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Journal of Computational Physics 222 (2007) 1–8

JOURNAL OF COMPUTATIONAL PHYSICS

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Short note

Padé–Gegenbauer suppression of Runge phenomenon in the diagonal limit of Gegenbauer approximations

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Received 27 November 2005; received in revised form 16 June 2006; accepted 20 June 2006
Available online 15 November 2006

Keywords: Padé–Gegenbauer reconstruction; Gegenbauer polynomials; Gibbs phenomenon; Runge phenomenon

1. Introduction

Gegenbauer reconstruction, developed by Gottlieb et al. [7,6,5,4,10], was developed to overcome the Gibbs oscillations introduced in a spectral expansion by a discontinuity. Since its appearance, Gegenbauer reconstruction has found numerous far reaching and diverse applications such as stiff differential equations, hyperbolic heat transfer, and the improvement in resolution of brain MRIs [2,9,11]. Although we will discuss Gegenbauer approximation, we approach the topic with the possible impact on Gegenbauer reconstruction in mind. Recently, a potential problem for Gegenbauer approximations was brought forth. Boyd demonstrated that for functions with singularities in the complex plane, the Gegenbauer approximation may introduce large oscillations near the boundaries, which he termed "generalized Runge phenomenon". These off-axis singularities are possibly troublesome for Gegenbauer approximations, leading to complications such as loss of accuracy and restricted parameters [3]. The purpose of this paper is to offer a method for sidestepping the generalized Runge phenomenon and the problems associated with it. In [8], an interpolation-based Padé–Jacobi reconstruction method was proposed for the reduction of oscillations induced by the Gibbs phenomenon. We introduce herein a new application of the interpolant defined in [8] – the Padé–Gegenbauer interpolant as a postprocessor to the Gegenbauer expansion. In the case where the Gegenbauer approximation of a function exhibits the generalized Runge phenomenon, application of the Padé–Gegenbauer postprocessor will suppress the oscillations. Let us first describe the framework of the problem in greater detail.

A Gegenbauer polynomial C_k^λ of degree k satisfies the orthogonality condition

$$\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}}C_k^\lambda(x)C_j^\lambda(x)\mathrm{d}x = \begin{cases} 0, & k \neq j, \\ \gamma_k^\lambda, & k = j, \end{cases} \tag{1}$$

where

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doi:10.1016/j.jcp.2006.06.032

$$\gamma_k^\lambda = \frac{\sqrt{\pi}\Gamma(k+2\lambda)\Gamma(\lambda+\frac{1}{2})}{k!\Gamma(2\lambda)\Gamma(\lambda)(k+\lambda)}. \tag{2}$$

A function $f(x)$ may be expressed by its Gegenbauer series on domain $[-1,1]$ as

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^\lambda C_k^\lambda(x), \tag{3}$$

where the coefficients $\hat{f}_k^\lambda$ are given by

$$\hat{f}_k = \frac{1}{\gamma_k^\lambda}\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}} f(x) C_k^\lambda(x)\mathrm{d}x. \tag{4}$$

For a fixed Gegenbauer order λ and truncation order N the maximum pointwise error of the approximant is defined as

$$E(\lambda, N) = \max_{x\in[-1,1]}\left| f(x) - \sum_{k=0}^{N} \hat{f}_k^\lambda C_k^\lambda(x)\right|. \tag{5}$$

Essentially, the Gegenbauer reconstruction method for eliminating the Gibbs phenomenon begins with the partial Fourier sum of a function and re-expands it as a partial sum of Gegenbauer polynomials, with coordinate changes so that the discontinuities occur at $x \pm 1$. By increasing the Gegenbauer order λ linearly with the truncation order N, the reconstruction is increasingly weighted away from the neighborhood of the discontinuity. Due to theory, we concern ourselves with the diagonal limit, $\lambda = \beta N$ as $N \to \infty$, of Gegenbauer approximants as this behavior is important in Gegenbauer reconstruction. For an appropriate choice of β, it can be shown that the diagonal limit converges [6]. In this work we restrict ourselves to examining the behavior of the Gegenbauer approximants of functions for the following reason. The Fourier approximation of a function $\tilde{f}$ will behave like the function itself except in the case where the number of Fourier coefficients is very small, of O(10) [3]. The Gegenbauer reconstruction, based on the Fourier approximation $\tilde{f}$, will therefore exhibit the same behavior as the Gegenbauer approximant. For restoration of exponential convergence, the Gegenbauer order of the polynomials λ must increase linearly with the Gegenbauer truncation order N [5].

Definition 1.1. The diagonal approximation is a sequence of approximations

$$\mathscr{E}(\beta, N) \equiv E(\beta N, N), \tag{6}$$

where $E(\beta N, N)$ is given by Eq. (5).

A sequence $\mathscr{E}(\beta, N)$ is generated by increasing the order of truncation N while the Gegenbauer order is determined by $\lambda = \beta N$ where β is a positive constant.

Boyd demonstrates numerically in [3] that the Gegenbauer approximation of a function with a singularity on the imaginary axis may diverge near the endpoints of the interval if the singularity is close enough to the real axis. Tests showed that this divergence can be so large that a sequence of approximations $\mathscr{E}(\beta, N)$ as defined by Eq. (6) may actually diverge for functions with poles sufficiently close to the real axis – the diagonal limit tends to infinity. Boyd rightfully suggests that this phenomenon could be problematic for the use of the Gegenbauer reconstruction. However the analysis of the behavior of the vertical limit, N is fixed and $\lambda \to \infty$, hints at a possible technique to deal with these problems. The vertical limit of the Gegenbauer approximant behaves like a power series centered around $x = 0$. Let us outline a proof of this fact which can also be found in [3].

Proposition 1.2 (Vertical limit of Gegenbauer approximation). *Suppose that we normalize the Gegenbauer polynomials $C_n^\lambda(x)$ by $C_n^\lambda(1)$ such that the normalized polynomial has a maximum value of* 1 *at* $x = 1$. *With this normalization, the nth Gegenbauer polynomial asymptotes to x^n for $x \in [-1,1]$.*

Proof. We can define the normalized polynomials as

$$\frac{C_n^\lambda(x)}{C_n^\lambda(1)} = \sum_{k=0}^{n/2} B_n^k x^{n-k}.$$

Then

$$B_n^k = \frac{(-1)^k \Gamma(\lambda + n - k) 2^{n-2k}}{\Gamma(\lambda) k! (n-2k)!}$$

using definitions for $C_n^\lambda(x)$, $C_n^\lambda(1)$ found in [1] (pp. 775, 777, respectively) we find using the asymptotics of the factorial function that

$$\lim_{m\to\infty} \frac{B_n^k}{B_n^0} = \frac{1}{k! 2^{2k} m^k}$$

and

$$\frac{C_n^\lambda(x)}{C_n^\lambda(1)} = x^n \left(1 + O\left(\frac{1}{m}\right)\right). \quad \square$$

We therefore propose the Padé–Gegenbauer interpolant specifically because it is a rational interpolant with a larger radius of convergence than a power series.

In Section 2 we give a brief introduction to the properties and construction of Padé–Gegenbauer interpolants. Section 3 is devoted to numerical examples illustrating the results of the Padé–Gegenbauer interpolation. We demonstrate the ability of the Padé–Gegenbauer interpolant to reduce or remove the oscillations caused by the singularity in the imaginary axis and restore the accuracy of the expansion. We close with concluding remarks in Section 4.

2. Padé–Gegenbauer reconstruction

We consider the same test function as Boyd,

$$f_1(x; z) = \frac{z^2}{z^2 + x^2}. \tag{7}$$

As another example we choose the function

$$f_2(x; z) = \frac{1}{\log(z^2 + x^2 + 1)}. \tag{8}$$

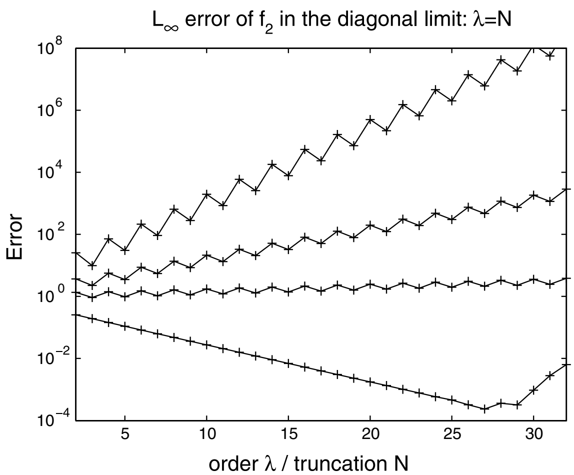

Fig. 1. Log of maximum pointwise errors of the sequences $\mathscr{E}(1, N) = E(N, N)$ for the function $f_2(x; z) = 1/\log(z^2 + x^2 + 1)$ for different values of z and $\beta = 1$. As z decreases, the pole moves closer to the real axis and causes divergence of the sequence of approximants.

This rational function with a non-polynomial denominator is a good test for Padé–Gegenbauer methods because it does not have an exact Padé approximant. Fig. 1 consists of various sequences for the test function f_2. It shows that for fixed $\beta = 1$, the sequence with a pole at $i\,(z = 1)$ converges, but as the pole moves closer to the real axis the sequence diverges exponentially. For smaller values of β the singularities must be moved closer to the origin to observe the same phenomenon-results for f_1 are similar and may be found in [3].

As Fig. 1 illustrates, singularities can be devastating for the Gegenbauer reconstruction. We propose the use of the Padé–Gegenbauer postprocessor as a method to recover accuracy for a function exhibiting this generalized Runge phenomenon. The construction of the postprocessor is described in detail in [8] for the Padé–Legendre case. Below we describe, in brief, the construction of the Padé–Gegenbauer interpolant.

We seek a Padé–Gegenbauer interpolant, $\mathscr{S}(x)$, of order (M, L) that interpolates the function f at $N + 1$ collocation points given by the form

$$\mathscr{S}(x) = \frac{\mathscr{P}(x)}{\mathscr{Q}(x)},$$

where

$$\mathscr{P}(x) = \sum_{i=0}^{M} a_i C_i^{\lambda}(x), \quad \mathscr{Q}(x) = \sum_{i=0}^{L} b_j C_j^{\lambda}(x).$$

Definition 2.1. Given integers M and L and polynomials $\mathscr{P} \in \mathbb{P}_M$, $\mathscr{Q} \in \mathbb{P}_L$ we call $(\mathscr{P}, \mathscr{Q})$ a solution to the (N, M, L) Padé–Gegenbauer interpolation problem of a function f if $\mathscr{Q}$ has a constant sign on the domain $[-1, 1]$ i.e.

$$\forall x \in [-1, 1], \quad \mathscr{Q}(x) > 0, \tag{9}$$

and

$$\forall \varphi \in \mathbb{P}_N, \quad \langle \mathscr{Q} f - \mathscr{P}, \varphi \rangle_N = 0. \tag{10}$$

We clarify the interpolation properties of $\mathscr{S}$ below.

Remark 2.2 (*Interpolation*). Given the polynomials $(\mathscr{P}, \mathscr{Q})$ that are a solution to the Padé–Gegenbauer interpolation problem, we take $\varphi \in \mathbb{P}_N$ in (10) to be ℓ_i, where ℓ_i is the Lagrange polynomial based on the quadrature points x_i. This gives the system

$$\forall i = 0, \ldots, N: \quad (\mathscr{P} - \mathscr{Q} f)(x_i) = 0. \tag{11}$$

Since $\mathscr{Q}(x_i) \neq 0$, the function $\mathscr{S}(x)$ interpolates f, i.e.

$$\forall i = 0, \ldots, N: \quad \mathscr{S}(x_i) = f(x_i). \tag{12}$$

We must also concern ourselves with the choice of parameters M and L. To ensure uniqueness we require throughout the rest of the paper that the parameters satisfy the following condition:

$$M + L \leqslant N. \tag{13}$$

Proof of uniqueness can be found in [8].

In order to formulate the computational system we take $\varphi_i = C_i^{\lambda}$ in Eq. (10) which gives the system

$$\forall C_n^{\lambda} \in \mathbb{P}_N, \quad \langle \mathscr{Q} f - \mathscr{P}, C_n^{\lambda} \rangle_N = 0. \tag{14}$$

From Eq. (14), we find that the coefficients $\{a_i\}$ and $\{b_j\}$ of the Padé–Gegenbauer expansion must satisfy two systems,

$$\sum_{j=0}^{L} b_j h_{kj} = 0, \quad k = M + 1, \ldots, N, \tag{15}$$

$$\sum_{j=0}^{L} b_j h_{kj} = a_k, \quad k = 0, \ldots, M, \tag{16}$$

where

$$h_{kj} = \frac{1}{\gamma_k^\lambda} \sum_{i=0}^{N} f(x_i) C_k^\lambda(x_i) C_j^\lambda(x_i) \omega_i.$$

The computation of the coefficients h_{kj} can be computed entirely as matrix products. We require the knowledge of the function value at the appropriate quadrature points, $(x_i)_{i=0}^N$ as well as the associated weights $(\omega_i)_{i=0}^N$, and define the following matrices:

$$D = \begin{bmatrix} C_0^\lambda(x_0) & \cdots & C_0^\lambda(x_N) \\ \vdots & & \vdots \\ C_N^\lambda(x_N) & \cdots & C_N^\lambda(x_N) \end{bmatrix}$$

and $F = \mathrm{diag}(u(x_0)\omega_0, \ldots, u(x_N)\omega_N)$. The entries h_{kj} can then be computed as

$$H = \begin{bmatrix} h_{00} & \cdots & h_{0N} \\ \vdots & & \vdots \\ h_{N0} & \cdots & h_{NN} \end{bmatrix} = (D \times F) \times D',$$

Note that Eq. (15) has L equations and $L + 1$ unknowns, therefore there exists a non-zero solution to the system. These equations can be solved in more than one way. Either they are solved by finding the null space of the system using some linear algebra toolbox or one of the unknown coefficients q_i can be fixed such that we have a square system. If we do choose to eliminate one degree of freedom we must choose which coefficient is fixed such that the resultant square matrix is invertible. For further details on the computation of the Padé–Gegenbauer interpolant we refer to [8].

3. Numerical tests

We now apply the Padé–Gegenbauer method to the two test functions we have presented. Let us be more specific about the setting of our tests. We shall begin our examination by requiring that the order of our interpolant satisfies the condition

$$N = M + L, \tag{17}$$

and choose to use Gegenbauer Gauss quadrature points for calculation of the Padé–Gegenbauer interpolant. The function values at the Gegenbauer Gauss points have been obtained by interpolation. This situation is close to what we would expect if reading a Gegenbauer reconstruction at the quadrature points - some error is present but not of the same magnitude as near the boundary.

As an example of the Padé–Gegenbauer method, Fig. 2 illustrates the Runge phenomenon observed for the Gegenbauer expansion of the function $f_1(x; 2/3)$ as well as a successful Padé–Gegenbauer interpolant where accuracy has been restored.

We consider sequences of Padé–Gegenbauer interpolants where the order of the denominator L scales with the order of the Gegenbauer expansion N, i.e. $L = N/2$. As the left plot of Fig. 3 illustrates, this choice of the denominator order L yields a reasonable reduction of the maximal error for all positions of the pole z. On the right in Fig. 3, we display the L_∞ error of sequences of Padé–Gegenbauer interpolants for our second test function, f_2. We point out that for the test functions presented, the case where $z = 1/4$ does not yield highly accurate results. However, we have shown only one Padé–Gegenbauer interpolant for each function when in fact there are many more possibilities, especially if we remove the condition of Eq. (17).

If instead we seek the order of the Padé–Gegenbauer interpolant that minimizes the error of the function, we find that we can achieve very good accuracy for all of the functions, regardless of the pole position. In order to illustrate the strength of the Padé–Gegenbauer interpolant we will use our knowledge of the exact function to find the interpolant that minimizes the error. We examine the interpolants that satisfy the looser condition

$$M + L \leqslant N.$$

Note that the construction of the interpolant was defined without constraints on the parameters M and L.

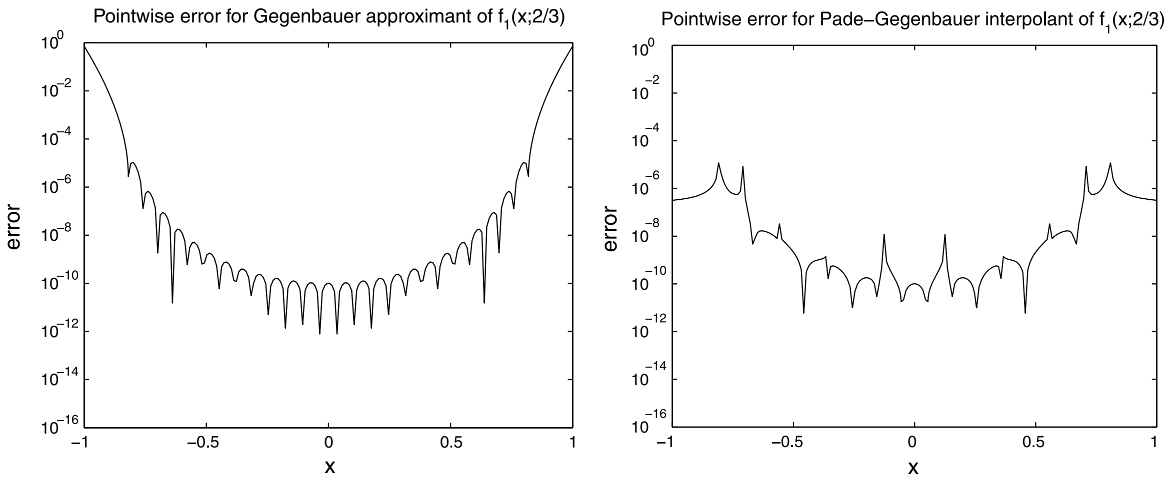

Fig. 2. On the left we have the pointwise error of the Gegenbauer approximant of order $N = 24$ to the function $f_1(x; 2/3)$. The large error in the narrow region near the boundaries is the Runge phenomenon. The right figure shows the Padé–Gegenbauer interpolant of order (12, 12) for the same function and shows the suppression of the Runge phenomenon. Both figures are shown on a uniform grid of 200 points.

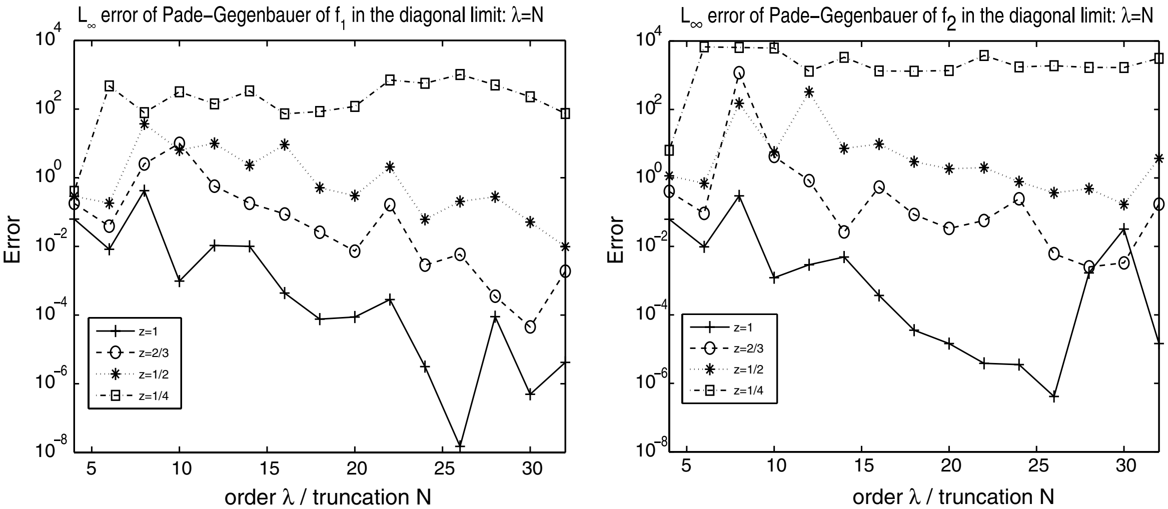

Fig. 3. Log of maximum pointwise error of sequences of Padé–Gegenbauer interpolants of the function for various values of z and fixed $M = N/2$, $L = N/2$ with $\beta = 1$. Left: f_1; right: f_2.

We consider the functions f_1 and f_2 for the pole positions, $z = 1/2, 1/4$, both leading to divergence of the Gegenbauer approximants. Equally good results are obtained for the other pole values as well. The top plots of Fig. 4 show the error of the most accurate interpolants of the function f_1. The function f_1 has an exact Padé–Gegenbauer interpolant of order $(0, 2)$ which yields extremely accurate results for all values of the pole z. The plots in Fig. 4 show that the orders of the interpolants hover around this exact order for all values of N and z, and differ only because of rounding error. The test function f_2 was constructed to display the same Runge behavior as f_1 although it does not have an exact Padé–Gegenbauer interpolant. The bottom plots of Fig. 4 show that the error drops off as N increases. Also, we note that the curves look similar regardless of the pole position, though the interpolant order (M, L) may be very different for the same truncation order N.

Of course in these examples knowledge of the exact function is used to determine the orders that give the best accuracy, which is not a realistic situation for computational problems. However the strength of the method lies in the ease and speed of computing many interpolants or every possible one. Choosing the ‘‘best’’ interpolant is thereafter user-defined. General guidelines and strategies for choosing the order of the Padé–Gegenbauer interpolant are found in [8].

4. Concluding remarks

In this work we have proposed a rational interpolant as a means of reducing the generalized Runge phenomenon observed in the Gegenbauer approximants of functions with off-axis singularities. This method requires the knowledge of the function values at Gegenbauer Gauss quadrature points but does not require that the user know the location of the singularities of the function. There is also no need to force β to be small as shown in the examples above. These properties, along with an efficient algorithm for computing the interpolants as laid out in [8] make the Padé–Gegenbauer postprocessor method as well suited for engineering and science applications as for exact functions. This does not mean that this Gegenbauer Runge phenomenon is no longer problematic, but rather that it may often be possible to circumvent the problem and regain accuracy of the expansion with minimal postprocessing.

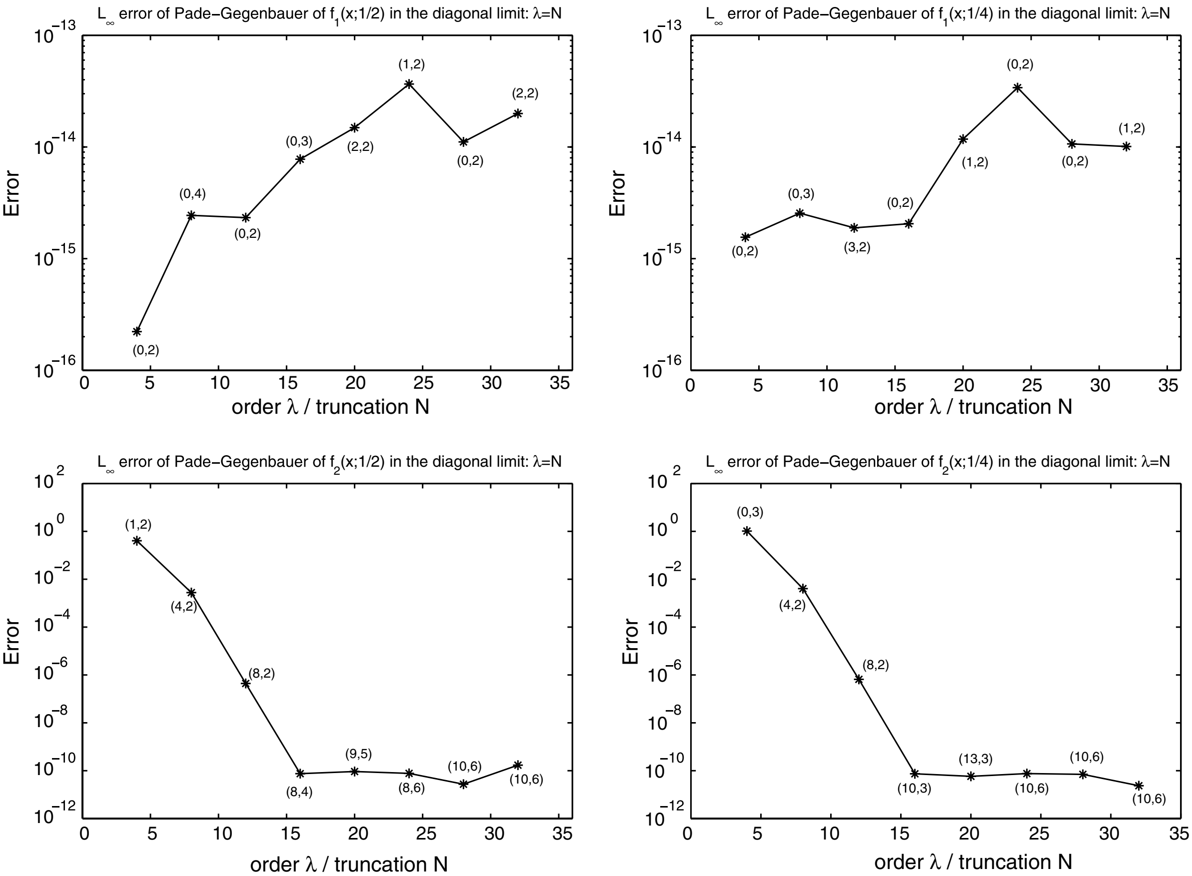

Fig. 4. L_∞ error of sequences of Padé–Gegenbauer interpolants for various values of z of both functions and $\beta = 1$. The interpolant of order (M, L) that minimizes the L_∞ error is shown on the plot. Top: $f_1(x; 1/2)$ and $f_1(x; 1/4)$; bottom: $f_2(x; 1/2)$ and $f_2(x; 1/4)$.

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