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ON THE INTERPOLATION BY PADÉ APPROXIMANTS

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1. INTRODUCTION

The scattering theory involves complex functions of complex arguments. These functions, which are known within some error corridor at discrete points of a segment of the real axis, are analytic complex functions and have zeros and poles in a cut-complex plane.

The physical problem is to use this information on the "experimentally" determined complex function to best represent it in order to extrapolate the function into the cut-complex plane. Or, in other words, to use this information in order to find the location of the zeros, poles, the cuts, the residues in poles and the imaginary parts on the cuts.

It is generally recognized that such extrapolations can be advantageous if done by Padé approximants (or rational fraction approximants).

In this paper we have formulated the general interpolation problem for error affected functions and using some numerical examples we show the existence of an optimum solution, i.e., the existence of an optimum set of interpolating points which can give the best Padé approximant.

Due to some symmetry properties of the complex functions involved in scattering physics we will use the diagonal and near-diagonal Padé approximants, i.e., those rational approximants which are connected with continued fractions.

2. FORMULATION OF THE GENERAL INTERPOLATION PROBLEM

Let $\tilde{f}(z)$ be a complex function of a complex variable z, given within an error at a set of points G_M of the finite interval of the real axis

$$\tilde{f}(z_k) \subsetneq \{ f(z_k) \pm \epsilon(z_k) \},$$

$$G_M = \{ x_k \}, \quad z_k = x_k + i0, \quad k = 1,2,\ldots, M,$$

where $f(z)$ is the exact but unknown function and $\epsilon(z)$ is the error.

The problem is to select a subset of interpolating N points G_N, with $N < M$, $G_N \subset G_M$ and to find the values of the approximant function $\tilde{\tilde{f}}(z_\ell)$ at these points for which the rational fraction interpolation of the type $[n \pm j/n]$, $j = 0;1$ is the best one in the χ^2 sense

$$\sum_{k=1}^{M} \left| \frac{1}{\epsilon(z_k)} [\tilde{f}(z_k) - R(x_\ell, \tilde{\tilde{f}}(z_\ell), z_k)] \right|^2 = \min, \quad (1)$$

where $R(x_\ell, \tilde{\tilde{f}}(z_\ell), z) = [n \pm j/n]$ is the interpolating Padé approximant which depends on the interpolating points $x_\ell \subseteq G_N$ $(\ell = 1,2,\ldots N)$, on the value of the interpolating function x_ℓ

$$\tilde{\tilde{f}}(z_\ell) = R(x_\ell, \tilde{\tilde{f}}(z_\ell), z_\ell), \qquad z_\ell = x_\ell + i0,$$

and on the complex variable z.

Here $\tilde{\tilde{f}}(z_\ell)$ can differ from $\tilde{f}(z_\ell)$ - the given value of the function which must be interpolated. If $\tilde{\tilde{f}}(z_\ell) = \tilde{f}(z_\ell)$ we refer to the normal N-point Padé approximants sometimes known as the Padé approximants of the second type - PAII.

This general problem can be separated into two subproblems:

a) the first one is the search for the best approximant:

$$R(x_\ell, f(z_\ell), z) = [n \pm j/n]$$

when the interpolating points $G_N = \{x_\ell\}$, $\ell = 1,2,\ldots,N$ are given.

b) The second one is to find the optimum set of interpolating points

$$G^o_N = \{x^o_\ell\} \subset G_M$$

which give the best rational approximant.

2a. The Padé Approximants of the Third Type

Using the so-called ν algorithm[1] for continued fractions the function is approximated by a rational fraction

$$\tilde{\tilde{f}}(z) = \frac{P_{(i)}}{Q_{(i)}} = \frac{P_n}{Q_m}, \quad (2)$$

where $P_{(i)}$ and $Q_{(i)}$ are polynomials of degree n and m, respectively, and are given by the recurrence formula:

$$P_{(i)} = P_{(i-1)} \cdot B_{i,i} + D_{i-1} \cdot P_{(i-2)},$$
$$Q_{(i)} = Q_{(i-1)} \cdot B_{i,i} + D_{i-1} \cdot Q_{(i-2)}. \quad (3)$$

The matrix $B_{i,j}$ depends on the interpolating points x_i and on the function values at these points $\tilde{f}(z_i)$

$$B_{i,1} = \tilde{f}(z_i) \qquad i = 1,2,\ldots,N, \quad (4a)$$

$$B_{i,j} = \frac{x_i - x_{j-1}}{B_{i,j-1} - B_{j-1,j-1}} \qquad j = 2,3,\ldots,i, \quad (4b)$$

$$D_i = z - x_i. \quad (4c)$$

The degrees of the P and Q polynomials are $n = N/2$, $m = N/2 - 1$ for even N and $n = m = (N-1)/2$ for odd N.

The best approximant in the χ^2 sense will be obtained if the function values $f(z_i)$ in eq. (4a) ($B_{i,1}$ is the first column of the triangular matrix $B_{i,j}$) are taken as free parameters in a χ^2 minimization over the set of M values of functions (a χ^2 procedure for M values of $\tilde{f}(z_k) \pm \epsilon(z_k)$ $k = 1,2,\ldots M$ with N parameters). We shall call the newly obtained Padé approximant-the Padé approximant of the third type (PAIII)[2]. Such a procedure was introduced in ref. [2] and applied for resonance searching in partial wave analysis[2,3].

Here we must note that such a method of finding the PAIII differs from the direct fit with Padé approximant ansatz where the coefficients of the power expansion of P_n and Q_m are taken as free parameters

$$P_n = \sum_{\ell=0}^{n} a_\ell z^\ell,$$

$$Q_m = 1 + \sum_{\ell=1}^{m} b_\ell z^\ell.$$

2b. The Optimum Set of Interpolating Points

As is well known for polynomial interpolation there are solutions for choosing the optimal set of interpolating points in order to obtain the best approximant in a given norm. For example, for the minmax problem the optimal set of interpolating points are the Chebyshev points ($x_k = \cos(\frac{2k-1}{N}\pi)$)or for the L_2 norm the zeros of Legendre polynomials. For interpolation by Padé approximants (for N-point Padé approximants) there are no such theorems.

This second part of the general interpolating problem can be easily analysed when $M = \infty$, i.e., when the function which must by approximated is known at each point of the interval $[x_a, x_b]$

of the real axis. Now, the best Padê approximant can be found by using the same ν algorithm (eqs. 2-4), but using as free parameters in a χ^2 procedure the N values of x_ℓ in which the function must be interpolated. This is a χ^2 fit with PAII ansatz plus a construction given by the function itself. The optimum set of interpolating points $G_N^o = \{x_\ell^o\}$ can now be found because the function which must be approximated is known as a continuum function in the interval $[x_a, x_b]$ and the χ^2 minimization can be easily done.

In the next section we show by a few numerical examples that the optimal set of N (N is given) interpolating points exist.

As free parameters in the above χ^2 procedure, the optimal points x_ℓ^o are uncorrelated in χ^2 = min.

We must remark that this type of analysis is only a searching procedure in order to put in evidence the existence of such an optimal set of interpolating points for Padê approximants.

In order to solve in practice the general interpolating problem we propose to use, as a first step, a smooth interpolation procedure (for example of spline type) and use it as a continuum function in a given interval $[x_a, x_b]$ (the construction in the above χ^2 procedure) in order to find the optimum set of points $G_N^o = \{x_\ell^o\}$ for Padê interpolation. Using this optimum set of points G_N^o, the Padê approximant of the third type ($\tilde{f}(z_\ell^o)$ as free parameters), we can obtain the best χ^2 and so, for a given set of error affected functions ($\tilde{f}(z_k) \pm \epsilon(z_k)$ $k = 1,2,\ldots M$) the best approximant.

3. NUMERICAL RESULTS

Using the method described in sect.2b, we have computed the optimal set of interpolating points for the following functions:

$$f(z) = \frac{1}{\sqrt{1-2az+a^2}} + i\,\frac{1}{\sqrt{1-2bz+b^2}}, \qquad (5)$$

$$f(z) = \frac{z - z_0}{\sqrt{1-2az+a^2}}, \qquad (6)$$

$$f(z) = \sqrt{1-2az+a^2} + i\sqrt{1-2bz+b^2}, \qquad (7)$$

where $a = 0.2$, $b = 0.3$ and $z_0 = 0.2 - i0.3$.

The function values were taken at $M = 41$ points on the real axis in the interval $x \in [-1,+1]$. In tables 1-3 are shown χ^2 obtained for the Chebyshev interpolating points and for the optimal set of points for different Padê approximants. Here χ^2 is

Table 1

χ^2 for PAII interpolating at Chebyshev and optimal points of eq. (5)

PAII	[2/1]	[2/2]	[3/2]	[3/3]	[4/3]
N	4	5	6	7	8
χ^2(Ch)	$6.515\cdot10^{-6}$	$2.607\cdot10^{-8}$	$3.235\cdot10^{-10}$	$1.550\cdot10^{-12}$	$2.509\cdot10^{-14}$
χ^2(op)	$3.060\cdot10^{-6}$	$5.770\cdot10^{-9}$	$5.375\cdot10^{-11}$	$1.390\cdot10^{-13}$	$1.600\cdot10^{-15}$

Table 2

As in table 1, but for eq. (6)

PAII	[3/2]	[3/3]	[4/3]
N	6	7	8
χ^2(Ch)	$2.620\cdot10^{-9}$	$2.550\cdot10^{-11}$	$2.530\cdot10^{-13}$
χ^2(op)	$5.731\cdot10^{-10}$	$3.410\cdot10^{-12}$	$1.990\cdot10^{-14}$

Table 3

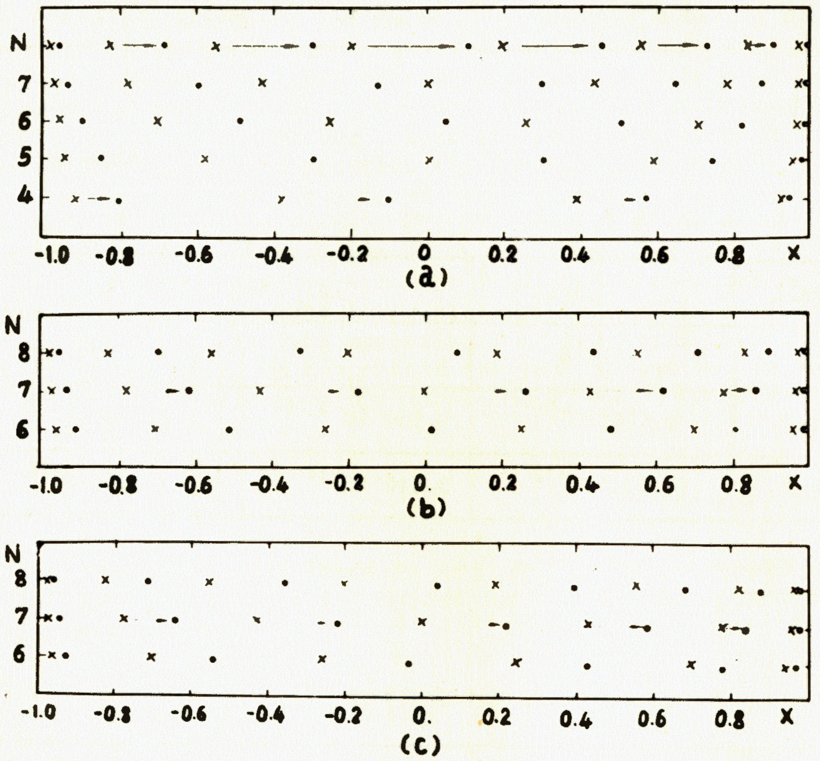
As in table 1, but for eq. (7)

PAII	[3/2]	[3/3]	[4/3]
N	6	7	8
χ^2(Ch)	$4.237\cdot10^{-11}$	$3.796\cdot10^{-13}$	$3.630\cdot10^{-15}$
χ^2(op)	$1.499\cdot10^{-11}$	$8.690\cdot10^{-14}$	$5.120\cdot10^{-16}$

given by

$$\chi^2 = \sum_{k=1}^{M} |f(z_k) - \tilde{\tilde{f}}(z_k)|^2 ,$$

where $\tilde{\tilde{f}}(z)$ is our optimal Padé approximant. The distribution of optimal points x°_{ℓ} in the interval $[-1,+1]$ is shown in the figure, where, for comparison, the Chebyshev points are also shown. The PAIII taken at the optimal set of points x°_{ℓ} give, of course, a better χ^2.



Distribution of the interpolating points: • - the optimal points, × - the Chebyshev points. a,b,c - for eq. (5), (6), and (7), respectively.

Concerning the first example (eq.5) we also must remark that expanding this optimal Padé approximant into a Legendre series

$$\frac{2\ell+1}{2}\int_{-1}^{+1} \tilde{\tilde{f}}(z) P_\ell(z)\, dz = \bar{a}_\ell + i\bar{b}_\ell$$

one can recover higher coefficients of the original Legendre

$$\frac{1}{\sqrt{1-2az+a^2}} + i\,\frac{1}{\sqrt{1-2bz+b^2}} = \sum_{\ell=0}^{\infty} (a^\ell + ib^\ell) P_\ell(z)$$

to a high precision, i.e., $r_\ell = \bar{a}_\ell / a^\ell \simeq 1$, $r'_\ell = \bar{b}_\ell / b^\ell \simeq 1$ even a higher precision than non-linear Padé approximants introduced by J.Fleischer /4,5/.

Finally, we must make an interesting observation concerning the PAIII and PAII at the optimal set of interpolating points. Solving the equation:

$$f(z) - \tilde{\tilde{f}}(z) = 0, \qquad (8)$$

where $\tilde{\tilde{f}}(z)$ is now the PAIII obtained by a χ^2 interpolation at the Chebyshev points, we can find the intersection between $f(z)$ and the PAIII (Ch) in the complex z plane. The solutions of the above equation (8) are near the real axis and are given by

$$z_\ell = x^{\circ}_{\ell} + iy_\ell ,$$

where x°_{ℓ} are to a good precision the optimal set of interpolating points for the given complex function, points which were previously found as shown in sect.2b.

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Богданова Н., Никитиу Ф. E5-83-228

Интерполяция с помощью паде-аппроксимантов

Исследуется проблема интерполяции для комплексных функций, заданных со своими ошибками, с целью наилучшим образом экстраполировать их в разрезанную комплексную плоскость. Для экстраполяции используются диагональный и околодиагональный паде-аппроксиманты /ПА/ второго сорта /ПАII/ и их модификация для χ^2-минимизации /ПАIII/. Сформулирована общая интерполяционная проблема для функций, заданных со своими ошибками; с помощью некоторых численных примеров показано, что существует оптимальный набор интерполяционных точек, и найдена связь между ПАIII и ПАII для этого набора. Таким образом, в интерполяционной проблеме для комплексных функций, заданных со своими ошибками, существует оптимальный набор интерполяционных точек, который обеспечивает наилучшую в смысле χ^2 ПА /паде-аппроксимацию/. Здесь предложен практический метод для нахождения этого набора.

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On the Interpolation by Padé Approximants

In this work we have studied the interpolation problem for error affected complex functions in order to best extrapolate them in the cut-complex plane. The methods used for interpolation are the diagonal and near-diagonal Padé approximants (PA) of the second type (PAII) and their modification for the χ^2 minimization (PAIII). We have formulated the general interpolation problem for error affected functions and, using some numerical examples, we have shown that there exists an optimum set of interpolating points and have revealed the connection between the PAIII and the PAII for this optimum set of interpolating points. To conclude, in the interpolation problem for error affected complex functions there exists an optimum set of interpolating points which can give the best PA in the χ^2 sense, and here we have proposed a practical method for finding it.

The investigation has been performed at the Laboratory of Nuclear Problems, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1983