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Self-similar power transforms in extrapolation problems

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A method is suggested allowing for the improvement of accuracy of self-similar factor and root approximants, constructed from asymptotic series. The method is based on performing a power transforms of the given asymptotic series, with the power of this transformation being a control function. The latter is defined by a fixed-point condition, which improves the convergence of the sequence of the resulting approximants. The method makes it possible to extrapolate the behaviour of a function, given as an expansion over a small variable, to the region of the large values of this variable. Several examples illustrate the effectiveness of the method.

KEY WORDS: power series, resummation and renormalization methods, extrapolation methods, self-similar approximants, computational methods

AMS subject classification: 40A05, 40A25, 40A30, 40G99, 40H05, 41A05

1. Introduction

In the majority of realistic computational problems, the sought function, satisfying a very complicated set of equations, cannot be defined for the whole range of its variable, but can be found only for asymptotically small values of this variable. At the same time, the most interesting could be the behaviour of the function at very large values of the variable. This is the standard situation in extrapolation problems, repeatedly appearing in various applications.

Suppose we are looking for a real function $f(x)$ of a real variable $x \in [0, \infty)$. By means of perturbation theory or an iterative procedure, we can find the behaviour of this function at asymptotically small $x \to 0$. But what of the most practical interest in many cases is the behaviour of $f(x)$ at very large x, say

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as $x \to \infty$. It is this the most difficult extrapolation problem that we address in the present paper: How, knowing the behaviour of $f(x)$ only at $x \to 0$, to define the value $f(\infty)$ for $x \to \infty$.

There exist several extrapolation methods, among which the most known are the Padé summation [1], Borel and Padé-Borel summations [2], and the optimized perturbation theory [3]. The latter was, first, advanced in [3] and nowadays is widely employed for various applications, as can be inferred from the review works [4, 5]. Another extrapolation method is based on the self-similar approximation theory [6–11]. Using the techniques of this theory, supplemented by the fractal transforms [12, 13], we have recently derived a novel types of approximants allowing for an effective summation of power series and, hence, for their extrapolation. These are the self-similar exponential approximants [14, 15], self-similar root approximants [16–18], and self-similar factor approximants [19, 20]. The exponential approximants are appropriate for extrapolating functions corresponding to exponentially varying processes, while the root and factor approximants suit well for extrapolating functions with power-law behaviour. The self-similar approximants were shown to be simpler and more accurate than the Padé approximants [16–20].

In the present paper, we aim at improving further the accuracy of the factor and root approximants by introducing a control function through a power transform of the initial asymptotic series. The new technique is illustrated by several examples of extrapolation from $f(x)$ at $x \to 0$ to $f(\infty)$.

2. Self-similar summation of power transforms

Assume that the behaviour of the sought function $f(x)$ is known only for asymptotically small $x \to 0$, when the function can be represented as an expansion in powers of x, being approximated by the series

$$f_k(x) = \sum_{n=0}^{k} a_n x^n , \tag{1}$$

where $k = 0, 1, 2, \ldots$ Without the loss of generality, we may consider such expansions for which $a_0 = 1$, so that $f(0) = 1$. Really, in the case when

$$f(x) \simeq f_0(x) \left(1 + a_1 x + a_2 x^2 + \cdots\right),$$

with a nontrivial $f_0(x)$, not expandable in a power series, we may always define

$$\overline{f}(x) \equiv \frac{f(x)}{f_0(x)},$$

after which the series for $\overline{f}(x)$ acquire the form (1), where $a_0 = 1$. Our aim is, being based on the behaviour of $f(x)$ at $x \to 0$, where it is approximated by the series (1), to find $f(\infty)$ at $x \to \infty$.

The novel trick, we advocate in this paper, is to introduce a control function $m = m_k(x)$ by means of the *power transform*

$$P_k(x, m) \equiv f_k^m(x). \tag{2}$$

Taking the power m of series (1), we reexpand the result in x obtaining

$$P_k(x, m) = \sum_{n=0}^{k} b_n(m) x^n \tag{3}$$

with $b_n(m)$ defined through a_n. A particular case of transform (2) is an inverted series with $m = -1$, which we have considered earlier. However, fixing the power m is not the best choice and here we shall advance a more general and rigorous way of selecting m. Expansion (3) serves as a basis for constructing in the standard ways [12–20] the self-similar factor and root approximants. Even-order factor approximants [19, 20] are defined as

$$F_{2k}(x, m) = \prod_{i=1}^{k} (1 + A_i x)^{n_i} \tag{4}$$

and odd factor approximants can be represented as

$$F_{2k+1}(x, m) = 1 + b_1 x \prod_{i=1}^{k} (1 + A_i x)^{n_i} \tag{5}$$

with the parameters $A_i = A_i(m)$ and $n_i = n_i(m)$ defined by the accuracy-through-order procedure with respect to series (3). This means that equations (4) or (5) are to be expanded in powers of x, and these expansions have to be compared with equation (3), equating the terms of like orders.

For the root approximants [16–18], we have

$$R_{2k}(x, m) = \left(\left(\dots (1 + A_1 x)^{n_1} + A_2 x^2 \right)^{n_2} + \dots + A_k x^k \right)^{n_k} \tag{6}$$

in even orders, and

$$R_{2k+1}(x, m) = 1 + b_1 x \left(\left(\dots (1 + A_1 x)^{n_1} + A_2 x^2 \right)^{n_2} + \dots + A_k x^k \right)^{n_k} \tag{7}$$

in odd orders. The parameters $A_i = A_i(m)$ and $n_i = n_i(m)$ could be defined in two ways. If the behaviour $f(x)$ at $x \to \infty$ would be known, this could be used for uniquely defining all parameters [4]. Another way is to determine these parameters by means of the accuracy-through-order procedure. The second way may yield multiple solutions, which, however, are usually close to each other [21]. In what follows, we shall present only the most accurate approximant. The advantage of the root approximants is their ability to catch rather complicated asymptotic behaviour at large x, including corrections to the main scaling.

Defining the parameters $A_i(m)$ and $n_i(m)$ by the accuracy-through-order procedure, we assume that the limit $f(\infty)$ exists and finite, which imposes an additional constraint on the sum $\sum_{i=1}^{k} n_i$.

After constructing a factor approximant $F_k(x, m)$ or a root approximant $R_k(x, m)$ for the power transform (3), we have to accomplish the transformation inverse to equation (2), thus, obtaining either

$$f_k(x, m) \equiv [F_k(x, m)]^{1/m} \tag{8}$$

or

$$r_k(x, m) \equiv [R_k(x, m)]^{1/m} . \tag{9}$$

The improvement of the accuracy, as compared to the factor and root approximants not involving the power transformation (2), is achieved by defining a control function $m{=}m_k(x)$ from a fixed-point condition. In general, there exist several types of such fixed-point conditions, which, actually, are equivalent to each other [4]. Here we use the simplest of them, the minimal sensitivity condition, which gives either

$$\frac{\partial}{\partial m} f_k(x, m) = 0, \quad m = m_k(x) \tag{10}$$

or

$$\frac{\partial}{\partial m} r_k(x, m) = 0, \quad m = m_k(x), \tag{11}$$

depending on whether the factor approximant (8) or root approximant (9) is considered. With the so defined control function $m_k(x)$, we get either

$$f_k^*(x) \equiv f_k(x, m_k(x)) \tag{12}$$

or

$$r_k^*(x) \equiv r_k(x, m_k(x)). \tag{13}$$

From here, keeping in mind our main aim to extrapolate the sought function to the limit $x \to \infty$, we obtain either

$$f_k^*(\infty) = \lim_{x\to\infty} f_k^*(x) \tag{14}$$

or

$$r_k^*(\infty) = \lim_{x\to\infty} r_k^*(x). \tag{15}$$

Below, we shall illustrate the method by several examples, confronting the found approximants $f_k^*(\infty)$ and $r_k^*(\infty)$ with known values of $f(\infty)$. Note that for defining the limits (14) or (15), we, actually, do not need to have the whole function $m_k(x)$, but what we need to have is just a limiting value $m_k = m_k(\infty)$, which is a constant.

3. Stirling series for factorial function

Let us consider the factorial function

$$f(x) = \frac{1}{\sqrt{2\pi}}\, e^{1/x} x^{1/x} \Gamma\left(1 + \frac{1}{x}\right),$$

where $\Gamma(\cdot)$ is a gamma function. As x tends to zero, one has

$$f(x) \simeq \frac{1}{\sqrt{x}} \quad (x \to 0).$$

Therefore, we define the reduced function

$$\overline{f}(x) \equiv \sqrt{x}\; f(x),$$

whose small-x expansion has the form of Equation (1), so that, as $x \to 0$, then

$$\overline{f}(x) \simeq 1 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5.$$

The expansion coefficients are

$$a_1 = \tfrac{1}{12}, \quad a_2 = \tfrac{1}{288}, \quad a_3 = -\tfrac{139}{51840}, \quad a_4 = -\tfrac{571}{2488320}, \quad a_5 = \tfrac{163879}{209018880}.$$

Thence, we shall apply the procedure of section 2 to the function $\overline{f}(x)$, and at the end, we will return to the sought function $f(x) = \overline{f}(x)/\sqrt{x}$, looking for the limit $f(\infty)$. The exact limit for the factorial is

$$f(\infty) = \frac{1}{\sqrt{2\pi}} = 0.398942.$$

Following the method, described in section 2, we find $r_5^*(\infty) = 0.458$, whose error, as compared with the exact $f(\infty)$, is 15%. The factor approximant $f_5^*(\infty) = 0.406$ is much better, with an error of only 2%. Comparing this with the Padé approximants, we should remember that these are not uniquely defined, yielding for each given order a whole table of approximants [1]. One often considers solely the diagonal approximants. For the present example, the diagonal Padé approximant $P_{[2/2]}$ describes [22] the factorial-function limit $f(\infty)$ with an error of 14%. Thus, the factor approximant $f_5^*(\infty) = 0.406$ is the most accurate. It is worth emphasizing that a direct application of the factor-approximation technique, without involving the power transformation (2), would give the limiting value 0.169, which is a very bad approximation. Hence, employing the power transformation is a crucial point in improving the accuracy of the approximants.

4. Debye-Hückel function for strong electrolytes

The function

$$D(x) = \frac{2}{x} - \frac{2}{x^2}\left(1 - e^{-x}\right)$$

arises in the Debye-Hückel theory of strong electrolytes [23]. At small $x \to 0$, this function possesses an expansion of the type (1), with

$$a_1 = -\tfrac{1}{3}, \quad a_2 = \tfrac{1}{12}, \quad a_3 = -\tfrac{1}{60}, \quad a_4 = \tfrac{1}{360}, \quad a_5 = -\tfrac{1}{2520}.$$

We shall be interested in finding the limiting value $f(\infty)$ of the reduced function

$$f(x) \equiv x D(x) \ ,$$

whose exact limit is $f(\infty) = 2$.

Using the technique of section 2, we get for the best root approximant $r_5^*(\infty) = 1.993$, whose error is -0.4%. For the uniquely defined factor approximant, we find $f_5^*(\infty)$=1.779, with an error of -11%. Note that without invoking the power transform, there are no real solutions for the sought limit. Thus, the usage of the power transformation (2) is principal here. The best Padé approximant, employing the same coefficients a_n, gives the limit $f(\infty)$ with an error of -33%.

5. Critical temperature of Bose gas

Bose-Einstein condensation in dilute Bose gas has attracted much attention in recent years (see reviews [24–27]). One of the interesting problems, which has been intensively studied, is the influence of atomic interactions on the shift of the critical temperature. One considers the relative variation of the critical temperature

$$\frac{\Delta T_c}{T_0} \equiv \frac{T_c}{T_0} - 1,$$

due to weak atomic interactions, as compared to the condensation temperature

$$T_0 = \frac{2\pi\hbar^2}{m k_B}\left[\frac{\rho}{\zeta(3/2)}\right]^{2/3}$$

of the ideal homogeneous Bose gas. The lowest term in the expansion of the critical-temperature shift with respect to the small gas parameter

$$\gamma \equiv \rho^{1/3} a_s,$$

where ρ is particle density and a_s, scattering length, is commonly represented as

$$\frac{\Delta T_c}{T_c} \simeq c_1 \gamma \quad (\gamma \to 0).$$

The coefficient c_1 has been calculated by a number of various methods. Review of the related literature up to 2004 can be found in [25, 27]. The most accurate are the results for c_1 obtained by means of the Monte Carlo simulations and using the optimized perturbation theory. Less accurate are the results based on a renormalization-group approach [28, 29]. Lattice Monte Carlo simulations by Arnold and Moore [30, 31] give $c_1 = 1.32 \pm 0.02$ and by Kashurnikov et al. [32] and Prokofiev and Svistunov [33], $c_1 = 1.29 \pm 0.05$. Path integral Monte Carlo simulations by Nho and Landau [34] give $c_1 = 1.32 \pm 0.14$. A variant [5] of optimized perturbation theory, employed by Kastening [35–37], yields $c_1 = 1.27 \pm 0.11$, and the optimized perturbation theory used by Kneur et al. [38] and Kneur and Pinto [39], results in $c_1 = 1.30 \pm 0.03$. Here, we shall calculate the coefficient c_1 by means of the technique of section 2.

The coefficient c_1 can be expressed as an asymptotic expansion

$$c_1(g) \simeq a_1 g + a_2 g^2 + a_3 g^3 + a_4 g^4 + a_5 g^5$$

in powers of an effective coupling parameter [36], where

$$a_1 = 0.223286, \quad a_2 = -0.0661032, \quad a_3 = 0.026446,$$

$$a_4 = -0.0129177, \quad a_5 = 0.00729073.$$

This expansion is valid for $g \to 0$. But the sought value of c_1 is given by the limit

$$c_1 = \lim_{g \to \infty} c_1(g).$$

Employing the factor approximants, complimented by the power transformation (2), we have $f_5^*(\infty) = c_1 = 1.09$, which is close to the values found by other methods. Summing the strong-coupling expansion with the help of the root approximants and defining the parameters from the weak-coupling expansion, we get $r_5^*(\infty) = 1.19$.

6. Structure factor of branched polymers

The structure factor of three-dimensional branched polymers is given [40, 41] by the confluent hypergeometric function

$$S(x) = F_1\left(1; \frac{3}{2}; \frac{3}{2}\, x\right).$$

We shall consider the reduced function

$$f(x) \equiv xS(x),$$

whose limit $f(\infty) = 1/3$ is finite. At asymptotically small $x \to 0$, the function $f(x)$ possesses an expansion of the form (1), with $a_0 = 1$. Several other expansion coefficients are

$$a_1 = -1, \quad a_2 = 0.6, \quad a_3 = -0.257, \quad a_4 = 0.086.$$

The best approximant, obtained by the method of Section 2, is $f_5^*(\infty) = 0.329$, whose error is -1.3%. This is much more accurate than the best Padé approximant of the same order having an error of -266%.

7. Discussion

In this paper, we suggested a method for improving the accuracy of self-similar approximants by introducing a control function through the power transformation (2). As is shown by several examples, the accuracy really becomes essentially better.

Here we have concentrated our attention on the extreme extrapolation problem, when from the behaviour of a function $f(x)$ at asymptotically small $x \to 0$ one has to find the limit $f(\infty)$ for $x \to \infty$. This extrapolation problem is one of the most difficult. If we are able to accurately predict the behaviour of a function $f(x)$ at $x \to \infty$, then, as is clear, it is even easier to approximate its behaviour for finite x.

As an illustration of the latter statement, we may consider the expansion factor of a polymer. The properties of polymers are of great importance for a variety of applications [42]. Let us, for example, consider the expansion factor $\alpha(z)$ for a three-dimensional polymer chain with excluded-volume interaction, where z is a dimensionless coupling parameter [43, 44]. From an asymptotic series of the type (1), derived by means of perturbation theory [43], we construct the expansion factor

$$\alpha^*(z) = 1.5286 z^{0.3543} \left[\left(1 + 0.1552 z^{-1}\right)^{-0.0749} + 0.3302 z^{-0.9252} \right]^{0.383}.$$

This is obtained by considering a large-z expansion, resumming it by means of the root approximants, and determining all unknown exponents and amplitudes from the weak-coupling expansion of fourth order. The strong-coupling exponent

$$\nu \equiv \frac{1}{2} + \frac{1}{4} \lim_{z \to \infty} \frac{\ln \alpha(z)}{\ln z}$$

for our approximant $\alpha^*(z)$ is $\nu = 0.5886$, which coincides with the value found numerically [43–45]. That is, the approximant $\alpha^*(z)$ possesses a correct scaling behaviour. It also gives a nontrivial correction to the scaling, with an exponent of -0.9552. The expression $\alpha^*(z)$ is valid for all $z \in [0, \infty)$, differing from the known numerical values [44] by not more than 0.3%.

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