

A Summation Procedure for Expansions in Orthogonal Polynomials

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Approximants to functions defined by formal series expansions in orthogonal polynomials are introduced. They are shown to be convergent even out of the elliptical domain where the original expansion converges.

Constroem-se aproximantes de funções definidas por expansões em séries formais em polinômios ortogonais. Mostra-se que esses aproximantes são convergentes mesmo fora do domínio elítico onde converge a expansão original.

INTRODUCTION

Perturbative series theory and orthogonal polynomials expansions are the two more usual methods to solve physical and engineering problems, which range from classical mechanics, and electromagnetism, to atomic and nuclear physics. A great effort has been devoted to the study of approximants to physical quantities defined by a perturbative series. The efforts were mainly aimed to obtain efficient methods, for either speeding up the convergence of the series, or obtaining an approximate analytical continuation of the physical quantity outside the region of convergence of its defining power series. The Padé rational approximants have

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been one of the most successful methods used in theoretical physics to deal with these problems. In spite of the importance of the polynomial expansions, only a few works, to our knowledge, have attempted to formulate methods in order to improve its properties.

In this paper, we introduce approximants to a function defined by a formal series expansion in orthogonal polynomials in the interval $[-1, 1]$ and such that its coefficients are those of a Stieltjes series. We prove their convergence even out of the elliptical domain where the original expansion converges, and they are intended to be an alternative way of summation. The field of application of these approximants is quite wide and covering Jacobi, Legendre, Chebyshev and Gegenbauer polynomial expansions, and they could be applied to collision processes, circuit theory and central potentials theory.

1. RATIONAL PADÉ APPROXIMANTS FOR POWER SERIES

Let us consider the Stieltjes series

$$g(z) = \sum_{n=0}^{\infty} a_n z^n ;$$

its coefficients are

$$a_n = \int_0^{1/r} u^n d\phi(u) , \quad (1.2)$$

where $\phi(u)$ is a bounded non decreasing function, taking on infinitely many values in the interval $0 \leq u \leq 1/r$. The upper integration limit is defined in such a way that

$$\limsup_{n \rightarrow \infty} |a_n|^{1/n} = \frac{1}{r} \quad (r > 1) , \quad (1.3)$$

which guarantees that the series (1.1) converges uniformly in the circular domain

$$C_r = \{z : |z| < r\} .$$

Rational Padé approximants to series (1.1) can be defined as ratios of two polynomials,

$$[N, M]g(z) = \frac{P_M(z)}{Q_N(z)},$$

where the numerator and denominator have degrees M and N , respectively. Their coefficients are determined by equating like powers of z in the following equations:

$$g(z) Q_N(z) - P_M(z) = O(z^{M+N+1}),$$

$$Q_N(0) = 1.$$
(1.4)

It can be proved that this definition gives an explicit and compact expression for the approximants:

$$[M, N] = \frac{\begin{array}{c} \left| \begin{array}{ccc} a_{M-N+1} & \dots & a_{M+1} \\ \vdots & & \vdots \\ a_M & \dots & a_{M+N} \\ \sum_{j=N}^M a_{j-N} x^j & \dots & \sum_{j=0}^M a_j x^j \end{array} \right| \end{array}}{\begin{array}{c} \left| \begin{array}{ccc} a_{M-N+1} & \dots & a_{M+1} \\ \vdots & & \vdots \\ a_M & \dots & a_{M+N} \\ x^N & \dots & 1 \end{array} \right| \end{array}}$$

When the conditions given by (1.2) are fulfilled, any sequence $[N, N+j]$ of Padé approximants converges in the complex z -plane, cut along the line $x \leq z < \infty$, to the analytic function defined by the power series¹. In particular, the convergence is uniform in any closed region which does not contain part of the branch cut. The poles of the successive approximants, corresponding to increasing values of N , can be shown to interlace. Furthermore, they are on the segment $x \leq z < \infty$. Consequently the following expression for the $[N, N+j]_g(z)$ approximants can be obtained:

$$[N, N+j]g(z) = \sum_{p=1}^N \frac{\alpha_{p,N}}{1 - \sigma_{p,N} z} + \sum_{q=0}^j \beta_{q,N} z^q ; 0 \leq \sigma_{p,N} \leq \frac{1}{r} , \quad (1.5)$$

where $j \geq -1$, and the last sum on the right should only be taken for $j \geq 0$. The $\{\alpha_{p,N}\}$, $\{\sigma_{p,N}\}$, and $\{\beta_{q,N}\}$ are solutions of the system of equations

$$\sum_{p=1}^N \alpha_{p,N} (\sigma_{p,N})^k + \beta_{k,N} = a_k , 0 < k < j ,$$

$$\sum_{p=1}^N \alpha_{p,N} (\sigma_{p,N})^k = a_k , j < k \leq 2N+j ,$$

which may be obtained by replacing (1.5) into (1.4), and using the fact that the series (1.1) has radius of convergence r .

In this way, the Padé approximants provide a direct analytical continuation of the series outside of its convergence domain. Furthermore, they can be used as a fast method for summation of the series.

In this paper, we consider the function

$$f(z) = \sum_{n=0}^{\infty} a_n P_n(z) , \quad (1.6)$$

where the a_n are the same coefficients used above. The $\{P_n(z)\}$ is a complete set of orthogonal polynomials in the interval $[-1, 1]$, with weight function $w(x)$ and inner product

$$(y(x), h(x)) = \int_{-1}^1 dx w(x) y(x) h(x) .$$

Condition (1.3) on the a_n coefficients, implies, by using a theorem due to Szegő², that Eq.(1.6) converges uniformly in the elliptical domain

$$E_r = \{z : z = \frac{t+t^{-1}}{2} ; r^{-1} < |t| < r\} . \quad (1.7)$$

Our aim is to define approximants able to give an analytic continuation of the expansion (1.6) out of the domain defined by (1.7). At the same time, they can be used as a summation procedure.

2. THE $f_{N,i}$ APPROXIMANTS

We shall here deal with Jacobi, Legendre, Gegenbauer and Chebyshev polynomials as defined by Abramovitz and Segun³. For these polynomials the generating functions are defined by

$$K(z,u) = \sum_{n=0}^{\infty} P_n(z) u^n \quad (2.1)$$

for $z \in E_n$, $u \in C_{1/h}$, $h > 1$. Their particular expressions can be found in Appendix I. For fixed z , the only singularities of $K(z,u)$ as a function of u are simple poles or branch points at the zeroes of:

$$R(z,u) = (u^2 - 2zu + 1)^{1/2} \quad , \quad (2.2)$$

which are

$$u_{\pm}(z) = z \pm (z^2 - 1)^{1/2} \quad . \quad (2.3)$$

This result is not straightforward for Jacobi polynomials, and we give the proof in Appendix II. For $z \notin E_h$, the following inequality can be readily verified:

$$1/h < |u_{\pm}(z)| < h \quad . \quad (2.4)$$

Let us now consider the series

$$G(z) = g\left(\frac{1}{z}\right) = \sum_{n=0}^{\infty} a_n z^{-n} \quad , \quad (2.5)$$

which converges uniformly for $|z| > 1/r$, and let R be such that $r > R > 1$. The coefficients a_n can be expressed by the integral

$$a_n = \frac{1}{2\pi i} \int_{\Gamma} G(u) u^{n-1} du \quad (2.6)$$

with $\Gamma = \{u : |u| = R^{-1}\}$. For R' such that $R > R' > 1$, we may be sure, from Eq. (2.4), that the series (2.1) converges uniformly to $K(z,u)$ for

$u \in \Gamma$ and $z \in E_R$. This allows us substituting Eq. (2.6) into Eq. (1.6), and interchanging the summation and integration, in order to obtain:

$$f(z) = \frac{1}{2\pi i} \int_{\Gamma} G(u) K(z, u) u^{-1} du; \quad z \in E_R, \quad (2.7)$$

We can introduce in this integral the Padé approximants to $G(u)$:

$$[N, N+j]_{G(u)} = [N, N+j]_{g\left(\frac{1}{u}\right)} = \sum_{p=1}^N \frac{u \alpha_{p,N}}{u - \sigma_{p,N}} + \sum_{q=0}^j \beta_{q,N} u^{-q} \quad (2.8)$$

in order to obtain a set $f_{N,j}$ of approximants to $f(z)$, for $j \geq -1$:

$$f_{N,j}(z) = \frac{1}{2\pi i} \int_{\Gamma} [N, N+j]_{G(u)} K(z, u) u^{-1} du. \quad (2.9)$$

By replacing (2.8) in (2.9) and taking into account the fact that, for $z \in E_R$, and $|u| < 1/R$, $K(z, u)$ is a regular function of u , we get

$$f_{N,j}(z) = \sum_{p=1}^N \alpha_{p,N} K(z, \sigma_{p,N}) + \sum_{q=0}^j \beta_{q,N} P_q(z). \quad (2.10)$$

The uniform convergence of these approximants to $f(z)$, for $N \rightarrow \infty$ and $z \in E_R$, follows from the defining equation (2.9) by recalling that the $[N, N+j]_{G(u)}$ converge uniformly to $G(u)$ for $u \in \Gamma$, and the fact that $K(z, u)$ is a regular function of u for $z \in E_R$, and $u \in \Gamma$.

Finally, we can note the analytical properties of the $f_{N,j}(z)$. From Eq. (2.10), we see that their singularities are determined by those of $K(z, \sigma_{p,N})$. That is, the $f_{N,j}(z)$ will have singularities at the zeroes of $R(z, \sigma_{p,N})$, which are the real quantities

$$z_{p,N} = \frac{1}{2} (\sigma_{p,N} + \sigma_{p,N}^{-1})$$

and by noticing (1.5)

$$z_{p,n} \geq \frac{1}{2} (x + x^{-1}).$$

The poles of the $f_{N,j}$ are on the positive real axis, outside the elliptical domain of convergence. Since the poles $(0, P, N)^{-1}$ of the successive $[N, N+j]$ Padé approximants are positive and interlace, also the singularities of the successive $f_{N,j}$ will interlace on the positive real axis. The nature of these singularities strongly suggest that, by means of the $f_{N,j}$ approximants, expansion (1.6) may be analytically continued to the complex z -plane cut along the real axis by the segment $z \geq \frac{1}{2} (r+r^{-1})$.

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APPENDIX I

We give here, the particular expressions for the generating functions $K(z, u)$ corresponding to the sets of polynomials considered, according to reference (3).

$P_n(z)$	$K(z, u) = \sum_{n=0}^{\infty} P_n(z) u^n$	Remarks
Jacobi $P_n^{\alpha, \beta}(z)$ $\alpha, \beta > -1$	$R^{-1}(1-u+R)^{-\alpha}(1+u+R)^{-\beta}$	$ u < 1$
Legendre $P_n(z)$	R^{-1}	$-1 < z < 1$ $ u < 1$
Gegenbauer $C_n^{\alpha}(z)$ $\alpha > -\frac{1}{2}$	$R^{-2\alpha}$	$ u < 1$ $\alpha \neq 0$
Gegenbauer $C_n^0(z)$	$-2n R^2$	$ u < 1$
Chebyshev first kind $T_n(z)$	$(1 - uz)R^{-2}$	$-1 < z < 1$ $ u < 1$
Chebyshev second kind $U_n(z)$	R^{-2}	$-1 < z < 1$ $ u < 1$

where $R \equiv R(z, u) = (u^2 - 2zu + 1)^{1/2}$.

By recalling a theorem by Szego², already cited, the domains of convergence of the expansions of $K(z,u)$ may be extended for $h > 1$, to $\{|u| < \frac{1}{h}, z \in E_h\}$.

APPENDIX II

Let us consider

$$K(z,u) = \sum_{n=0}^{\infty} P_n^{\alpha, \beta}(z) u^n = 2^{\alpha+\beta} R^{-1} (1-u+R)^{-\alpha} (1+u+R)^{-\beta},$$

with

$$R(z,u) = (u^2 - 2zu + 1)^{1/2} = (u-u_+)(u-u_-)$$

where

$$u_{\pm}(z) = z \pm (z^2 - 1)^{1/2}, \quad u_+ = \frac{1}{u_-},$$

and the branch of $(z^2-1)^{1/2}$ considered is that for which

$$\lim_{|z| \rightarrow \infty} \left[\frac{1}{z} z^2 - 1 \right] = 1.$$

We intend to prove that, at least for one of the branches of R we have for $z \in E_p$

$$\begin{aligned} 1 - u + R &\neq 0, \\ 1 + u + R &\neq 0, \end{aligned}$$

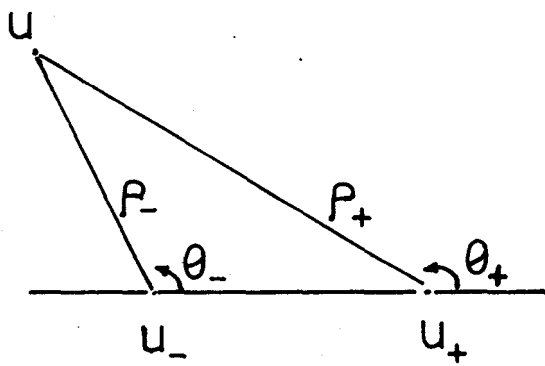
for every u .

This fact assures that, for fixed $z \in E_p$, the singularities of $K(z,u)$ as a function of u are only those of R . By defining

$$\rho_{\pm} = |u - u_{\pm}|$$

and phases θ_{\pm} , as in Fig.1, with the conditions

$$0 \leq \theta_{\pm} < 2\pi$$



and

$$\rho_+ + \rho_- > |u_+ - u_-| ,$$

we may define the two branches of R in the following way:

$$\begin{aligned} R_I &= (\rho_- \rho_+)^{1/2} \exp \left[i \frac{(\theta_- + \theta_+)}{2} \right], \\ R_{II} &= (\rho_- \rho_+)^{1/2} \exp \left[i \frac{(\theta_- + \theta_+ + 2\pi)}{2} \right]. \end{aligned} \tag{II.1}$$

It is easy to see that

$$\begin{aligned} A = 1 - u + R &= 0 \text{ for } z = 1 , \\ B = 1 + u + R &= 0 \text{ for } z = -1 , \end{aligned}$$

and that for these singular values of z , one has

$$R(1, u) = \sqrt{(u-1)^2} , \quad R(-1, u) = \sqrt{(u+1)^2} .$$

This implies that if A (or B) vanishes, this will occur for all values of u . Having this in mind, it will suffice to show that at least for one of the branches (II.1), A and B do not vanish for $z = \pm 1$ in some non empty subset of the u -plane.

Let us consider u real such that $|u| < r^{-1}$. This condition for $z \in E_r$ and $r^{-1} < u_{\pm}(z) < r$, requires $|u| < \text{Min} \{ |u_-|, |u_+| \}$. By taking notice of (II.1), we see that for $z \in E_r$ such that $z > 1$

$$R_{II}(z, u) > 0 ,$$

and we must have

$$R_{II}(\pm 1, u) = |u - 1| ,$$

and

$$1 \pm u + R_{II}(\pm 1, u) > 0 .$$

We then can conclude that for, $z \in E_r$, the only singularities of

$$K(z, u) = 2^{\alpha+\beta} R_{II}^{-1} (1 - u + R_{II})^{-\alpha} (1 + u + R_{II})^{-\beta} ,$$

$\alpha, \beta > -1$, as a function of u , are those of R_{II}^{-1} , which depending on the values of α and β , may be either branch points or simple poles in the u -plane.

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