Shafer (Hermite-Pade) Approximants for Functions with Exponentially Small Imaginary Part with Application to Equatorial Waves with Critical Latitude

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Abstract

Quadratic Shafer approximants and their generalization to higher degree polynomials called *Hermite-Padé approximants* have been successfully used in quantum mechanics for calculation of exponentially small escape rates.

In this paper we test quadratic Shafer approximants in representing growth rates typical for equatorial atmosphere. One of the characteristic features of the equatorial Kelvin wave — the dominant mode in equatorial dynamics — is its exceptionally small linear growth rate. For example, Kelvin wave evolving on the zonal basic state with small linear shear ϵ has growth rate $O(\exp(-1/\epsilon^2))$ in contrast to $\Im(E) \sim O(\exp(-1/\epsilon))$ common to similar problems in quantum mechanics. It is interesting to know how well Hermite-Padé approximants handle this more computationally expensive problem.

First we apply the quadratic Shafer approximants to calculate the imaginary part of the Gauss-Stieltjes function defined as

$$G_S(\epsilon) \equiv \lim_{\delta \to 0} \int_0^\infty \frac{\exp\left(-t^2\right)}{t - [1 + i\delta]/\epsilon} \, dt \tag{1}$$

on its branch cut. The imaginary part of $G_S(\epsilon)$ can be shown to be

$$\Im(G_S)(\epsilon) = \pi \exp\left(-\frac{1}{\epsilon^2}\right) \tag{2}$$

which is of the same order of magnitude as Kelvin-in-shear growth rate. Next, we use this technique to sum the divergent Rayleigh-Schrödinger perturbation series of the Hermite-with-Pole equation

$$u_{yy} + \left(\epsilon \frac{1}{1 + \epsilon y} - \lambda - y^2\right) u = 0 \tag{3}$$

which is a simple model for equatorial waves in shear. The Hermite-with-Pole equation has been previously studied numerically and analytically in [**?**]. We compare Shafer approximants against numerical integration and find that for small ϵ Shafer approximants are more efficient, primarily because with rational coefficients one does not need multiple precision at the main stage of the calculation.

Although the higher order approximants are usually more accurate, the overall improvement of accuracy is not monotonic due to the appearance of nearly coincident zeros in the approximants.

1 Introduction

In solving eigenvalue problems by singular perturbation technique the answer usually comes in a form of a divergent series. One is then faced with a task of extracting useful information from a sequence of fast growing coefficients.

Ordinary Padé approximants help to accelerate summation and improve the accuracy over optimal truncation in many cases, but they also can miss important information. For example, they are incapable of representing multivalued functions, or giving any hints that the function that corresponds to the real-valued divergent series in hand actually has nonzero imaginary part.

A family of generalizations called *Hermite-Padé approximants*, that includes the quadratic Shafer form as a special case, has been successfully used in quantum mechanics, theory of water waves, series analysis of multivalued functions and other applications [**?**, **?**, **?**, **?**, **?**]. On the theoretical side many illuminating and useful theorems have been proven about convergence properties of the Hermite-Padé approximants. However, the accuracy required in some applications can make a problem intractable for modern day computers, or at least make the approximants less efficient than other methods.

The quadratic Shafer approximant $f[K/L/M]$ is defined to be the solution of the quadratic equation (Shafer[**?**])

$$P(f[K/L/M])^2 + Q\, f[K/L/M] \,+\, R = 0 \tag{4}$$

where the polynomials P, Q and R are of degrees K, L and M, respectively. These polynomials are chosen so that the power series expansion of $f[K/L/M]$ agrees with that of f through the first $N = K+L+M+1$ terms. The constant terms in P and Q can be set arbitrarily without loss of generality since these choices do not alter the root of the equation, so the total number of degrees of freedom is as indicated. As for ordinary Padé approximants, the coefficients of the polynomials can be computed by solving a matrix equation and the most accurate approximations are obtained by choosing the polynomials to be of equal degree, so-called “diagonal” approximants.

2 Gauss-Stieltjes Problem

The integral

$$G_S(\epsilon) \equiv \lim_{\delta\to 0} \int_0^\infty \frac{\exp\left(-t^2\right)}{t - [1+i\delta]/\epsilon}\, dt \tag{5}$$

cannot be evaluated in closed form. However, because the limit $\delta \to 0$ of $\delta/(\delta^2 + z^2)$ is π times the Dirac delta-function, the imaginary part of the integral gives [1]

$$\Im(G_S)(\epsilon) = \pi \exp\left(-\frac{1}{\epsilon^2}\right) \tag{6}$$

without approximation.

The real part of the integral can be approximated by the asymptotic series

$$G_S(\epsilon) \sim \sum_{n=1}^{\infty} b_n \, \epsilon^n \tag{7}$$

where, by expanding the denominator of the integrand as a power series in ϵ,

$$b_j \equiv -\int_0^{\infty} \exp(-t^2)\, t^{j-1} dt = -\frac{\Gamma\left(\frac{j}{2}\right)}{2}, \qquad j = 1, 2, \ldots \tag{8}$$

where Γ is the usual factorial function.

Divergent series usually have terms that diverge as $j!$; the error of an optimally-truncated series is then $O(\exp(-\text{constant}/\epsilon))$. For the Gaussian-Stieltjes integral, $\Im(G_S)$ is proportional to $\exp(-1/\epsilon^2)$ and the series diverges as the square root of $j!$. (Note that $\log((j/2)!) \sim \log(\sqrt{j!})$.

Fig.1 shows the relative error for the first 10 Shafer approximants.

One has to remember to keep adequate number of digits in floating point representation of π to evaluate $\Im(G_S)(\epsilon)$ numerically for different values of ϵ, because the magnitude of the coefficients in P, Q, R varies dramatically for high order approximants. We can reformulate the problem in such way that all coefficients are rational and this complication disappears. This will also show that evaluation of the Gauss-Stieltjes function on its branch cut can be reduced to a problem in which the imaginary part is only exponentially small in the reciprocal of the small parameter, similarly to previously studied quantum mechanical problems.

Define the symmetric and antisymmetric parts of $G_S(\epsilon)$ by

$$\sigma(\epsilon) \equiv G_S(\epsilon) + G_S(-\epsilon) \tag{9}$$

$$\alpha(\epsilon) \equiv G_S(\epsilon) - G_S(-\epsilon) \tag{10}$$

Since the imaginary part of G_S is symmetric in ϵ for either choice of branch cut, it follows that $\alpha(\epsilon)$ is always a real-valued function. Therefore, we should apply approximants only to the symmetric function,

[1] Note correction from published version; the factor of π on the R. H. S. of Eq. 6 was omitted in the published version.

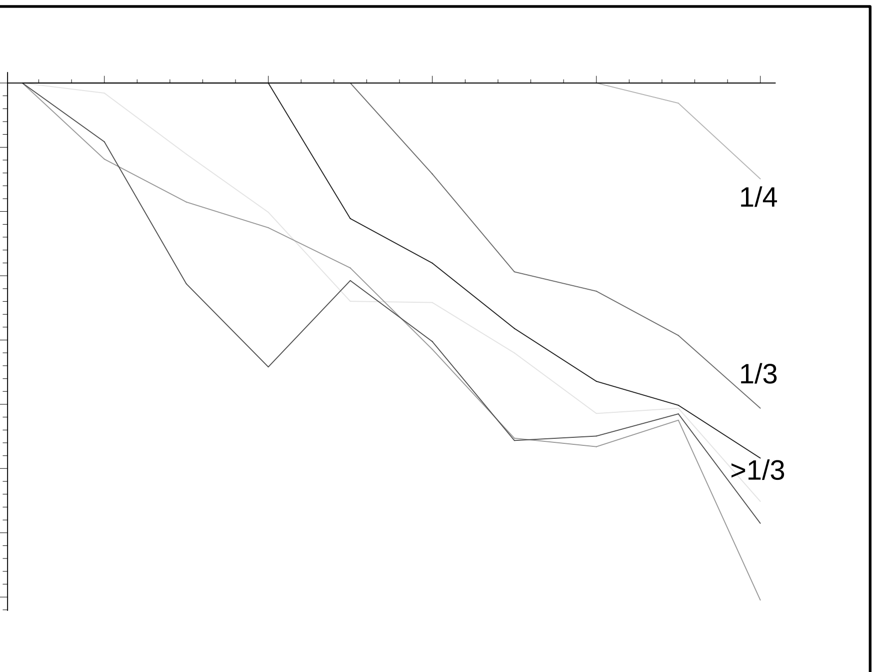

Figure 1: Relative errors (absolute error divided by the true imaginary part) for the imaginary part of $\Im(G_S)(\epsilon)$

which has the expansion

$$\sigma(\epsilon) = \sum_{j=1}^{\infty} -(j-1)!\epsilon^{2j} \tag{11}$$

This implies that

$$\sigma(\epsilon) = -\epsilon^2 S(-\epsilon^2) \tag{12}$$

where the usual Stieltjes function is defined by

$$S(\epsilon) = \sum_{j=1}^{\infty} (-1)^j j!\epsilon^j \tag{13}$$

This implies

$$\Im(\sigma(\epsilon)) = \pm\pi \exp(-1/\epsilon^2) \tag{14}$$

Since we have added two copies of G_S, it would seem as though the imaginary part should be twice what is given by Eq. 14. However, matching the coefficients and using the known imaginary part of the Stieltjes function on its branch cut says otherwise.

Note also that by using its definition

$$\sigma(\epsilon) \equiv \lim_{\delta\to 0} \int_0^{\infty} \exp\left(-t^2\right) \left\{ \frac{1}{t - [1+i\delta]/\epsilon} + \frac{1}{t + [1+i\delta]/\epsilon} \right\} dt \tag{15}$$

Although there are two singular terms, only one of them has a pole on the integration interval — the other is at $t = -1/\epsilon$, so the imaginary part of σ is $\pi \exp(-1/\epsilon^2)$.

3 The Rayleigh-Schrödinger Series of the Hermite-with-Pole Equation

The Hermite-with-Pole Equation

$$u_{yy} + \left(\epsilon \frac{1}{1+\epsilon y} - \lambda - y^2\right) u = 0 \tag{16}$$

models a combination of effects of critical latitude (the term $\frac{1}{1+\epsilon y}$) and equatorial trapping (potential well $\lambda - y^2$) on equatorial waves. Although it is much simpler than the actual shallow water equations, it captures the essentials.

The Rayleigh-Schrödinger perturbation series of the Hermite-with-Pole equation is real. In [**?**] we showed that the leading order behavior of the imaginary part of the ground state eigenvalue is $\sqrt{\pi}(1 - 2\epsilon \log\epsilon +$

Table 1: Hermite-with-Pole Equation:Imaginary Part

ϵ	$\Im(\lambda)$	[6/6/6]	[13/13/13]	[20/20/20]	[20/20/20] Rel. err.
1	0.63002304156	0.**63**230	0.**6300**5297	0.**63002**2014	0.0000016
3/4	0.386770686076	0.**3**914	0.**3867**474	0.**38677**1895	3.1E-6
1/2	0.07805030263	0.**07**712	0.**0780**434	0.**078050**6125	1.4E-6
2/5	0.01023260167	0.**01**104	0.**010232**505	0.**010232**6406	6.E-5?
1/3	0.00065934248	I	0.**000659**771	0.**000659**343119	5.E-4?
1/4	0.00000053831	I	**5**888	0.**5383**683848E-6	1.3E-4?
1/5	0.000000000059815	I	I	0.817E-10	0.36

Table 2: Hermite-with-Pole Equation:Imaginary Part

ϵ	$\Im(\lambda)$	[27/27/27]	[27/27/27] Rel. err.	[33/33/33]	Rel. Err.
1	0.63002304156	0.**630023**615	9.1E-7	0.**63002**28836	2.5E-7
3/4	0.386770686076	0.**38677**10999	1.1E-6	0.**386770**7246426	2.9E-10
1/2	0.07805030263	0.**078050**6478618	4.4E-6	0.**07805030**01249	3.3E-8
2/5	0.01023260167	0.**01023260**7136699788	5.3E-7	0.**01023260**23764	6.9E-8
1/3	0.00065934248	**000659342**780021111	4.5E-7	0.**6593424**	6.8E-8
1/4	0.00000053831	0.**000000538**30718417	$<$ **5.E-6**	0.**5383**08437555	$<$ **5.E-6**
1/5	0.000000000059815	0.**5981**42597235	$<$ **2.E-5**	0.**5981**4142299068	$<$ **2.E-5**

$(\gamma + \log 2)\epsilon) \exp(-1/\epsilon^2)$. The singularity structure of this function is more complicated than that of the Gauss-Stielties integral.

The tables 1 and 2 and Fig.2 show the relative error as a function of the order of an approximant for diagonal sequences. Here we assume that the numerical solution obtained by method of shooting in [[**?**]] can be taken for exact. It could be, however, that the higher order approximants are more accurate than the shooting solution. The correct digits are shown in bold typeface in tables.

Note that accuracy improves nonmonotonically with the order of the approximant. This is due to the fact that for some N the polynomials P, Q acquire nearly-coincident roots in the interior of the interval $[0, 1]$. Since these roots do not cancel out exactly in $-Q/2P$, this allows a singularity to form at the location of the zero of P and deteriorate the accuracy over the entire interval $[0, 1]$.

The imaginary part of the eigenvalue is approximated by $\sqrt{Q^2 - 4PR}$. It is therefore important to find the zeros of $Q^2 - 4PR$ to know when the radical becomes real and thus non-approximant. It turns out that the radical has a double root at $x = 0$ and a couple of nearly-coincident zeros in the vicinity of the close roots of P and Q.

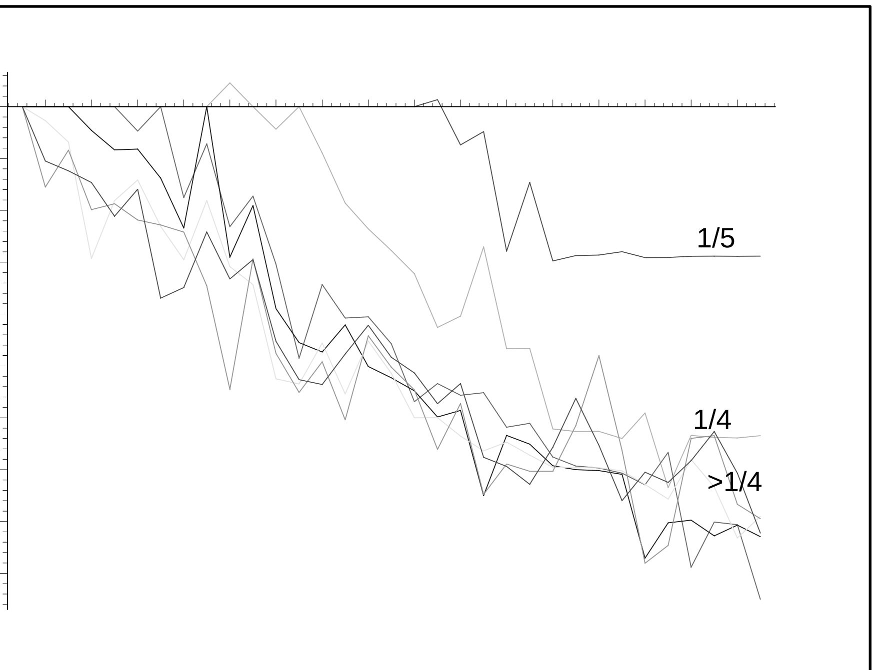

Figure 2: Relative errors (absolute error divided by the true imaginary part) for the imaginary part of the Hermite-with-Pole eigenvalue

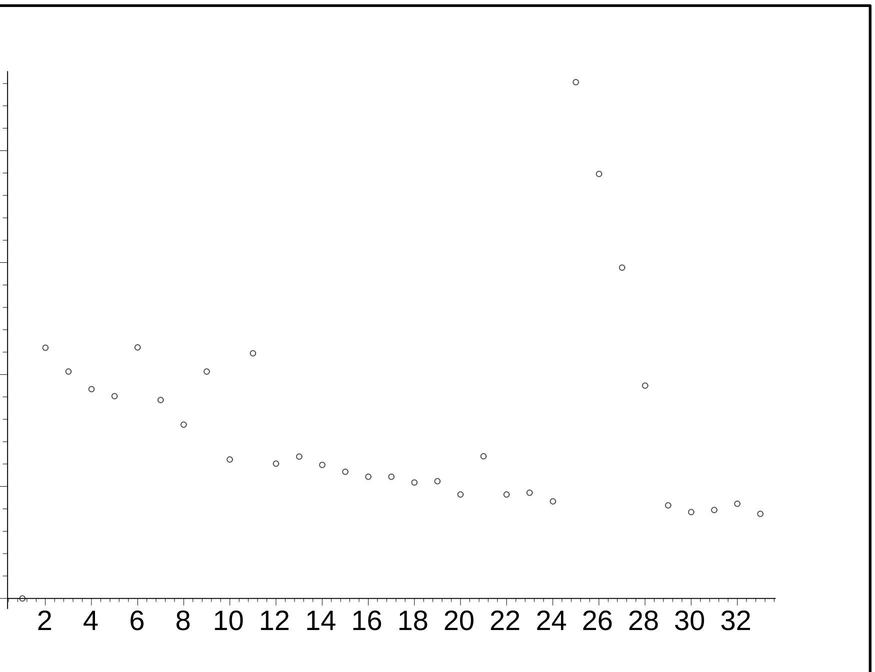

Figure 3: The largest root of the radical

Fig.3 shows the points where the radical first becomes real. Note that the points that lie off the curve actually represent nearly-coincident zeros and the radical is real only in a small neighborhood below the marked point.