theory and practice of iteration processes. They were rediscovered several times and expressed in different forms during the last 140 years. In this paper we consider the question of possible link between these two families of iteration methods, posed as an open problem by Steven Smale in 1994. We show that the method of the first kind (often called the Schröder-Euler basic sequence) is obtained from the method of the second kind (often called the Schröder-König method)

$$S_r(x) = x - \frac{u(1 + a_1(x)u + \cdots + a_{r-3}(x)u^{r-3})}{1 + b_1(x)u + \cdots + b_{r-2}(x)u^{r-2}}, \quad u = f(x)/f'(x),$$

by the development of the reciprocal of denominator into the power series and constructing a polynomial in u of degree r by neglecting the terms containing the powers of u higher than u^{r-1}.

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1. Introduction

Schröder's remarkable paper [10] (1870) on the solution of nonlinear equations stayed unrecognized for almost a century, until the appearance of Traub's monograph [12], where it was exposed to the wide scientific audience. A further contribution to the recognition of Schröder's results is due to the Stewart's translation of the original paper from 1870, together with his comments [11].

Considering the problem of finding the roots of the equation $f(z) = 0$, where f is analytic about the roots, Schröder distinguishes two kinds of methods with the arbitrary order of convergence. The Schröder's method of the first kind $E_r(x)$ is typified by Newton's method and consists of the successive substitution of iterates in a fixed formula. Schröder's method of the second kind $S_r(x)$ consists essentially of constructing a sequence of functions with the property to converge to a root of the equation, the particular root depending on the choice of z. Although the interpretation of Schröder's methods is today modernized

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through the application of König's theorem, the generality of his approach makes him the rediscoverer of some iterative methods but the discoverer of infinitely many more. Moreover, his method of the first kind (often called the Schröder-Euler basic sequence) is frequently used in the analysis of the convergence order of iterative methods for establishing the order of convergence.

The aim of this paper is to give the answer to an open problem posed by Steven Smale in 1994 (Section 3). Actually, he asked wheather there is a possible connection between Schröders's families of the first and second kind. Surprisingly, this question has not been considered for almost 140 years, although the issue is very natural. In Section 4 we show that the method of the first kind $E_r(x)$ is obtained from the method of the second kind

$$S_r(x) = x - \frac{u(1 + a_1(x)u + \cdots + a_{r-3}(x)u^{r-3})}{1 + b_1(x)u + \cdots + b_{r-2}(x)u^{r-2}}, \quad u = f(x)/f'(x),$$

by the development of the reciprocal of denominator into the power series and constructing a polynomial in u of degree r, omitting the terms that contain the powers of u higher than u^{r-1}.

2. Schröder's methods of the first and second kind

Let us consider a single equation $f(x) = 0$ assuming that f is sufficiently many times differentiable. In his remarkable paper [10] from 1870 (see, also, [11]) Schröder proposed two general methods with arbitrary order of convergence, referred to as the methods of the first and second kind (in Schröder's terminology).

Schröder presented **the method of the first kind** in the form

$$E_r(x) = x + \sum_{\nu=1}^{r-1} (-1)^\nu \frac{f(x)^\nu}{\nu!} (f^{-1})^{(\nu)}(f(x)), \tag{1}$$

where f^{-1} is the inverse of f. The convergence order of the method (1) is r. The following formula is useful for the evaluation of the derivative of f^{-1} :

$$(f^{-1})^{(\nu)}(f(x)) = \frac{Z_\nu}{(f')^{2\nu-1}}, \; Z_{\nu+1} = f' Z'_\nu - (2\nu-1) Z_\nu f'', \; (Z_1 = 1, \; \nu = 1, 2, \ldots),$$

where Z_ν is a polynomial in $f', f'', \ldots, f^{(\nu)}, \; f^{(j)} \equiv f^{(j)}(x)$.

Theorem 1 (Schröder [10]). *Any root-finding algorithm of the order r can be presented in the form*

$$F_r(x) = E_r(x) + f(x)^r \varphi_r(x), \tag{2}$$

where φ_r is a function bounded in α which depends on f and its derivatives.

Let us introduce the abbreviations

$$u(x) = \frac{f(x)}{f'(x)}, \quad C_\nu(x) = \frac{f^{(\nu)}(x)}{\nu! f'(x)} \quad (\nu = 1, 2, \ldots).$$

A convenient technique for generating basic sequences E_r is based on Traub's difference-differential relation (see [12, Lemma 5-3])

$$E_{k+1}(x) = E_k(x) - \frac{u(x)}{k} E'_k(x), \quad E_2(x) = x - u(x), \quad (k \geq 2). \tag{3}$$

According to (3) we obtain the first few E_k (omitting the argument x):

$$\begin{aligned}
E_3 &= E_2 - C_2 u^2, \quad \text{(Chebyshev's method)},\\
E_4 &= E_3 - (2C_2^2 - C_3)u^3,\\
E_5 &= E_4 - (5C_2^3 - 5C_2C_3 + C_4)u^4,\\
E_6 &= E_5 - (14C_2^4 - 21C_2^2C_3 + 6C_2C_4 + 3C_3^2 - C_5)u^5,\\
E_7 &= E_6 - (42C_2^5 - 84C_2^3C_3 + 28C_2^2C_4 + 28C_2C_3^2 - 7C_5C_2 - 7C_3C_4 + C_6)u^6.
\end{aligned}$$

Schröder [10] defined **the method of the second kind** of the order r by the iteration function

$$S_r(x) = x - \frac{A_{r-2}(x)}{A_{r-1}(x)}, \tag{4}$$

where $A_r(x)$ is calculated from the recursive relation

$$A_0(x) = 1/f(x), \quad A_r(x) = \sum_{\nu=1}^{r} (-1)^{\nu-1} \frac{f^{(\nu)}(x)}{\nu! f(x)} A_{r-\nu}(x) \quad (r = 1, 2, \ldots). \tag{5}$$

Schröder derived the iteration formulas (4) and (5) using suitable development to partial fractions and restricting himself to a rational function whose roots are sought. Today the natural approach to Schröder's method (4) would be through König's theorem [7], so that some authors call (4) the Schröder-König method.

Remark 1. Hamilton [3] (1946) and later Wang [13] (1966) showed that the function $A_r(x)$ can be evaluated by the functional determinant

$$A_r(x) = \frac{1}{f(x)} \det \begin{pmatrix} B_1 & B_2 & B_3 & \ldots & B_r \\ 1 & B_1 & B_2 & \ldots & B_{r-1} \\ 0 & 1 & B_1 & \ldots & B_{r-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & B_1 \end{pmatrix},$$

where $B_k(x) = f^{(k)}(x)/(k! f(x))$. Actually, both authors rediscovered the Schröder method of the second kind and expressed it by the functional determinants.

Using the abbreviation C_ν $(\nu = 1, 2, \ldots)$ introduced above, let us define

$$P_0(x) = 1, \quad P_r(x) = \det \begin{pmatrix} 1 & C_2 & C_3 & \ldots & C_r \\ u & 1 & C_2 & \ldots & C_{r-1} \\ 0 & u & 1 & \ldots & C_{r-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}.$$

Considering the last two determinants, it is easy to see that

$$P_r(x) = f(x)u(x)^r A_r(x). \tag{6}$$

Taking into account (6) we observe that the Schröder method of the second kind (4) can be presented in the form

$$S_r(x) = x - u(x)\frac{P_{r-2}(x)}{P_{r-1}(x)}, \quad (r \geq 2). \tag{7}$$

According to (5) and (6) we conclude that the following recursive relation is valid

$$P_r(x) = \sum_{\nu=1}^{r}(-1)^{\nu+1}u(x)^{\nu-1}C_\nu(x)P_{r-\nu}(x), \quad C_1(x) = 1, \quad (r \geq 1). \tag{8}$$

This relation, together with (7), is convenient to generate an array of iteration methods. For example, suppressing the argument of functions for brevity, we obtain for $r = 2, \ldots, 7$:

Newton's method of the order 2:

$$S_2 = x - u;$$

Halley's method [2] *of the order* 3:

$$S_3 = x - \frac{u}{1 - C_2 u};$$

Kiss' method [8] *of the order* 4:

$$S_4 = x - \frac{u(1 - C_2 u)}{1 - 2C_2 u + C_3 u^2};$$

Kiss' method [8] *of the order* 5:

$$S_5 = x - \frac{u(1 - 2C_2 u + C_3 u^2)}{1 - 3C_2 u + (2C_3 + C_2^2)u^2 - C_4 u^3};$$

Method of the order 6:

$$S_6 = x - \frac{u\big[1 - 3C_2 u + (2C_3 + C_2^2)u^2 - C_4 u^3\big]}{1 - 4C_2 u + (3C_2^2 + 3C_3)u^2 - (2C_2C_3 + 2C_4)u^3 + C_5 u^4};$$

Method of the order 7:

$$S_7 = x - \big(u\big[1 - 4C_2 u + (3C_2^2 + 3C_3)u^2 - (2C_2C_3 + 2C_4)u^3 + C_5 u^4\big]\big) \,/\, \big(1 - 5C_2 u + (6C_2^2 + 4C_3)u^2 - (C_2^3 + 6C_2C_3 + 3C_4)u^3 + (C_3^2 + 2C_2C_4 + 2C_5)u^4 - C_6 u^5\big)$$

and so on. Let us note that the methods S_4 and S_5, often attributed to Kiss [8], can be found in Schröder's paper [10].

3. Smale's conjecture

From the paper [5] we have learned that Steve Smale posed a question of finding possible link between Schröder's methods of the first kind (given by (1)) and second kind (given by (7)). Investigating this problem by experimentation, we came to the conjecture which can be expressed in the following symbolic form:

Conjecture 1. $x - u * P_{r-2}(u) * \texttt{truncation}_{r-1}\Big[\texttt{Series}[1/P_{r-1}(u), \{u, 0, r - 2\}]\Big] = E_r.$

Here $*$ denotes the multiplication, `Series` executes the development into the power series at the point $u = 0$ taking $r - 1$ members (including the constant term 1), and $\texttt{truncation}_{r-1}$ means that the terms in the bracket containing the powers of u higher than $r - 1$ should be neglected.

We have started to investigate this conjecture using symbolic computation in the programming package *Mathematica* 6 in three steps:

1° We note that the denominator $P_{r-1}(x)$ in (7) is a polynomial in u of degree $r - 2$,

$$P_{r-1}(x; u) = 1 - \psi_1 u + \psi_2 u^2 + \cdots + (-1)^{r-2}\psi_{r-2}u^{r-2},$$

where $\psi_{r-2} = C_{r-1}$ and ψ_k depends of $C_2, \ldots, C_{k+1}$ $(k = 1, \ldots, r-3)$. Developing the function $G(x; u) = 1/P_{r-1}(x; u)$ into the power series (about the point $u = 0$) and taking $r - 1$ members (including the first term 1), we obtain

$$G(x; u) = 1 + \lambda_1 u + \lambda_2 u^2 + \cdots + \lambda_{r-1}u^{r-2} + O(u^{r-1}),$$

where $\lambda_k = \lambda_k(C_2, \ldots, C_{k+1})$.

2° We multiply

$$uP_{r-2}(x; u)G(x; u) = Q_r(x; u)$$

and neglect (in $Q_r(x; u)$) the terms containing the powers of u higher than $r - 1$ to obtain the truncated $\widetilde{Q}_r(x; u) = \sum_{k=1}^{r-1} h_k(x)u^k$.

3° Since the Schröder method of the first kind is of the form $E_r(x; u) = x - \sum_{k=1}^{r-1} Y_k(x)u^k$, where $Y_1 = 1$ and Y_k depends of $C_2, \ldots, C_k$ $(k \geq 2)$ (see Traub [12, p. 83]), we check the identity

$$\widetilde{Q}_r(x; u) = \sum_{k=1}^{r-1} h_k(x)u^k = \sum_{k=1}^{r-1} Y_k(x)u^k = E_r(x; u) \tag{9}$$

by comparing the corresponding functional coefficients h_k and Y_k.

We performed the above procedure and found that the identity (9) holds true for $r = 3, 4, \ldots, 13$. For example, taking $r = 6$ we find by (8)

$$\begin{aligned} P_4(x; u) &= 1 - 3C_2u + (C_2^2 + 2C_3)u^2 - C_4u^3, \\ P_5(x; u) &= 1 - 4C_2u + (3C_2^2 + 3C_3)u^2 - (2C_2C_3 + 2C_4)u^3 + C_5u^4. \end{aligned}$$

In the programming package *Mathematica* 6 we obtain:

Step **1°**

$$\begin{aligned} G(x;u) &= \texttt{Series}\big[1/P_5(u),\{u,0,4\}\big] \\ &= 1+4C_2u+(13C_2^2-3C_3)u^2+(40C_2^3-22C_2C_3+2C_4)u^3 \\ &\quad +(121C_2^4-110C_2^2C_3+9C_3^2+16C_2C_4-C_5)u^4+O(u^5) \end{aligned}$$

Step **2°**

$$\begin{aligned} \tilde{Q}_6(x;u) &= \texttt{truncation}_5\big[uP_4(x;u)G(x;u)\big] \\ &= u+C_2u^2+(2C_2^2-C_3)u^3+(5C_2^3-5C_2C_3+C_4)u^4 \\ &\quad +(14C_2^4-21C_2^2C_3+3C_3^2+6C_2C_4-C_5)u^5 \end{aligned}$$

Step **3°**

We check the validity of the equality $\tilde{Q}_6(x;u)=E_6(x;u)$ and conclude that it holds.

Theoretically, it is possible to verify the validity of Conjecture 1 for any specific r. However, in practice, the exponentially growing complexity of the checking procedure for large r kept us to work with relatively small r. For this reason we were forced to search for a theoretical proof.

4. The proof of the conjecture

Let

$$x_{k+1}=g_r(x_k)\quad (k=0,1,\dots) \tag{10}$$

define an iteration method of the order r for finding a simple zero α of a given function f (sufficiently many times differentiable), that is,

$$g_r(x_k)-\alpha=O((x_k-\alpha)^r)=O(\varepsilon_k^r), \tag{11}$$

where we put $\varepsilon_k=x_k-\alpha$. According to Theorem 2.2 of Traub [12, p. 20], then

$$g_r(\alpha)=\alpha,\quad g_r'(\alpha)=\cdots=g_r^{(r-1)}(\alpha)=0,\quad g_r^{(r)}(\alpha)\neq 0. \tag{12}$$

Using the relations (12), we find by Taylor's series

$$g_r(x_k)=\alpha+\frac{1}{r!}g_r^{(r)}(\alpha)\varepsilon_k^r+O(\varepsilon_k^{r+1}), \tag{13}$$

$$g_r'(x_k)=\frac{1}{(r-1)!}g_r^{(r)}(\alpha)\varepsilon_k^{r-1}+O(\varepsilon_k^r). \tag{14}$$

By (11), (13) and (14) we obtain

$$\begin{aligned} \frac{1}{r}g_r'(x_k)(x_k-g_r(x_k)) &= \frac{1}{r}g_r'(x_k)(x_k-\alpha-(g_r(x_k)-\alpha)) \\ &= \frac{1}{r!}g_r^{(r)}(\alpha)\varepsilon_k^r-\frac{1}{r!}g_r^{(r)}(\alpha)\varepsilon_k^{2r-1}+O(\varepsilon_k^{r+1}), \end{aligned}$$

wherefrom

$$\frac{1}{r}g_r'(x_k)(x_k - g_r(x_k)) = \frac{1}{r!}g_r^{(r)}(\alpha)\varepsilon_k^r + O(\varepsilon_k^{r+1}). \tag{15}$$

Combining (13) and (15), we get

$$g_r(x_k) - \frac{1}{r}g_r'(x_k)(x_k - g_r(x_k)) = \alpha + O(\varepsilon_k^{r+1}). \tag{16}$$

The relation (16) suggests the following iteration method

$$x_{k+1} = F_{r+1}(x_k) := g_r(x_k) - \frac{1}{r}g_r'(x_k)(x_k - g_r(x_k)). \tag{17}$$

According to the relation (16), it follows immediately that the order of convergence of the iteration method (17) is $r+1$. Let us note that the iteration method (17) was previously derived in [4] and [1].

By virtue of Theorem 1, we have

$$F_{r+1}(x) = E_{r+1}(x) + f(x)^{r+1}\varphi_{r+1}(x). \tag{18}$$

Taking $g_2(x) = E_2(x) = x - u(x)$ and neglecting the term of higher order $f(x)^{r+1}\varphi_{r+1}(x)$ in (18), we conclude that the iteration formula (17) generates the same sequence of iteration methods as the Schröder family of the first kind (1). Regarding (18) we have particular cases

$$\varphi_3(x) = 0, \quad \varphi_4(x) = \frac{f(x)f''(x)f'''(x)}{12f'(x)^3} - \frac{f(x)f''(x)^3}{4f'(x)^4}, \quad \text{etc.}$$

The expressions of φ_r for $r \geq 5$ are very complicated. For this reason and having in mind that the iteration formula (17) produces not only the basic sequence but also unnecessary "parasite" terms (members of higher order), it is clear that the Schröder method of the first kind (1) is considerably simpler and thus preferable in theory and practice in comparison to the method (17).

Substituting $g_r(x_k) = x_{k+1}$ in the second term of (17) and solving the equation

$$x_{k+1} = g_r(x_k) - \frac{1}{r}g_r'(x_k)(x_k - x_{k+1})$$

in x_{k+1}, the following iteration method was derived in [4]:

$$x_{k+1} = x_k - \frac{x_k - g_r(x_k)}{1 - \dfrac{1}{r}g_r'(x_k)}. \tag{19}$$

This method also has the order $r+1$, see [4]. The methods (17) and (19) were referred in [4] and [1] as the methods for accelerating convergence. Indeed, if g_r is the method of the order r, then the methods (17) and (19) are of the order $r+1$.

Theorem 2.

$$S_r(x) = x - \frac{A_{r-2}(x)}{A_{r-1}(x)} = x - u(x)\frac{P_{r-2}(x)}{P_{r-1}(x)} \equiv x - \frac{x - g_{r-1}(x)}{1 - \dfrac{1}{r}g'_{r-1}(x)}. \tag{20}$$

The proof follows from the proof of equivalence of the iteration method (19) and Wang's method [13], given in [9]. On the other hand, Wang's method is actually rediscovered Schröder's method of the second kind (4) (or (7)) (see Remark 1).

According to Theorem 2, searching for a link between the Schröder methods of the first and second kind, it is sufficient to consider the connection between the iteration formulas (17) and (19) (or (20)). In our analysis we assume that x_k is sufficiently close to the zero α, meaning that $|\varepsilon_k| = |x_k - \alpha|$ is sufficiently small. According to (14) we conclude that $|g'_r(x_k)| = O(|\varepsilon_k^{r-1}|)$ is also a very small quantity, so that we can apply the approximation

$$\frac{1}{1 - \dfrac{1}{r}g'_r(x_k)} \approx 1 + \frac{1}{r}g'_r(x_k)$$

in (19). In this way we obtain the iteration formula (17). Furthermore, neglecting the higher order member $f(x)^{r+1}\varphi_{r+1}(x)$ in (17) (compare with (18)), we obtain the Schröder method of the first kind $E_{r+1}(x)$. Therefore, we have confirmed Conjecture 1:

The method of the first kind (1) *is obtained from the method of the second kind* (20) *by the development of the reciprocal of the denominator of* (20) *into the power series and constructing a polynomial in u of degree $r-1$ by neglecting the terms containing the powers of u higher than u^{r-1} (or f^{r-1}, according to* (18)).

In fact, the construction of E_r (given by (1)) from S_r (given by (7) or (20)) is performed using the steps **1°**–**3°** presented above.

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