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Note

On the Zeroes of Infinite Series

1. Introduction

In a number of situations it is necessary to find zeroes of an infinite series. An example of such cases is the search for bound states or resonance states of confined quantum systems. Usually, the zeroes are found by truncating the series in such a way to define polynomials of successive degrees. The hope of that method lies in obtaining a succession of approximate roots that is convergent. If convergence is not achieved, the series is truncated to define a polynomial of higher degree and the search must be reinitiated under the same steps.

Another difficulty of the described method is the necessity of determining the domain containing the desired roots.

In this paper, we describe a method for finding one zero, if it exists, of an infinite series. The method is iterative and there is no need to guess the eventual localization of the root. Besides, in some cases, the convergence is assured by convergence theorems of the subjacent theory.

In all examples we applied the algorithm described here, the attained root was the closest one to zero (excluding the zero itself if a root). To date we cannot prove a formal theorem, guaranteeing this result.

The next section contains a brief discussion of the theory of Padé approximants which is the base for the method described here. In Section 3, we define the algorithm. A table with some numerical examples is presented in the last section.

2. The Padé Approximants

The method presented in this paper is based on the theory of Padé approximants. For the sake of completeness, we outline the points of that theory which are essential to our algorithm. The reader interested in more details is referred to the excellent books listed in the references.

Given the series

$$f(z) = 1 + f_1 z + f_2 z^2 + \cdots \tag{2.1}$$

the associated Padé approximant $[L/M]$ is defined by

$$[L/M] = \frac{p_{0M} + p_{1M} z + p_{2M} z^2 + \cdots + p_{LM} z^L}{1 + q_{1M} z + q_{2M} z^2 + \cdots + q_{MM} z^M} \doteq f(z) + \mathcal{O}(z^{L+M+1}). \tag{2.2}$$

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The choice $q_{0M} = 1$ in (2.2) is the usual "normalization" election. With this normalization, the family of Padé approximants $[L/0]$, $L = 0, 1, 2,\ldots$, coincides with a succession of truncated series.

The Padé approximants are thus quotients of two polynomials (rational functions). The coefficients of these polynomials are uniquely determined by the condition (2.2) which provides the following two sets of algebraic linear equations

$$\begin{aligned} &f_{L-M+1} q_{MM} + f_{L-M+2} q_{M-1M} + \cdots + f_{L+1} = 0 \\ &f_{L-M+2} q_{MM} + f_{L-M+3} q_{M-1M} + \cdots + f_{L+2} = 0 \\ &\vdots \\ &f_L q_{MM} + f_{L+1} q_{M-1M} + \cdots + f_{L+M} = 0 \end{aligned} \tag{2.3}$$

and

$$\begin{aligned} &p_{0M} = 1 \\ &p_{1M} = f_1 + q_{1M} \\ &p_{2M} = f_2 + f_1 q_{1M} + q_{2M},\ldots \end{aligned}$$

or

$$p_{lM} = f_l + f_{l-1} q_{1M} + \cdots + f_{l-n} q_{nM}, \qquad n = \min(L, M), \quad l = 0, 1, 2,\ldots, L. \tag{2.4}$$

The system of M equations (2.3) is known as the q-equations, and the p-equations are the system of $L + 1$ equations (2.4). Notice that the q-equations determine completely the q coefficients in terms of the series coefficients only.

The convergence of this class of approximants is discussed in Refs. [1, 2]. Loosely, the smaller the value $L + M$ the poorer the approximation.

3. The Algorithm

Based on definition (2.2) we can approach the zeroes of $f(z)$ by the roots of the numerator polynomial. Now, as $L + M$ increases we expect that the corresponding Padé approximants "improve." So, we devise a method to approach zeroes of an infinite series through the roots of a polynomial of fixed degree. We maintain the degree L of the polynomial in the numerator and vary the value of M. In this way, i.e., as M increases, more and more coefficients of the series (2.1) will contribute to the solutions for the q coefficients which will transfer more and more information of the series to the roots of the numerator through the p coefficients.

Clearly, we cannot obtain all the zeroes of $f(z)$ since this requires the exact treatment of the series. But we can approach a finite number of them.

Choosing $L = 1$ allows us to define a closed recursive algorithm to obtain one zero of $f(z)$ at the desired accuracy.

Consider the Padé approximant

$$[1/M] = (1 + p_{1M}z)/(1 + q_{1M}z + \cdots + q_{MM}z^M). \tag{3.1}$$

For $f(z_0) = 0$, we have

$$1 + p_{1M}z_0 = 0, \tag{3.2}$$

and hence the approximation of order M

$$z_0^{(M)} = -1/p_{1M}. \tag{3.3}$$

From (2.4) we see that

$$p_{1M} = f_1 + q_{1M}, \tag{3.4}$$

so all we have to do with the q-equations is to obtain the solution for the unknown q_{1M}.

In the following, we list the first three approximations to z_0, namely,

$$z_0^{(1)} = f_1/(f_2 - f_1^2), \tag{3.5}$$

$$z_0^{(2)} = (f_2 - f_1^2)/(f_1^3 - 2f_1f_2 + f_3), \tag{3.6}$$

$$z_0^{(3)} = (f_1^3 - 2f_1f_2 + f_3)/(f_4 - 2f_3f_1 - f_2^2 + 3f_2f_1^2 - f_1^4). \tag{3.7}$$

We can infer an expression for $z_0^{(n)}$ that is at once compact and proper for recursive calculations. To accomplish this subject define the quantities A_n through the recurrence relation

$$A_n = -\sum_{m=1}^{n} f_m A_{n-m}, \qquad n = 1, 2, \ldots, \tag{3.8}$$

with $A_0 = -1$.

In terms of these quantities,

$$z_0^{(n)} = A_n/A_{n+1}, \qquad n = 1, 2, \ldots . \tag{3.9}$$

So, to obtain the approximation of order n, we need $n+1$ coefficients of the original series.

From the relation (3.9),

$$z_0^{(n)} = (A_{n-1}/A_{n+1})/z_0^{(n-1)} \tag{3.10}$$

$$= (f_1/A_{n+1})\bigg/\prod_{m=1}^{n-1} z_0^{(m)}. \tag{3.11}$$

If a previously chosen accuracy is not attained, all we have to do is to calculate the quantity A_{n+2}, which depends only on the coefficients of the series, and apply relation (3.9), (3.10) or (3.11). It is not necessary to find the roots of a new polynomial of higher order. Finally, it is clear that no "initial guess" is necessary.

Rounding error accumulation is well controlled by Eq. (3.9).

4. Some Examples

We applied the method described here to some specific cases. We asked for accuracy to seven significative digits, and, with the help of a TRS80 pocket computer, obtained the results displayed in the following table:

$f(z)$	$z_0^{(n)}$	n
$\cos z$	1.570796	6
$j_0(z)$	3.141593	12
$j_1(z)$	4.493409	14
$M(-0.1, 1, z)$	3.387796	16
$Ai(z)$	−2.338107	25

In the table, $j_0(z)$ and $j_1(z)$ are spherical Bessel functions while M and Ai stand for the confluent hypergeometric function and the Airy function, respectively, as defined in Ref. [3], for example.

Finally, the $z_0^{(n)}$ shown in the table coincide with the more accurate ones up to the displayed figures, according to Ref. [3].

References

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2. G. A. Baker, Jr., and P. Graves-Morres, Padé approximants, *in* "Encyclopedia of Mathematics and its Applications" (G. C. Rota, Ed.), Vols. 13 and 14, Addison–Wesley, Reading, Mass., 1981.
3. M. Abramowitz and I. Stegun, "Handbook of Mathematical Functions," Dover, New York, 1965.

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