NONLINEAR CONVERGENCE ACCELERATION FOR ORTHOGONAL SERIES

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ABSTRACT

Nonlinear convergence acceleration methods are useful tools for the evaluation of slowly convergent sequences and series. Many of these algorithms can also be applied to extrapolation and summation problems. Slowly convergent Fourier and other orthogonal series pose special problems for usual convergence accelerators. These problems are due to the complicated sign pattern of the terms of the series. In the present contribution, a new iterative convergence accelerator for orthogonal series is introduced. It is based on the three-term recurrence relations which are characteristic for orthogonal polynomials. Numerical tests are presented.

1. Introduction

Convergence acceleration methods are currently a rapidly developing field. This is proved by a look at the literature. An excellent recent introduction from a mathematical point of view is the book of Brezinski and Redivo Zaglia [1]. Rational approximation and acceleration methods have been applied to such diverse fields as critical phenomena, strong interactions, atomic physics, molecular integrals and polymer calculations (for references see Ref. [2]). These methods can also be used for the summation of divergent series, as for instance the perturbation series for anharmonic oscillators (compare [3] and references therein.) References to several monographs and review articles which contain more comprehensive descriptions of these methods, and of their application to the computational sciences, can be found in Ref. [2].

Most convergence acceleration methods are based on some space of model sequences. Usually, the methods allow the exact calculation of the limits of these model sequences. Applied to other sequences, the methods give rise to sequence transformations which transform a slowly convergent input sequence into another sequence. The basic expectation is that these transformations are able to accelerate the convergence for those sequences which are well approximated by the model sequence.

In order to apply the known methods, or to develop new ones, it is necessary to classify the type of convergence problems. In the present article, we limit ourselves to convergent series. There are many excellent methods for the convergence acceleration of most power series [1]. However, for complicated sign patterns of the terms, special complications arise. Fourier series and other expansions in orthogonal systems show such patterns. Many methods which

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work for other types of problems cannot cope with these sign patterns. Special methods have to be developed. Some progress was made recently by the author in the case of Fourier series [4], [2]. Convergence acceleration of Fourier series is somewhat easier to handle than that of other orthogonal expansions because the recursion relations of the trigonometric functions are simpler than those of orthogonal polynomials since they involve only constant coefficients. Also, real Fourier series can be rewritten as the real part of some complex power series; for the latter, many usual methods are effective (cf. [1], pp. 282-284, and [2]). In the present contribution, some algorithms are presented that are useful in the case of real orthogonal series. Some test results will be given and discussed.

2. Algorithms

For model sequences of the form

$$s_n = s + \omega_n \left(\exp(\,i\,\omega n) \sum_{j=0}^{k-1} c_j (n+\beta)^{-j} + \exp(-\,i\,\omega n) \sum_{j=0}^{k-1} d_j (n+\beta)^{-j} \right) , \tag{1}$$

with arbitrary constants c_j and d_j, frequency ω, and a shift β of n which in most cases can be set to 1, the following algorithm is exact (cf. Eq. (26) of Ref. [2])

$$\begin{aligned}
\mathcal{N}_n^{(0)} &= (n+\beta)^{-1}\, s_n/\omega_n \,, \qquad \mathcal{D}_n^{(0)} = (n+\beta)^{-1}/\omega_n \,, && \text{(2a)}\\
\mathcal{N}_n^{(k)} &= (n+\beta)\,\mathcal{N}_n^{(k-1)} + (n+2k+\beta)\,\mathcal{N}_{n+2}^{(k-1)} - 2\cos(\omega)\,(n+k+\beta)\,\mathcal{N}_{n+1}^{(k-1)} \,, && \text{(2b)}\\
\mathcal{D}_n^{(k)} &= (n+\beta)\,\mathcal{D}_n^{(k-1)} + (n+2k+\beta)\,\mathcal{D}_{n+2}^{(k-1)} - 2\cos(\omega)\,(n+k+\beta)\,\mathcal{D}_{n+1}^{(k-1)} \,, && \text{(2c)}\\
\mathcal{H}_n^{(k)}(\,\omega,\beta,\{s_n\},\{\omega_n\}) &= \mathcal{N}_n^{(k)}/\mathcal{D}_n^{(k)} \,. && \text{(2d)}
\end{aligned}$$

The s_n represent the partial sums of the Fourier series with remainder estimates $\omega_n \neq 0$.

By iterating the expression for $\mathcal{H}_n^{(1)}(\omega,\beta,\{s_n\},\{\omega_n\})$, one obtains the algorithm (cf. Eq. (28) of Ref. [2])

$$\begin{aligned}
\mathrm{N}_n^{(0)} &= s_n/\omega_n \,, \qquad \mathrm{D}_n^{(0)} = 1/\omega_n \,, && \text{(3a)}\\
\mathrm{N}_n^{(k)} &= (n+\beta)^{\gamma}\left(\mathrm{N}_n^{(k-1)} + \mathrm{N}_{n+2}^{(k-1)} - 2\cos(\omega)\,\mathrm{N}_{n+1}^{(k-1)}\right) \,, && \text{(3b)}\\
\mathrm{D}_n^{(k)} &= (n+\beta)^{\gamma}\left(\mathrm{D}_n^{(k-1)} + \mathrm{D}_{n+2}^{(k-1)} - 2\cos(\omega)\,\mathrm{D}_{n+1}^{(k-1)}\right) \,, && \text{(3c)}\\
\mathrm{I}_n^{(k)}(\omega,\beta,\gamma,\{s_n\},\{\omega_n\}) &= \mathrm{N}_n^{(k)}/\mathrm{D}_n^{(k)} \,. && \text{(3d)}
\end{aligned}$$

Here, $\gamma \geq 0$ is an additional free parameter which can be set equal to two in most applications. This algorithm can be generalized for expansions in orthogonal polynomials $P_n(x)$ with partial sums of the form

$$s_n = \sum_{j=0}^{n} c_j\, P_j(x) \tag{4}$$

as

$$\begin{aligned}
\mathrm{N}_n^{(0)} &= s_n/\omega_n \,, \qquad \mathrm{D}_n^{(0)} = 1/\omega_n \,, && \text{(5a)}\\
\mathrm{N}_n^{(k+1)} &= \left(\gamma_{n+k}^{(0)}\mathrm{N}_n^{(k)} + \gamma_{n+k}^{(1)}\,\mathrm{N}_{n+1}^{(k)} + \gamma_{n+k}^{(2)}\mathrm{N}_{n+2}^{(k)}\right) \Big/ \,\delta_n^{(k)} \,, && \text{(5b)}\\
\mathrm{D}_n^{(k+1)} &= \left(\gamma_{n+k}^{(0)}\mathrm{D}_n^{(k)} + \gamma_{n+k}^{(1)}\,\mathrm{D}_{n+1}^{(k)} + \gamma_{n+k}^{(2)}\mathrm{D}_{n+2}^{(k)}\right) \Big/ \,\delta_n^{(k)} \,, && \text{(5c)}\\
\mathrm{K}_n^{(k)}(\{\delta_n^{(k)}\},\{\gamma_n^{(j)}\},\{s_n\},\{\omega_n\}) &= \mathrm{N}_n^{(k)}/\mathrm{D}_n^{(k)} \,. && \text{(5d)}
\end{aligned}$$

Here, the auxiliary quantities $\delta_n^{(k)} \neq 0$ generalize the factors $(n+\beta)^{-\gamma}$ of the I algorithm. The $\gamma_n^{(j)}$ are the (x dependent) coefficients of the usual three-term recursion of the orthogonal polynomials $P_n(x)$:

$$\gamma_n^{(0)} P_n(x) + \gamma_n^{(1)} P_{n+1}(x) + \gamma_n^{(2)} P_{n+2}(x) = 0 \, . \tag{6}$$

It may be noted that the sequence transformation

$$\mathrm{K}_n^{(1)}(\{\delta_n^{(k)}\}, \{\gamma_n^{(j)}\}, \{s_n\}, \{\omega_n\}) = \frac{\gamma_n^{(0)} s_n/\omega_n + \gamma_n^{(1)} s_{n+1}/\omega_{n+1} + \gamma_n^{(2)} s_{n+2}/\omega_{n+2}}{\gamma_n^{(0)} 1/\omega_n + \gamma_n^{(1)} 1/\omega_{n+1} + \gamma_n^{(2)} 1/\omega_{n+2}} \tag{7}$$

is exact for model sequences of the form

$$s_n = s + \omega_n \left(c\, P_n(x) + d\, Q_n(x) \right) \tag{8}$$

where $Q_n(x)$ is the second solution of the recursion of Eq. (6), and $c \neq 0$ and $d \neq 0$ are arbitrary constants. If the ω_n depend on the s_n or the expansion coefficients c_j in Eq. (4) these sequence transformations are nonlinear.

3. Numerical Tests

Numerical tests for Fourier series have been reported in Ref. [2] in the context of the inversion of the Laplace transform, and also for series occurring in the Matsubara formalism. Here, results are given for expansions in Legendre polynomials $P_n(x)$. Expansions of this type are for instance solutions of Laplace's equation in spherical coordinates for problems of azimuthal symmetry (cf. Ref. [5]). The calculations were done in FORTRAN QUADRUPLE PRECISION (30-32 digit accuracy).

As a simple test case the sequence transformation

$$\{s_n\} \longrightarrow \{s'_n = \mathrm{K}_{n-2[\![n/2]\!]}^{([\![n/2]\!])}(\{(n+1)^{-1}\}, \{\gamma_n^{(j)}\}, \{s_n\}, \{(n+1)^{-1}\})\} \tag{9}$$

where $[\![x]\!]$ denotes the integer part of x, is applied with $\gamma_n^{(0)} = n+2$, $\gamma_n^{(1)} = -(2n+5)x$, and $\gamma_n^{(2)} = n+3$, to the sequence

$$s_n = \sum_{j=0}^{n} \frac{1}{j+1} \, P_j(x) \tag{10}$$

of partial sums of the series (cf. p. 700, Eq. 5.10.1.5 of Ref. [6])

$$\sum_{k=0}^{\infty} \frac{1}{k+1} \, P_k(x) = \ln \left(1 + \sqrt{\frac{2}{1-x}} \right) \, . \tag{11}$$

This corresponds to the choice $\omega_k = c_k$ where $c_k = 1/(k+1)$ are the coefficients in Eq. (11). Also, it should be noted that the coefficients $\gamma_n^{(j)}$ are n–shifted by one in comparison to Eq. (8) since the Legendre polynomials satisfy the recursion relation (cf. p. 736 of Ref. [6])

$$(n+2)\, P_{n+2}(x) - (2n+3)\, x\, P_{n+1}(x) + (n+1)\, P_n(x) = 0 \, . \tag{12}$$

Table 1

Acceleration of the expansion (11) for different values of x. Plotted are the numbers n_j such that the transformed sequence s'_n of Eq. (9) has j accurate digits for $n \geq n_j$. An asterisk means that $0 \leq n_j \leq 30$ does not hold. Plotted are also the number of accurate digits of the partial sums s_n of Eq. (10).

x	n_6	n_{10}	n_{12}	n_{14}	Digits (s_{30})
–2.0	12	20	24	26	divergent
–1.0	6	10	12	14	< 2
–0.9	6	11	12	16	< 3
–0.7	8	12	15	17	< 3
–0.5	8	14	16	18	< 3
–0.3	9	15	18	21	< 3
–0.1	9	16	19	22	< 3
0.1	10	17	20	23	< 3
0.3	11	18	21	26	< 3
0.5	12	21	24	28	3
0.7	13	23	29	$*$	< 3
0.9	18	30	$*$	$*$	< 3

From the data displayed in Table 1, it is seen that the convergence acceleration is very effective for any $x \in (-1, 1)$ far from the singularity $x = 1$. The nearer the argument x is to the singularity, the less effective is the convergence acceleration. Such effects are known for Fourier series (see Ref. [2]). For $x = 0.9$, one is rather near the singularity. Using the K transformation, one obtains the first 6 digits of the exact result using only 18 terms of the series and 10 digits for $n = 30$. Thus, the accuracy of the transformed sequence is much higher than the accuracy of the term-by-term summation of the series. The latter accuracy is low, approximately 2-3 digits for $n = 30$, as may be seen from the last column of Table 1. For $x < -1$ the expansion Eq. (11) diverges but can be summed using the sequence transformation Eq. (9) as may be seen from the first line in Table 1. Only in the case of this summation heavy loss of accuracy is observed when repeating the calculations in DOUBLE PRECISION. It may be noted that the numerical effort for the convergence acceleration is very low.

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