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PROBLEM OF THE CONVERGENCE OF PADE APPROXIMANTS***

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THE LINEAR, FUNCTIONAL EQUATION APPROACH TO THE
PROBLEM OF THE CONVERGENCE OF PADÉ APPROXIMANTS*

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ABSTRACT

The Padé approximant problem is related to a (not necessarily orthogonal) projection of a linear functional equation of the Fredholm type. If the kernel is of trace class and its upper Hessenberg form is tridiagonal (this class includes Hermitian operators), then we prove that not only do the diagonal Padé approximants converge, but so do their numerators and denominators separately. The generalization of these results to C_p classes of compact operators is given. For kernels which are not only compact, but also satisfy an additional mild restriction, a pointwise convergence theorem is proven. The application of these results to quantum scattering theory is indicated.

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Considerable progress in the study of the convergence of Padé approximants can be made, I think, by the use of the techniques of functional equations. What I will report here is probably just a beginning, and is drawn in part from a previous paper.[1] First we will review the known relation of Padé approximants to linear functional equations, then we review the properties of some special classes of compact operators, and give convergence results for these classes. Finally we indicate how these results lead to convergence of Padé approximants to the partial wave scattering amplitudes in certain quantum mechanical scattering problems.

PROJECTIONS IN THE CINI-FUBINI SUBSPACE

Suppose we consider the functional equation

$$f = g + \lambda A f \quad (1)$$

where f , g , and h belong to some Hilbert space H , and A is a linear operator whose properties are yet to be defined. We also introduce the associated sets of elements

$$\varphi_i = A^{i-1} g, \quad \varphi_i' = (A^\dagger)^{i-1} h \quad i = 1, 2, \dots, \quad (2)$$

where $A^\dagger$ is the Hermitian conjugate operator to A . We need as well the $N \times N$ matrix

$$R_{i,j} = (\varphi_i', \varphi_j) = (h, A^{i+j-2} g) \quad (3)$$

defined in terms of the inner products of the φ_j and φ_i' . We are now in a position to define our projection operator onto the Cini-Fubini subspace [2]

$$P_N = \sum_{i,j=1}^N \varphi_i (R^{-1})_{ij} (\varphi_j', \cdot), \quad (4)$$

provided $\det|R| \neq 0$. (It can be shown [3] that there exists an infinite number of such N 's.) The operator P_N is a projection on $\mathcal{S}_N$ from $\mathcal{S}_N'$. (The spaces $\mathcal{S}_N$ and $\mathcal{S}_N'$ are respectively those spaces spanned by φ_i and φ_i' for $i = 1, \dots, N$.) It has the properties

$$P_N P_M = P_M P_N = P_M, \quad M \leq N. \quad (5)$$

However, it may not be an orthogonal projection. If it is not, then its norm $\|P_N\|$ will be greater than unity! We show in fig. 1 the projection on non-orthogonal directions. It is clear in this figure that the "length" $(a^2 + b^2)^{1/2}$ of the projection can be greater than the length of the original vector.

Fig. 1

Projection on non-orthogonal directions
(heavy lines) of a vector (arrow)

With this machinery, let us consider the truncated equation

$$f_N = g + \lambda P_N A P_N f_N. \quad (6)$$

By the properties of P_N , we expect a solution of the form

$$f_N = \sum_{j=1}^N a_j \varphi_j. \quad (7)$$

The substitution of (7) leads to the solution

$$f_N = \left(\sum_{i=1}^N \sum_{j=1}^N \varphi_i v_{ij} w_{j-1} \right) / \det |u_{ij}|, \quad (8)$$

where

$$\begin{aligned} u_{ij} &= w_{i+j-2} - \lambda w_{i+j-1} \\ v_{ij} &= i, \text{ } j\text{th minor of } (u_{kl}). \end{aligned} \quad (9)$$

Then

$$(h, f_N) = \sum_{i=1}^N \sum_{j=1}^N w_{i-1} v_{ij} w_{j-1} / \det |u_{ij}|. \quad (10)$$

However this formula is Nuttall's compact form [4,5] for the $[N-1/N]$ Padé approximant to $h(\lambda)$ defined by the Liouville-Neumann series

$$\begin{aligned} f &= g + \lambda Ag + \lambda^2 A^2 g + \lambda^3 A^3 g + \dots, \\ h(\lambda) &= (h, f) = w_0 + \lambda w_1 + \lambda^2 w_2 + \dots \end{aligned} \quad (11)$$

Thus by use of the projection operator (4) we generate directly the Padé approximants as the solutions of the truncated equations.

RESULTS FOR THE TRACE CLASS OF COMPACT OPERATORS

Here we will assume that P_N is orthogonal. What does this restriction imply about the linear operator A ? To examine this question we use a basis e_i determined by the w_i so that the e_i are orthonormal and the first N of them span $\mathcal{S}_N$. Using this basis, we see that A is of the form

$$\begin{pmatrix} x & x & x & x & \dots \\ x & x & x & x & \dots \\ 0 & x & x & x & \dots \\ 0 & 0 & x & x & \dots \\ 0 & 0 & 0 & x & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (12)$$

that is, upper right triangular plus one subdiagonal. This form is called the upper Hessenberg form. Now if $A = A^\dagger$, this Hermiticity condition implies at once that A is tridiagonal. Therefore if we choose h of eq. (2) equal to g , then the φ_i define the same spaces as the ψ_i , and P_N is orthogonal. But this conclusion depends only on the tri-diagonality of A which is more general than Hermiticity. The restriction $A = A^\dagger$ would yield only generalized series of Stieltjes, however our results extend them.

Now let us define trace class operators. If the operator is trace class and A is tridiagonal in its upper Hessenberg form, then it turns out that the numerator and denominator converge separately. In order to define the trace class of compact operators we introduce the non-negative, definite, Hermitian operator

$$T = A^\dagger A, \quad (13)$$

which has the eigenvalues and eigenvectors

$$T \psi_i = \alpha_i^2 \psi_i. \quad (14)$$

The trace norm of A is then

$$\|A\|_1 = \sum_i \alpha_i, \quad (15)$$

which is something like $\text{Tr}(|A|)$, and the trace class consists of those operators with a finite trace norm. Standard theory [6] insures that for an operator of trace class we can define

$$D(\lambda) = \det |I + \lambda A| = \lim_{N \rightarrow \infty} D_N(\lambda), \quad (16)$$

where the D_N are the determinants in a sequence of subspaces. The resulting $D(\lambda)$ is an entire function of λ . We note at this point that

some condition related to the trace of A is required as the Padé' denominator must go to

$$1 - \lambda \sum_i \lambda_i^{-1} + O(\lambda^2), \quad (17)$$

and, if

$$\sum_i \lambda_i^{-1} = \text{Tr}(A) = \infty, \quad (18)$$

then the denominator can't possibly converge separately.

In order to see the convergence in this case, it is convenient to construct the Fredholm solution to the truncated equations. To this end we introduce an orthonormal basis $\chi_i, i=1, \dots, N$ spanning $S_N = S_N^+$. Then

$$A_{ij} = (\chi_i, A\chi_j), \quad f_N = \sum b_i \chi_i, \quad (19)$$

$$b_j = (\chi_j, g) + \lambda \sum_{k=1}^N A_{jk} b_k. \quad (20)$$

If

$$D_N(\lambda) = \det_N |\delta_{ij} - \lambda A_{ij}| \neq 0, \quad (21)$$

then the Fredholm solution is given by

$$f_N = g + \lambda \sum_j \chi_j D_{N,jk}(\lambda) (\chi_k, g) / D_N(\lambda), \quad (22)$$

where

$$D_{N,jk}(\lambda) = A_{jk} - \frac{\lambda}{1!} \sum_{l=1}^N \begin{vmatrix} A_{jk} & A_{jl} \\ A_{lk} & A_{ll} \end{vmatrix} + \frac{\lambda^2}{2!} \sum \begin{vmatrix} & & \\ & & \end{vmatrix} + \dots, \quad (23)$$

and are automatically polynomials of degree at most $N - 1$ in λ . If we choose the χ_i to be eigenfunctions of

$$T_N = (P_N A P_N)^\dagger (P_N A P_N), \quad (24)$$

and use Hadamard's determinant inequality

$$\left| \det \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix} \right| \leq \prod_{i=1}^n \left(\sum_{j=1}^n |a_{ij}|^2 \right)^{1/2}, \quad (25)$$

then we can show [1] for any z in $\mathbb{H}$, of unit length

$$\left[\sum_{j=1}^N \left| \sum_{k=1}^N D_{N,jk}(\lambda) z_k \right|^2 \right]^{1/2} \leq \|A\|_2 \quad (1) \\ + \frac{|\lambda|}{1!} 2^{2/2} \|A\|_1 + \frac{|\lambda|}{2!} 3^{3/2} \|A\|_1^2 + \dots \quad (26)$$

Thus the operators that give the numerator in the Fredholm solution are a sequence of uniformly bounded operators in N for all λ provided the series in (26) converges. As $\|A\|_1$ is finite the series does and $\|A\|_1$ finite makes $\|A\|_2$ automatically finite also. Standard arguments then insure the convergence of the numerators and eq. (16) gives that of the denominators. Hence we have the separate convergence of the numerator and denominator of the Padé approximants to the ratio of the two entire functions given by the Fredholm solution.

C_p CLASSES OF COMPACT OPERATORS

We may define larger classes of operators than the trace class and obtain special convergence results for them. We say a compact operator belongs to class C_p if, using (13) and (14),

$$\|A\|_p = \left[\sum_i \alpha_i^p \right]^{1/p} < \infty. \quad (27)$$

The trace class is C_1 and these classes have the properties that $C_{p-1} \subset C_p$. We use the convenient notation, due to Nuttall,

$$\left[\sum_{i=0}^{\infty} F_i x^i \right]^P = \sum_{i=0}^P F_i x^i \quad (28)$$

for any formal power series. The results for operators of class C_p are based on rewriting the Padé approximants as

$$[N-1/N] = \frac{P_N(\lambda)}{Q_N(\lambda)} = \frac{P_N(\lambda) \exp[-\{\ln Q_N(\lambda)\}^{P-1}]}{Q_N(\lambda) \exp[-\{\ln Q_N(\lambda)\}^{P-1}]} \quad (29)$$

By applying arguments parallel to those of Dunford and Schwartz [6], we can show for P_N orthogonal and A in C_p that if we define

$$D_{N,p}(\lambda) = \det_N(\delta_{ij} - \lambda A_{ij}) \exp[-\{\ln \det_N(\delta_{ij} - \lambda A_{ij})\}^{P-1}] \quad (30)$$

then

$$\begin{aligned} \lim_{N \rightarrow \infty} D_{N,p}(\lambda) &= \text{entire function of } \lambda \\ &\leq \exp(\Gamma \|A\|_p^P \lambda^P), \end{aligned} \quad (31)$$

and in the $N \times N$ truncated space $\mathcal{S}_N = \mathcal{S}_N^*$

$$\begin{aligned} \lim_{N \rightarrow \infty} \|D_{N,p}(\lambda) \{(\delta_{ij} - \lambda A_{ij})^{-1} - \delta_{ij} - \lambda A - \dots - \lambda^{P-2} A^{P-2}\}\|_{\frac{p}{p-1}} \\ \leq \exp[\Gamma(\lambda^P \|A\|_p^P + 1)] \end{aligned} \quad (32)$$

where Γ is a finite, N -independent constant. By combining eq. (11), (29)-(32) we deduce that we have the form

$$\lim[N-1/N] = \sum_{j=0}^{p-2} \lambda^j h_j + \frac{\text{entire function}}{\text{entire function}}, \quad (33)$$

where for A in C_p both entire functions in (33) satisfy

$$|\text{entire function}| \leq k \exp(B \lambda^P). \quad (34)$$

The modified numerator and denominator defined in this way converge separately to entire functions, and thus, of course, the Padé approximant does too. The result for the Padé approximant itself is more general than for the numerator and denominator separately as we shall see below.

COMPACT OPERATORS

First let us consider the case where P_N is an orthogonal projection ($g_N = g_N^i$). If we subtract eq. (6) from eq. (1) we get

$$f - f_N = \lambda A (f - f_N) + \lambda (A - P_N A P_N) f_N. \quad (35)$$

Now if $\|f_N\| < \infty$, then the second term on the right hand side of (35) goes to zero as A is compact. Then eq. (35) becomes the form

$$d \simeq \lambda A d. \quad (36)$$

Thus, if λ is not a singular point of eq. (1), we may conclude $d = 0$ by the Fredholm alternative theorem. Hence

$$\begin{aligned} f_N &= f, \\ [N-1/N] &= (h, f_N) - (h, f) = h(\lambda). \end{aligned} \quad (37)$$

If, on the other hand, $\|f_N\| \rightarrow \infty$ for all N , we can define

$$d_N = f_N / \|f_N\|, \quad (38)$$

an element of unit norm. Eq. (6) becomes

$$d_N - \lambda P_N A d_N = 0. \quad (39)$$

As A is compact, there exists a subsequence of N 's such that the limit over the subsequence exists and has the value

$$\lim \lambda A d_N = d, \quad (40)$$

which implies, as A is compact,

$$d - \lambda A d = 0. \quad (41)$$

Since we are assuming λ is not a singular point of (1), we conclude by the Fredholm alternative theorem that $\|d\| = 0$, which is a contradiction. Therefore there does not exist an infinite sequence of f_N whose norm tends to infinity, but at most a finite number of such equations. Therefore we conclude if A is a compact operator and the P_N are orthogonal projection operators that when λ is not a singular point of eq.

(1)

$$\lim [N-1/N] = h(\lambda), \quad (42)$$

where the limit is taken over the infinite number of N 's for which the Padé approximants exist.[3]

In the case P_N is not orthogonal, less complete results have been obtained. The problem here is that the magnitude of $\|P_N\|$ is uncontrolled. In particular, insofar as we are concerned it is only the magnitude of the element,

$$P_N A e_N, \quad (43)$$

where the e_j are defined before eq. (12), that is uncontrolled, as by construction

$$P_N A e_j = A e_j, \quad j \leq N-1. \quad (44)$$

If we make the additional mild assumption that (note that this equation is misprinted in ref. 1)

$$\lim_{N \rightarrow \infty} \inf \|P_N A P_N A e_N\| = 0, \quad (45)$$

where

$$P_N = \sum_{j=1}^N e_j (e_j, \cdot) \quad (46)$$

is the orthogonal projection on $\mathcal{S}_N$. Then we can prove:[1]

Theorem: Let Λ be any closed bounded region in the complex λ plane not containing a singular point of eq. (1). Then either (i) a finite order Padé approximant to $h(\lambda)$ of eq. (11) is exact, or (ii) eq. (42) holds, or (iii) for each λ in Λ for which (i) and (ii) fail, there exists an infinite subsequence of N 's such that (ii) holds for all other λ in Λ .

APPLICATION TO QUANTUM SCATTERING THEORY

This application is a generalization of that of Garibotti and Villani.[7] We consider the problem of potential scattering in non-relativistic quantum mechanics. The fundamental equation is the Schrodinger equation

$$-\nabla^2 \psi(\vec{r}) + \lambda V(r) \psi(\vec{r}) = k^2 \psi(\vec{r}). \quad (47)$$

We restrict the potential function by assuming that $V(r)$ is of single sign, spherically symmetric, and satisfies

$$\int_0^\infty |V(r)| \exp(2|v|r) r dr < \infty. \quad (48)$$

Then, for the partial wave decomposition of (47) we can show: (i) a slightly recast version of the kernel of the usual corresponding integral equation is of trace class. (ii) The upper Hessenberg form of the kernel is tridiagonal. Thus the results we have reported show that the numerator and denominator of the $[M/M]$ Padé approximants

converge separately, and the denominator converges to the Jost function, as one would hope. These conclusions hold if $|\operatorname{Im}(k)| \leq \nu$.

In as much as Fredholm equations appear very frequently throughout the field of mechanics, the potential applications of these convergence results in the area of this conference seems to me to be very large.

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