



Trouble with Gegenbauer reconstruction for defeating Gibbs' phenomenon: Runge phenomenon in the diagonal limit of Gegenbauer polynomial approximations

John P. Boyd *

Laboratory for Scientific Computation, Department of Atmospheric, Oceanic and Space Science, University of Michigan, 2455 Hayward Avenue, Ann Arbor, MI 48109-2143, USA

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Abstract

To defeat Gibbs' phenomenon in Fourier and Chebyshev series, Gottlieb et al. [D. Gottlieb, C.-W. Shu, A. Solomonoff, H. Vandeven, On the Gibbs phenomenon I: recovering exponential accuracy from the Fourier partial sum of a nonperiodic analytic function, *J. Comput. Appl. Math.* 43 (1992) 81–98] developed a "Gegenbauer reconstruction". The partial sums of the Fourier or other spectral series are reexpanded as a series of Gegenbauer polynomials $C_n^m(x)$, recovering spectral accuracy even in the presence of shock waves or other discontinuities. To achieve a rate of convergence which is exponential in N , however, Gegenbauer reconstruction, requires increasing the order m of the polynomials linearly with the truncation N of the series: $m = \beta N$ for some constant $\beta > 0$. When the order m is fixed, it is well-known that the Gegenbauer series converges as $N \rightarrow \infty$ everywhere on $x \in [-1, 1]$ if $f(x)$, the function being expanded, is analytic on the interval. But what happens in the diagonal limit in which m, N tend to infinity simultaneously? We show that singularities of $f(x)$ off the real axis can destroy convergence of this diagonal approximation process in the sense that the error diverges for subintervals of $x \in [-1, 1]$. Gegenbauer reconstruction must therefore be constrained to use a sufficiently small ratio of order m to truncation N . This "off-axis singularity" constraint is likely to impair the effectiveness of the reconstruction in some applications.

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Keywords: Gegenbauer polynomials; Gibbs' phenomenon; Shocks; Gegenbauer reconstruction of discontinuities; Fourier series

* Tel.: +1 734 764 3338; fax: +1 734 764 5137.

E-mail address: jpboyd@umich.edu.

1. Introduction

When a function $f(x)$ is expanded as series of basis functions that depend upon a parameter m as well as upon a degree n , the error in truncating the approximation after the N th term defines the two-dimensional array of maximum pointwise errors

$$E(m, N) \equiv \max_{x \in [-1,1]} \left| f(x) - \sum_{n=0}^N a_n^m C_n^m(x) \right|. \tag{1}$$

In our application, the C_n^m are the Gegenbauer polynomials. For a fixed m , these polynomials are defined by the orthogonality integral

$$\int_{-1}^1 C_n^{(m)} C_{n'}^{(m)} (1-x^2)^{m-1/2} dx = \begin{cases} 0 & n \neq n', \\ \frac{\pi 2^{1-2m} \Gamma(n+2m)}{n!(n+m)\Gamma(m)^2} \equiv h_n^m & n = n', \end{cases} \tag{2}$$

where n is the degree of the polynomial. We shall usually plot the error array and so on for $m = \text{integer} + 1/2$ so that the weight function inside the integral is non-singular.

A typical error array for a particular $f(x)$ is illustrated in Fig. 1. Standard convergence theory is what we shall dub the “horizontal limit”: $N \rightarrow \infty$ while the Gegenbauer order m is fixed. What happens is described by the following:

Theorem 1.1 (Gegenbauer ellipse of convergence). *The Gegenbauer series of $f(x)$ for FIXED m converges in the largest ellipse with foci at $x = \pm 1$ in which $f(x)$ is analytic. (Stated for the more general family of Jacobi polynomials on p. 243 of [33].)*

This theorem is very powerful because it implies that if $f(x)$ is analytic on the expansion interval, $x \in [-1,1]$, then the Gegenbauer polynomial series for fixed m is guaranteed to converge everywhere on the expansion interval.

The “vertical” limit describes what happens for fixed N but Gegenbauer order tends to infinity. Since the Gegenbauer series is a least-squares approximation with the weight function $(1-x^2)^{m-1/2}$, which becomes more and more concentrated around the origin as m increases, the vertical Gegenbauer approximation tends to the $(N + 1)$ -term truncation of the power series about $x = 0$. This is rigorously proved in Appendix A.

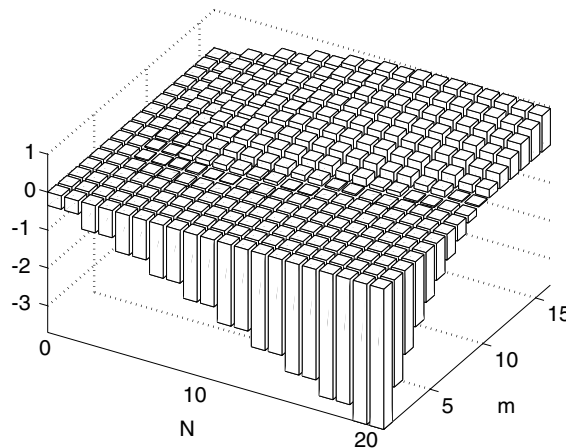


Fig. 1. The base-10 logarithm of the error array $E(m, N)$ is plotted for $f(x) = (1/4)/([1/4] + x^2)$, which has poles at $\pm i/2$.

This is rather alarming because the power series – and therefore the vertical Gegenbauer limit – will *diverge* over part of the expansion interval, $x \in [-1,1]$, unless $f(x)$ is free of singularities in the unit disk in the complex plane, $|x| \leq 1$.

Our goal is to understand the diagonal approximations defined formally by the following.

Definition 1.1 (Diagonal Gegenbauer approximation). With the error $E(m,N)$ as defined by (1), a “diagonal limit” or “diagonal approximation” is a sequence of approximations

$$\mathcal{E}(\beta; N) \equiv E(\beta N, N), \tag{3}$$

which are obtained by varying the order with truncation N according to the rule

$$m = \beta N, \tag{4}$$

where β is a positive constant.

If the diagonal limit of Gegenbauer approximation behaves similarly to the vertical limit, then the approximation may diverge for some x on the expansion interval – a possible land-mine exploding the validity of the Gegenbauer reconstruction of Gibbs’ phenomenon.

In the following section, we show numerically that this divergence does happen and analyze the details.

2. Generalized Runge phenomenon for diagonal Gegenbauer approximations

Fig. 2 shows the maximum pointwise error for four different $f(x)$ in the diagonal limit with $\beta = 1$. Just as for an ordinary power series, the error falls exponentially when the singularity is sufficiently far from the real axis. However, when the poles are moved closer to the origin, the approximation *diverges* exponentially!

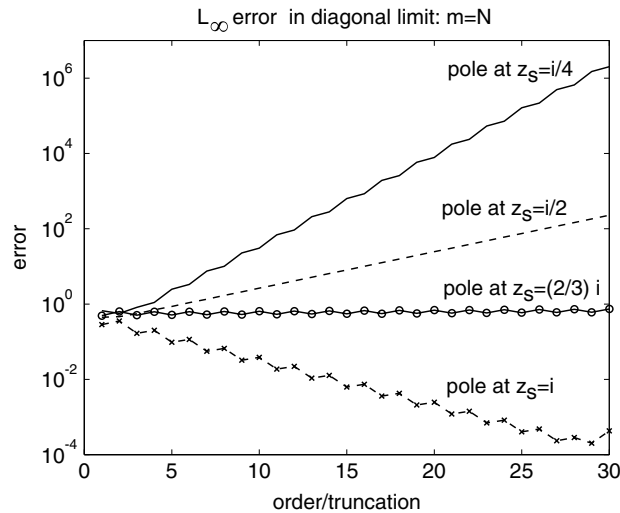


Fig. 2. The maximum pointwise errors for the approximation of four different functions of the form $f(x) = y^2/(y^2 + x^2)$ in the diagonal limit with $\beta = 1$. That is, $E(m,m)$ is plotted, where m is the Gegenbauer order, which is set equal to the truncation N for each approximation. This $f(x)$ has complex conjugate poles on the imaginary axis at $x = \pm iy$. We arbitrarily chose $\beta = 1$ for ease of visualization; $\beta = 1/4$ is more typical in Gegenbauer reconstruction. However, the same phenomenon is observed for smaller β ; it is only necessary to move the singularities closer to the expansion interval as β decreases.

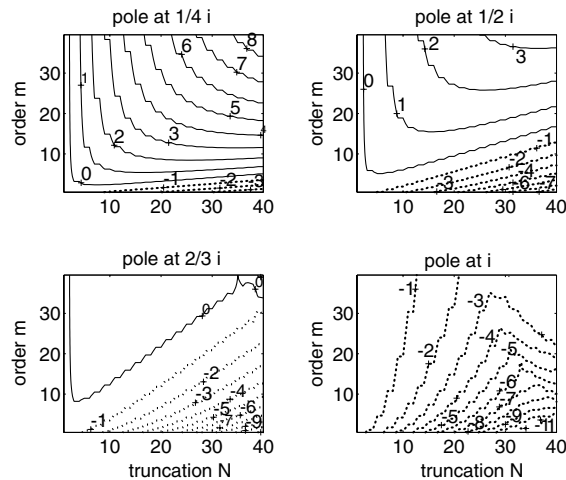


Fig. 3. Isolines of the base-10 logarithm of the maximum pointwise errors for the approximation of functions of the same form as in the previous graph, $f(x) = y^2/(y^2 + x^2)$ for four different imaginary values of y , as Gegenbauer series for various orders m (vertical axis) and truncation N (horizontal axis). Solid contours denote 100% or larger error relative to the maximum of each function; negative contours are dashed, and indicate that the approximation has an absolute error of 0.1 or less.

Fig. 3 shows the contours in the N – m plane of the logarithm of the error for the same four functions as in Fig. 2. The contours of zero or positive logarithm – 100% or larger error – are solid while the dotted contours (negative powers-of-ten) denote at least a moderate accuracy. The lower right panel, which is almost all dashes, shows that when the singularity is at one or further from the real axis, almost all diagonal approximations converge, regardless of the value of the parameter $\beta \equiv m/N$. When the pole is at $2/3 i$, the error contours are roughly parallel to the diagonal line $m = N$. The error neither increases nor decreases along this line. However, it is possible to obtain convergence by moving on a line of shallower slope, that is, by setting $m = \beta N$ for $\beta < 1$ so that the order m increases more slowly than the truncation. The top panels show that as the poles move closer to the real axis, the region of accuracy in the m – N plane shrinks, and it is necessary to use a shallower and shallower slope, i.e., smaller and smaller $\beta = m/N$, in order to obtain any accuracy at all.

Fig. 4 shows what happens as a function of x : the diagonal Gegenbauer approximations do not diverge over the entire expansion interval, but only in subintervals near the boundaries. The subintervals of divergence for the case illustrated are roughly $|x| \in [0.8, 1]$; these widen as the singularity moves closer to the real axis, and shrink to nothing – convergence everywhere on $x \in [-1, 1]$ – when the singularity at $z_s = i$ or farther.

Runge showed at the turn of the twentieth century that polynomial interpolation at evenly spaced points could diverge. Just as here, the interpolant converged on the center part of the interval while diverging near the boundaries of the interval spanned by the interpolation points. Since something very similar is happening here – divergence near the endpoints because of complex-plane singularities – it is reasonable to dub the Gegenbauer-diagonal-limit divergence a “generalized Runge phenomenon”.

3. Convergence domain in the complex plane

The preceding examples have employed functions which are singular on the imaginary axis. An obvious question is: What happens when the location of the singularity is different?

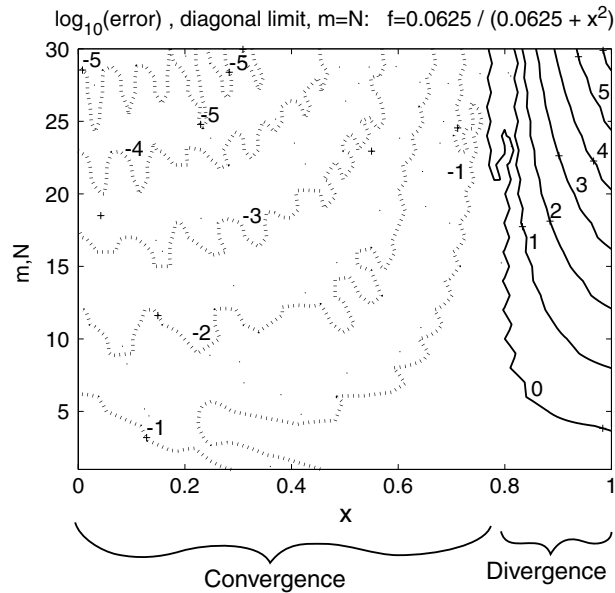


Fig. 4. Isolines of the base-10 logarithm of the maximum pointwise errors for the approximation of $f = (1/16)/([1/16] + x^2)$ as Gegenbauer series in the diagonal limit, $m = N$, for various orders m (vertical axis) and x (horizontal axis). Solid contours denote 100% or larger error relative to the maximum of each function; negative contours are dashed, and indicate where the approximation is accurate. Because this function (and the errors) are symmetric with respect to $x = 0$, only the right half of the interval is shown.

Fig. 5 shows the errors for the $m = N$ approximant as functions of the location z_s of the pole in the upper right quadrant of the function

$$f^{\text{symm,pole}}(x; z_s) \equiv [\Im(z_s)]^2 \left\{ \frac{1}{[\Im(z_s)]^2 + (x - \Re(z_s))^2} + \frac{1}{[\Im(z_s)]^2 + (x + \Re(z_s))^2} \right\}. \tag{5}$$

The form is chosen so that $f^{\text{symm,pole}}$ is symmetric with respect to both the real and imaginary axes, making it sufficient to graph only the upper right quadrant of the z_{sing} plane.

The zero isoline, that is, where the maximum pointwise error is equal to one, is roughly the boundary between convergence and divergence. The large errors in the region of solid contours show that a pole in that region will force the diagonal Gegenbauer approximation (with $m = N$) to diverge. However, the Gegenbauer diagonal approximation converges when the singularity is outside the heavy contour. The graph illustrates the errors for $m = N = 30$ and the contours are rather wiggly; as a check, the zero contours for both $m = N = 20$ and $m = N = 30$ are shown as the dashed lines and the heavy solid curve is a smooth fit between them. The three curves are barely distinguishable, showing that the boundary is rather well-defined.

The divergence region is widest for singularities on the imaginary axis and then curves closer and closer to the real axis as $\Re(z_s)$ approaches one. As the parameter β decreases, that is, as the ratio m/N decreases, the region of divergence will shrink (not illustrated).

4. Theory of Gegenbauer approximation

Gottlieb and Shu [20] review two theorems on convergence of diagonal approximants. We combine these into one, altering their notation into ours, as follows:

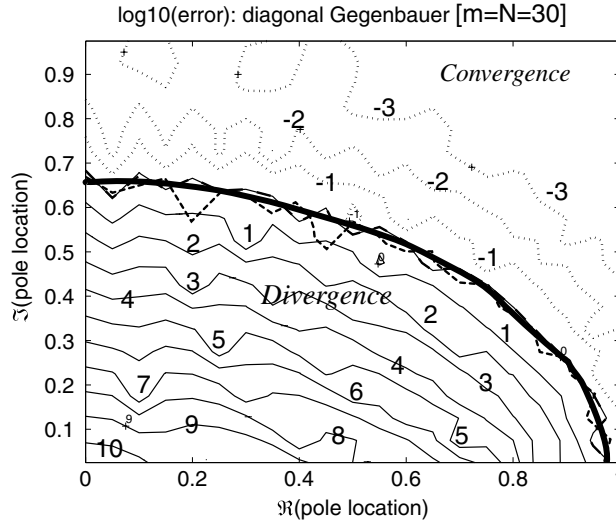


Fig. 5. Isolines of the base-10 logarithm of the error in the diagonal Gegenbauer approximation with $m = N = 30$ of the function $f^{\text{symm,pole}}(x; z_s)$ in the complex z_s -plane, where the parameter z_s is the location of the simple pole of $f^{\text{symm,pole}}$ in the upper right quadrant. The zero isoline (i.e., an error of 10^0) is the boundary between convergence and divergence. The heavy solid curve is a slightly smoothed representation of this contour, which ceases to change with the truncation when N is sufficiently large.

Theorem 4.1. Let $m = \beta N$ where m is the order of the Gegenbauer polynomials and N is the Gegenbauer truncation and $\beta > 0$ is a constant. Define the error for the Gegenbauer polynomials, as in (1), to be

$$E(m, N) \equiv \max_{x \in [-1, 1]} \left| f(x) - \sum_{n=0}^N a_n^m C_n^m(x) \right|. \tag{6}$$

1. If $f(x)$ is analytic everywhere in an ellipse in the complex x -plane with foci at ± 1 and axes $(\cosh(\mu), \sinh(\mu))$, then

$$E(\beta N, N) \leq \text{constant } N Q^N \exp(-N\mu), \tag{7}$$

where

$$Q(\beta) \equiv \frac{(1 + 2\beta)^{(1+2\beta)/2}}{(2\beta)^\beta}. \tag{8}$$

2. If $f(x)$ is analytic at all points in the complex x -plane which lie a distance ρ or closer to any point of the interval $x \in [-1, 1]$, then

$$E(\beta N, N) \leq \text{constant } N \tilde{Q}^N \rho^{-N}, \tag{9}$$

where

$$\tilde{Q}(\beta) \equiv \frac{(1 + 2\beta)^{1+2\beta}}{\beta^\beta 2^{1+2\beta} (1 + \beta)^{1+\beta}}. \tag{10}$$

3. For any $f(x)$ that satisfies the first assumption, the diagonal Gegenbauer approximation will converge exponentially fast if β is chosen sufficiently small, that is, if the slope of order/truncation is sufficiently small, so that

$$Q(\beta) < \exp(\mu). \tag{11}$$

4. For any fixed $\beta > 0$, it is always possible to find functions that are analytic on the real interval $x \in [-1, 1]$ for which both bounds fail to guarantee convergence.

Fig. 6 shows representative curves for the two conditions in the theorem. The fourth proposition in the theorem is not in their review, but is easily proved by considering a function with singularities at $x = \pm i\epsilon$: for any β , one can always find a sufficiently small $\epsilon > 0$ such that Q and \tilde{Q} are insufficiently small to guarantee convergence.

The good news is that the third condition shows that for any function which is analytic on the interval and within an ellipse of finite eccentricity around it, the diagonal Gegenbauer approximation can be guaranteed to converge.

The first piece of bad news is that small β seriously degrades the accuracy of the Gegenbauer reconstruction of functions with shock waves or other discontinuities which is discussed in the following section.

The second piece of bad news is that the theorem is consistent with the numerical results given earlier: for fixed β , it is always possible to find f that are analytic on $x \in [-1, 1]$, but break the theorem.

Gottlieb and Shu give both bounds because the geometry of the curves of constant μ and ρ are different, and one bound or the other may be best for a given $f(x)$. Unfortunately, neither bound is tight. When $\beta = 1$, for example, $Q = 2.6$ and $\tilde{Q} = 0.84$. For a singularity on the imaginary axis, the theorem guarantees convergence only when the singularity is further than 1.1 and 0.84 from the real axis, respectively. The

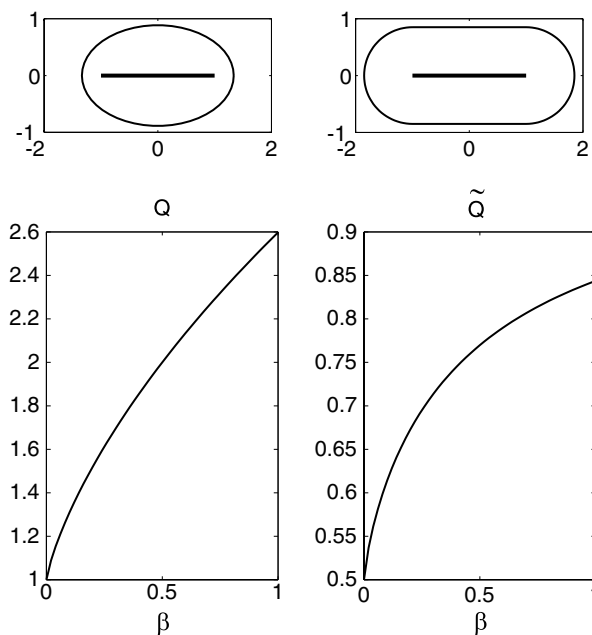


Fig. 6. Upper left: a typical ellipse in the complex x -plane with foci at $x = \pm 1$. Upper right: a typical set of points which lie a distance ρ from the nearest point of the interval $x \in [-1, 1]$, which is shown in both panels as the thick horizontal line segment. Lower graphs: the functions Q and \tilde{Q} which appear in Gottlieb and Shu’s theorem.

numerical calculations show that with $m = N$, the approximation converges until the singularity is within about 0.66 of the real axis.

The important point is that there is no contradiction between the theorems and the numerical results: complex-plane singularities can destroy convergence for any finite ratio of order to truncation, β .

5. Gegenbauer reconstruction of shocks and discontinuities

The strategy of Gottlieb et al. [21] is simple: the Fourier partial sums are reexpanded as a Gegenbauer series (the shocks can always be moved to $x = \pm 1$ by stretching the coordinate; their method applies to Chebyshev and other spectral series, too, but for simplicity we shall discuss only Fourier series with a discontinuity at $x = \pm 1$). If the order m is fixed, the Gibbs' oscillations in the partial sums of the Fourier series will poison the polynomial series, too. The polynomial expansion will converge only as $O(N^{-k})$ for some finite $k > 0$ that increases with m . By increasing the order m linearly with the truncation N , the polynomial approximation is weighted more and more heavily away from the “danger zone” of the neighborhood of the discontinuities and of large oscillations in the Fourier sums. By judiciously choosing the parameter $\beta = m/N$ and also the ratio of the Gegenbauer truncation N to the Fourier truncation N_f , always so that N is much smaller than N_f , one can prove that the diagonal limit converges, and yields a good approximation to the discontinuous function [20]. The success of Gegenbauer reconstruction has spawned an industry of theoretical papers [21,16–19,12,9,10,23–25,32,26,11] and applications in fluid mechanics [29–31,7], hyperbolic waves [15], local Fourier methods [35,36] and medical imaging [2,1,3,14]. The reconstruction procedure has recently been extended to high order finite difference (WENO) computations by Gottlieb et al. [22].

The only worry is that in applications, most functions are not free of singularities everywhere in the complex x -plane, but rather have poles or branch points at finite x . We have already seen that such singularities are a potential disaster for diagonal Gegenbauer approximations.

However, there is a subtlety: the reconstruction is not applied to $f(x)$ itself, but rather to a function \tilde{f} which is a *trigonometric polynomial*. By definition, \tilde{f} is an entire function, free of all singularities. Does this exempt the Gegenbauer reconstruction from difficulties?

The answer is no. We have carried out a thorough study with several figures which were deleted from the final draft, but is available from the author. Unless the number of Fourier terms, N_f , is $O(10)$, far smaller than in any reasonable reconstruction procedure, the trigonometric polynomial \tilde{f} will impersonate the singular function $f(x)$ sufficiently well so that, insofar as the Gegenbauer Runge Phenomenon is concerned, there is no meaningful difference between them.

6. Conclusions

When the order m increases with the truncation N , what we have dubbed the “diagonal limit” of an approximation process for a class of polynomials that contain a parameter m , new numerical phenomena may appear and convergence theory must be completely rethought. In particular, the theorem that Gegenbauer polynomials always converge on the expansion interval $x \in [-1, 1]$ as $N \rightarrow \infty$ for fixed order m must be replaced by the statement that the diagonal approximation may diverge near the ends of the interval even for a function $f(x)$ which is analytic everywhere on the expansion interval.

This discovery of a generalized Runge phenomenon has been made by numerical experiments. Future work should try to capture this Runge divergence in asymptotic approximations. Szegő [33, p. 249] gives the exact expansion coefficients for the function $f = 1/(y - x)$, proportional to associated Legendre functions of the second kind, $Q_n^m(y)$. An asymptotic approximation for the Legendre functions, *uniformly* valid

in the limit (m, n) go to infinity *simultaneously*, would give theoretically what here has been explored only numerically. But this would be only the beginning of a rich new area of “diagonal” approximation theory.

Does the Runge Phenomenon foretell the death of Gegenbauer reconstruction? No; the method has triumphed in a number of demanding real-world applications such as [7,2,1,30,3]. The mere presence of a minefield does not guarantee an explosion. Indeed, Gottlieb and Shu [20] proved that the Gegenbauer expansion can be guaranteed to converge in the diagonal limit if the ratio of order divided by truncation is sufficiently small. However, their theorems only show that small $\beta \equiv m/N$ is *sufficient* for convergence. We have here shown that small β is unfortunately *necessary* for convergence when $f(x)$ has poles or branch points close to the interval $x \in [-1,1]$.

Unfortunately, the location of off-axis singularities is usually unknown for most real science and engineering problems; the exceptions prove only that there are such singularities [4–6,28,34]. Gelb and Jackiewicz [13] describe a procedure to estimate the parameter ρ , which measures proximity of off-axis singularities. Unfortunately, the singularity structure can be very complicated with an infinity of poles or branch points forming a fractal natural boundary for the region of analyticity [5,6,28,34]. And yet we have shown that such singularities can wreck a diagonal Gegenbauer expansion. The choice of parameters for the reconstruction must be constrained so that the Gegenbauer approximation will converge in spite of off-axis poles or branch points of $f(x)$. Our work suggests that the problem of off-axis singularities is more serious than previously thought.

Acknowledgement

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Appendix A. The “vertical limit”: a proof that Gegenbauer series tend to power series as the order m tends to infinity

Theorem A.1 (Large order limit of Gegenbauer expansions). *Suppose a function $f(x)$, analytic on $x \in [-1,1]$ and in a small disk about the origin, is expanded as*

$$f(x) = \sum_{n=0}^{\infty} b_n \frac{C_n^m(x)}{C_n^m(1)}, \tag{A.1}$$

that is, the b_n are the coefficients of the Gegenbauer series when the polynomials are normalized so as to have a maximum value of one at $x = 1$.

Then in the limit $m \rightarrow \infty$ for fixed n

1. The Gegenbauer coefficients asymptote to the power series coefficients of $f(x)$:

$$b_n \sim \frac{1}{n!} \frac{d^n f}{dx^n}(0) \{1 + O(1/m)\}. \tag{A.2}$$

2. The n th Gegenbauer polynomial with this normalization asymptotes to x^n

$$\frac{C_n^m(x)}{C_n^m(1)} \sim x^n \{1 + O(1/m)\}, \quad x \in [-1, 1] \tag{A.3}$$

3. It follows that the N -term truncation of the Gegenbauer series asymptotes to the N -term power series.

Table 1
Coefficients of the $N = 8$ Gegenbauer approximations, converted to powers-of- x form, for $f = 1/(1 + x^2)$ and various m

m	1	x^2	x^4	x^6	x^8
20	0.99999913	-0.999772	0.9915	-0.898	0.514
40	0.99999925	-0.99965	0.9978	-0.955	0.660
100	0.999999984	-0.999983	0.99975	-0.989	0.822
250	0.9999999976	-0.99999940	0.999979	-0.9978	0.918
500	0.99999999917	-0.99999958	0.999971	-0.99942	0.957
1000	0.999999999972	-0.999999972	0.9999962	-0.99985	0.978
Power series	1	-1	1	-1	1

Fox and Parker [8, p. 17–18] prove the first proposition above, borrowing some arguments from [27]. However, since their book discusses Gegenbauer polynomials only to condemn them, and explain why the rest of the book is about Chebyshev polynomials only, they do not formally prove the rest of the theorem, but merely assert that from the Gegenbauer differential equation “We deduce... that the Taylor series... corresponds to the limiting ultraspherical orthogonal expansion as $m \rightarrow \infty$ ”. The remaining propositions are obvious consequences of the following lemma.

Lemma A.1. (Power series of Gegenbauer polynomials) *Define the power series expansion coefficients as*

$$\frac{C_n^m(x)}{C_n^m(1)} = \sum_{k=0}^{\lfloor n/2 \rfloor} B_n^k(x) x^{n-2k}. \tag{A.4}$$

Then

$$B_n^k = (-1)^k \frac{\Gamma(n+1)\Gamma(2m)}{\Gamma(m)\Gamma(n+2m)} \frac{\Gamma(n-k+m)}{\Gamma(k+1)\Gamma(n-2k+1)} 2^{n-2k}, \tag{A.5}$$

$$B_n^0 = \frac{\Gamma(n+m)\Gamma(2m)}{\Gamma(m)\Gamma(n+2m)} 2^n \tag{A.6}$$

$$\sim 1 + (45/2)/m + (585/4)/m^2, \quad m \rightarrow \infty, \quad \text{fixed } n, \tag{A.7}$$

$$\lim_{m \rightarrow \infty} B_n^k/B_n^0 = \frac{1}{\Gamma(k+1)2^{2k}} \frac{1}{m^k}. \tag{A.8}$$

Proof. The exact formula for the power series coefficients is (4.7.31) [33, p. 85]. Using the formula for $C_n^m(1)$, which is (4.7.3) on p. 81 of [33], cancelling common factors and using the definition and asymptotics of the factorial function proves the remaining propositions. \square

Table 1 shows an example of asymptoting-to-the-power-series. Gegenbauer polynomials become increasingly ill-conditioned as m increases; the last line of the table required 1200-digit arithmetic! A good discussion of the ill-conditioning is [11].

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