Recovering exponential accuracy in spectral methods involving piecewise smooth functions

Zheng Chen

chenz1@ornl.gov

CAM Semiar
Oak Ridge National Laboratory
March 3, 2016

Overview

1. Motivation
   - Gibbs phenomenon
   - Preliminaries
2. Gegenbauer reconstructions for non-periodic analytic functions
   - Recovering from spectral partial sums
   - Recovering from collocation point values
   - Practical Applications
3. Recovery processes for smooth function with singularities
   - Collocation cases
   - Galerkin cases
4. Summary

Outline

Fourier Series

- For a function periodic in $[-1, 1]$, the Fourier series is

$$f(x) = \sum_{n=-\infty}^{\infty} \tilde{f}_n e^{in\pi x}, \qquad -1 \leq x \leq 1$$

  where,

$$\tilde{f}_n = \frac{1}{2} \int_{-1}^{1} f(x) e^{-in\pi x} dx$$

- The Fourier series of an analytic and periodic function, truncated after 2N+1 terms, converges *exponentially* with N, even in the maximum norm.

$$\max_{-1 \leq x \leq 1} |f(x) - f_N(x)| \leq Ce^{-\alpha N}, \qquad C, \alpha > 0.$$

a good way to reconstruct $f(x)$ EVERYWHERE

Gibbs Phenomenon

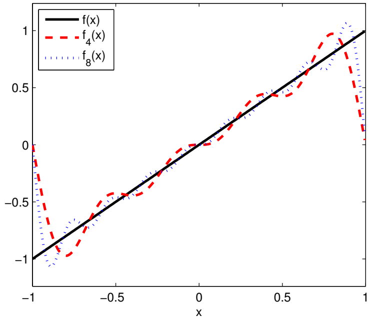
If the function is not periodic, the rate of convergence deteriorates.

Example:

For a piecewise continuous function

$$f(x) = x, \qquad x \in [-1, 1]$$

We use the continuous Fourier series to approximate it, with $N = 4, 8$.



- Away from the discontinuity, only first-order accuracy is achieved.
- Near the discontinuity, there are $\mathcal{O}(1)$ oscillations that do not decrease with increasing N.
- There is no convergence in the maximum norm, although the function is still analytic.

Gibbs Phenomenon(cont'd)

Reasons for the slow convergence:

- the slow decay of the Fourier coefficients $\tilde{f}_n$
- the global nature of the Fourier series

To resolve the Gibbs phenomenon:

- enhancing the decay rate of the given Fourier coefficients
- localizing the information that determines the Fourier coefficients
- finding a set of complementary basis to represent the function

History of overcoming the Gibbs phenomenon

- **Filters** enhance the accuracy but only away from the discontinuity
- **Gegenbauer reconstructions** completely overcome the Gibbs phenomenon for piecewise analytic functions

Outline

Gegenbauer polynomials

Definition: $C_{\mathbf{n}}^{\lambda}(x)$

$$(1-x^2)^{\lambda-\frac{1}{2}} C_n^{\lambda}(x) = \frac{(-1)^n}{2^n n!} G(\lambda, n) \frac{d^n}{dx^n}\left[(1-x^2)^{n+\lambda-\frac{1}{2}}\right], \qquad \lambda \geq 0$$

with

$$G(\lambda, n) = \begin{cases} \frac{\Gamma(\lambda+\frac{1}{2})\Gamma(n+2\lambda)}{\Gamma(2\lambda)\Gamma(n+\lambda+\frac{1}{2})} & \lambda > 0 \\ \frac{2\sqrt{\pi}(n-1)!}{\Gamma(n+\frac{1}{2})} & \lambda = 0, n \geq 1 \\ 1 & \lambda = 0, n = 0 \end{cases}$$

Remark Chebyshev polynomials $T_n(x)$ are special cases.

$$C_n^0(x) = \lim_{\lambda \to 0^+} \frac{1}{\lambda} C_n^{\lambda}(x) = \frac{2}{n} T_n(x), \qquad n > 0$$

Gegenbauer polynomials(cont'd)

- **Orthogonality** under the weight function $(1-x^2)^{\lambda-\frac{1}{2}}$:

$$\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}}C_k^\lambda(x)C_n^\lambda(x)dx=\delta_{k,n}h_n^\lambda$$

where

$$h_n^\lambda=\begin{cases}\pi^{\frac{1}{2}}C_n^\lambda(1)\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda)(n+\lambda)} & \lambda>0\\ \frac{2\pi}{n^2} & \lambda=0, n\geq 1\\ \pi & \lambda=0, n=0\end{cases}$$

- **Gegenbauer expansion** under the basis $C_k^\lambda(x)$, for L_1 function $f(x)$:

$$f(x)=\sum_{k=0}^{\infty}\hat{f}_k^\lambda C_k^\lambda(x),\qquad -1\leq x\leq 1$$

with the Gegenbauer coefficients $\hat{f}_k^\lambda$ defined by

$$\hat{f}_k^\lambda=\frac{1}{h_k^\lambda}\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}}f(x)C_k^\lambda(x)dx,\qquad k\geq 0$$

Regularization error of Gegenbauer expansion

Approximation error of Gegenbauer expansion:

Definition

The **regularization error** is defined by

$$RE(\lambda, m) = \max_{-1\leq x\leq 1} \left| f(x) - \sum_{k=0}^{m} \hat{f}_k^{\lambda} C_k^{\lambda}(x) \right|$$

Theorem

Let $\lambda = \gamma m$ with a constant $\gamma > 0$, then for analytic function $f(x)$

$$RE(\gamma m, m) \leq C q_R^m, \qquad q_R(\gamma) < 1.$$

Gegenbauer reconstructions

In 1990s, a framework has been developed to remove the Gibbs phenomenon completely for piecewise analytic functions, which means recovering exponential accuracy in the maximum norm in any sub-interval of analyticity, from the knowledge of the Fourier or Gegenbauer series of a piecewise analytic but non-periodic function.

Regularity	**Given Info**	**Recovery region**
analytic, non-periodic	first $2N + 1$ Fourier coeffs	$[-1, 1]^*$
piecewise analytic	first $2N + 1$ Fourier coeffs	$[a, b]$ †
piecewise analytic	first $N + 1$ Gegenbauer coeffs	$[a, b]$
analytic, non-periodic	uniform point values	$[-1, 1]$
piecewise analytic	uniform point values	$[a, b]$
piecewise analytic	Gauss or Gauss-Lobatto point values	$[a, b]$

*whole interval

†sub-interval of analyticity

†D. Gottlieb and C.-W. Shu (1997). "On the Gibbs phenomenon and its resolution". In: *SIAM Review* 30, pp. 644–668

Outline

case 1

Given the first $2N + 1$ Fourier coefficients

Reconstruction

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

with

$$\hat{f}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1 - x^2)^{\lambda - \frac{1}{2}} f(x) C_k^{\lambda}(x) dx$$

Error

$$\left\| f - f^{\lambda,m} \right\|_{L_\infty}$$

Regularization

[†] D. Gottlieb et al. (1992). "On the Gibbs phenomenon I: recovering exponential accuracy from the Fourier partial sum of a non-periodic analytic function". In: *Journal of Computational and Applied Mathematics* 43, pp. 81–98

case 1

Given the first $2N+1$ Fourier coefficients

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^{\lambda} C_k^{\lambda}(x) \sim \sum_{k=0}^{m} \hat{g}_k^{\lambda} C_k^{\lambda}(x) = f_N^{\lambda,m}(x)$$

with

$$\hat{f}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} f(x) C_k^{\lambda}(x) dx$$

$$\hat{g}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} f_N(x) C_k^{\lambda}(x) dx$$

Error

$$\left\| f - f_N^{\lambda,m} \right\|_{L_\infty} \leq \underbrace{\left\| f - f^{\lambda,m} \right\|_{L_\infty}}_{\textit{Regularization}} + \underbrace{\left\| f^{\lambda,m} - f_N^{\lambda,m} \right\|_{L_\infty}}_{\textit{Truncation}}$$

† D. Gottlieb et al. (1992). "On the Gibbs phenomenon I: recovering exponential accuracy from the Fourier partial sum of a non-periodic analytic function". In: *Journal of Computational and Applied Mathematics* 43, pp. 81–98

Error estimate: Two steps

Provided that both λ and m are proportional to N, we have:

- the truncated Gegenbauer series converges exponentially with N, for any analytic function.

$$RE(\lambda, m) = \max_{-1 \le x \le 1} \left| f(x) - \sum_{k=0}^{m} \hat{f}_k^\lambda C_k^\lambda(x) \right|$$

- the first m coefficients of the Gegenbauer expansion of any L_2 function can be obtained from $f_N(x)$, within exponential accuracy.

$$TE(\lambda, m, N) = \max_{-1 \le x \le 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(x) \right|$$

Theorem

Theorem: Removal of the Gibbs Phenomenon

For $\lambda = m = \beta N$ with $\beta < \frac{2\pi e}{27}$

$$\max_{-1\leq x\leq 1} |f(x) - \sum_{l=0}^{m} \hat{g}^{\lambda}(l) C_l^{\lambda}(x)| \leq A q_T^N + B q_R^N, \qquad 0 < q_T, q_R < 1$$

Here, A and B depend on N at most in polynomial growth.

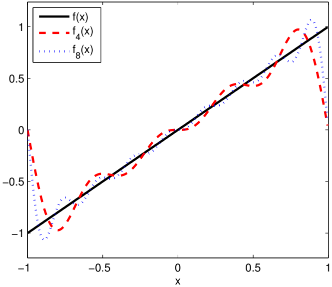
Remark The reconstruction is not optimal.

Numerical example (revisit)

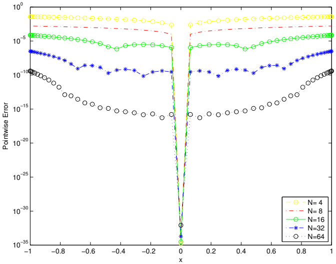
Example:

$$f(x) = x, \qquad x \in [-1, 1]$$

Use Gegenbauer procedure to recover the function from $f_N(x)$ with $\lambda = m = \frac{N}{4}$.



$f(x) = x$ and its Fourier series $f_N(x)$ with $N = 4, 8$



Pointwise errors for Gegenbauer reconstruction in log scales, with $N = 4, 8, 16, 32, 64$.

Outline

case 2

Given the point values $f(x_i)$ at the N Gauss or Gauss-Lobatto points

Reconstruction

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

with

$$\hat{f}_k^\lambda = \frac{1}{h_k^\lambda} \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} f(x) C_k^\lambda(x) dx$$

† D. Gottlieb and C.-W. Shu (1995b). "On the Gibbs phenomenon V: recovering exponential accuracy from collocation point values of a piecewise analytic function". In: *Numerische Mathematik* 71, pp. 511–526

case 2

Given the point values $f(x_i)$ at the N Gauss or Gauss-Lobatto points

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^\lambda C_k^\lambda(x) \sim \sum_{k=0}^{m} \hat{g}_k^\lambda C_k^\lambda(x) = f_N^{\lambda,m}(x)$$

with

$$\hat{f}_k^\lambda = \frac{1}{h_k^\lambda} \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} f(x) C_k^\lambda(x) dx$$

$$g_N(x) = I_N((1-x^2)^{\lambda-\frac{1}{2}} f(x))$$

$$\hat{g}_k^\lambda = \frac{1}{h_k^\lambda} \int_{-1}^{1} g_N(x) C_k^\lambda(x) dx$$

Error

$$\left\| f - f_N^{\lambda,m} \right\|_{L_\infty} \leq \underbrace{\left\| f - f^{\lambda,m} \right\|_{L_\infty}}_{\textit{Regularization}} + \underbrace{\left\| f^{\lambda,m} - f_N^{\lambda,m} \right\|_{L_\infty}}_{\textit{Truncation}}$$

† D. Gottlieb and C.-W. Shu (1995b). "On the Gibbs phenomenon V: recovering exponential accuracy from collocation point values of a piecewise analytic function". In: *Numerische Mathematik* 71, pp. 511–526

Theorem

Theorem: Removal of the Gibbs Phenomenon

For $\lambda = m = \beta N$ where $\beta < \frac{2e}{27(1+\frac{1}{2\rho})}$

$$\max_{-1 \le x \le 1} |f(x) - \sum_{l=0}^{m} \hat{g}^{\lambda}(l) C_l^{\lambda}(x)| \le A q_T^N + B q_R^N, \qquad 0 < q_T, q_R < 1.$$

Remark The reconstruction is not optimal.

Numerical example

Example:

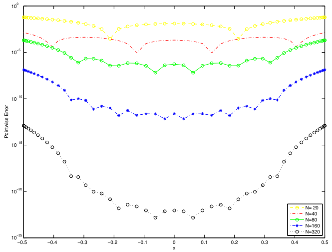
$$f(x) = I_{[-0.5,0.5]}(x) \cdot \sin(\cos(x)), \qquad x \in [-1,1]$$

where $I_{[-0.5,0.5]}(x)$ is a characteristic function of the sub-interval $[-0.5, 0.5]$. Recover point values over $[-0.5, 0.5]$ with Gegenbauer reconstruction:

Given $f(x_i)$ at the $N+1$ Gauss-Lobatto points

$$x_i = \cos(\frac{i\pi}{N}), \qquad 0 \le i \le N,$$

with $N = 20, 40, 80, 160, 320$ and $\lambda = N/10, m = N/20$.



Pointwise errors in log scales, Gegenbauer reconstruction

Numerical example

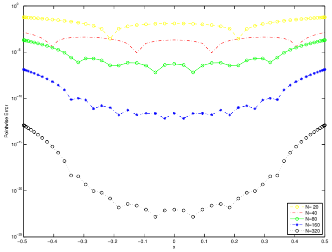
Example:

$$f(x) = I_{[-0.5,0.5]}(x) \cdot \sin(\cos(x)), \qquad x \in [-1, 1]$$

where $I_{[-0.5,0.5]}(x)$ is a characteristic function of the sub-interval $[-0.5, 0.5]$. Recover point values over $[-0.5, 0.5]$ with Gegenbauer reconstruction:

Table: Maximum error table

N	L^∞ error	order
20	5.96E-02	
40	1.37E-03	5.45
80	2.02E-04	2.76
160	1.32E-07	10.58
320	1.23E-13	20.02



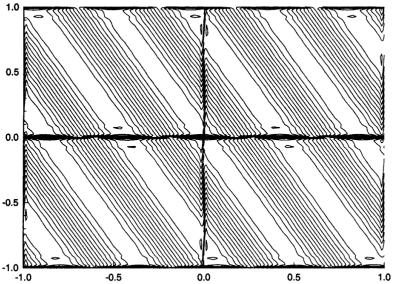
Pointwise errors in log scales, Gegenbauer reconstruction

Outline

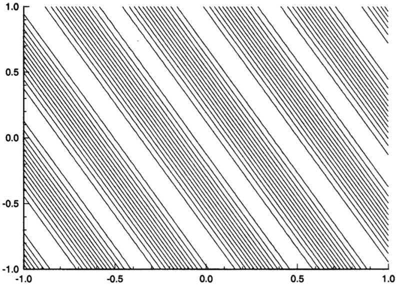
"Spliced" functions in two dimensions

Given the first $2N + 1$ Fourier coefficients of the "spliced" function in each quadrant ($N = 32$)

$$f(x, y) = e^{i2.3\pi x + i1.2\pi y}$$



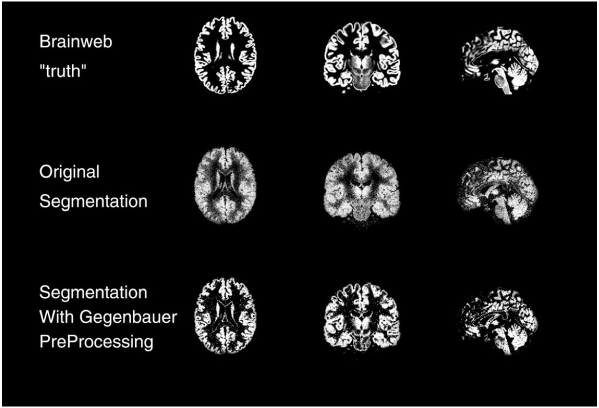
Fourier partial sum in each subdomain



Gegenbauer method in each subdomain

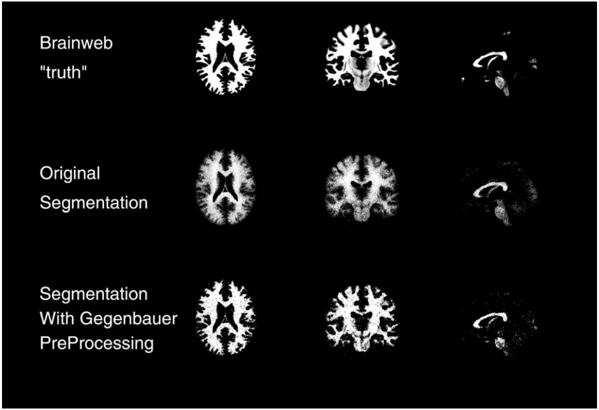
† A. Gelb and D. Gottlieb (1997). "The resolution of the Gibbs phenomenon for spliced functions in one and two dimensions". In: *Computers & Mathematics with Applications* 33.11, pp. 35–58

Improving tissue segmentation of human brain MRI



† R. Archibald et al. (2003). "Improving tissue segmentation of human brain MRI through preprocessing by the Gegenbauer reconstruction method". In: *NeuroImage* 20.1, pp. 489–502.

Improving tissue segmentation of human brain MRI



† R. Archibald et al. (2003). "Improving tissue segmentation of human brain MRI through preprocessing by the Gegenbauer reconstruction method". In: *NeuroImage* 20.1, pp. 489–502.

More applications

- Recover high order information of the discontinuous solutions of scalar nonlinear hyperbolic PDEs[‡]
- Simulate sophisticated problems, such as high Mach number reactive flows[§]
- Recover lost order of accuracy in other types of approximations, such as weighted essentially non-oscillatory (WENO) solutions of hyperbolic PDEs[¶]
- Post processing in radial basis functions approximations of linear and nonlinear hyperbolic PDEs[‖]

[‡] C.-W. Shu and P. Wong (1995). "A note on the accuracy of spectral method applied to nonlinear conservation laws". In: *Journal of scientific computing* 10.3, pp. 357–369

[§] D. Gottlieb and S. Gottlieb (2005). "Spectral methods for compressible reactive flows". In: *Comptes Rendus Mecanique: High-order methods for the numerical simulation of vortical and turbulent flows* 333.1, pp. 3–16

[¶] S. Gottlieb, D. Gottlieb, and C.-W. Shu (2006). "Recovering high-order accuracy in WENO computations of steady-state hyperbolic systems". In: *Journal of Scientific Computing* 28.2-3, pp. 307–318

[‖] J.-H. Jung et al. (2010). "Recovery of high order accuracy in radial basis function approximations of discontinuous problems". In: *Journal of Scientific Computing* 45.1-3, pp. 359–381

Question: What if the function has some singularities? Does the current Gegenbauer Reconstruction work?

Question: What if the function has some singularities? Does the current Gegenbauer Reconstruction work?

Answer: Unfortunately, NO. 

Consider a smooth function with one-end singularity:

$$f(x) = a(x) + b(x)(1+x)^s$$

where, $a(x)$ and $b(x)$ are both unknown analytic functions , and s is given

$$0 < s = \frac{p}{q} < 1$$

New techniques are developed to recover such functions with exponential accuracy everywhere, from the knowledge of

- point values on the standard collocation points[**],
- first $2N+1$ Fourier coefficients[††].

Joint work with Prof. Chi-Wang Shu (Brown University)

[**] Z. Chen and C.-W. Shu (2014). "Recovering exponential accuracy from collocation point values of smooth functions with end-point singularities". In: *Journal of Computational and Applied Mathematics* 265, pp. 83–95

[††] Z. Chen and C.-W. Shu (2015). "Recovering exponential accuracy in Fourier spectral methods involving piecewise smooth functions with unbounded derivative singularities". In: *Journal of Scientific Computing* 65.3, pp. 1145–1165

Consider a smooth function with one-end singularity:

$$f(x) = a(x) + b(x)(1+x)^s$$

where, $a(x)$ and $b(x)$ are both unknown analytic functions , and s is given

$$0 < s = \frac{p}{q} < 1$$

Under the one-to-one transformation between $x \in [-1, 1]$ and $y \in [-1, 1]$:

$$2^{q-1}(1+x) = (1+y)^q$$

$f(x(y))$ is an analytic function of the variable y, thus has Gegenbauer expansion:

$$f(x(y)) = \bar{f}(y) = \sum_{k=0}^{\infty} \hat{f}_k^\lambda C_k^\lambda(y)$$

with

$$\hat{f}_k^\lambda = \frac{1}{h_k^\lambda} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} f(x(y)) C_k^\lambda(y) dx$$

Outline

Reconstruction from collocation point values

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^\lambda C_k^\lambda(y(x)) \sim \sum_{k=0}^{m} \hat{f}_k^\lambda C_k^\lambda(y(x)) = f_q^{\lambda,m}(x)$$

with

$$\hat{f}_k^\lambda = \frac{1}{h_k^\lambda} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} f(x(y)) C_k^\lambda(y) dy$$

Reconstruction from collocation point values

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^{\lambda} C_k^{\lambda}(y(x)) \sim \sum_{k=0}^{m} \hat{g}_k^{\lambda} C_k^{\lambda}(y(x)) = f_{N,q}^{\lambda,m}(x)$$

with

$$\hat{f}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} f(x(y)) C_k^{\lambda}(y) dy$$

$$\hat{g}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1+y)^{\frac{q-1}{2}} g_N^{\lambda}(x(y)) C_k^{\lambda}(y) dy$$

$$g_N^{\lambda}(x) = I_N \left(\frac{(1-y(x)^2)^{\lambda-\frac{1}{2}} f(x)}{\sqrt{A \frac{dx}{dy}}} \right)$$

Error

$$\left\| f - f_{N,q}^{\lambda,m} \right\|_{L_\infty} \leq \underbrace{\left\| f - f_{q}^{\lambda,m} \right\|_{L_\infty}}_{Regularization} + \underbrace{\left\| f_{q}^{\lambda,m} - f_{N,q}^{\lambda,m} \right\|_{L_\infty}}_{Truncation}$$

Error estimate: Two steps

We estimate the errors in the following fashion:

- Regularization error:

$$RE(\lambda, m) = \max_{-1\leq x\leq 1} \left| f(x) - \sum_{k=0}^{m} \hat{f}_k^\lambda C_k^\lambda(y(x)) \right|$$
$$= \max_{-1\leq y\leq 1} \left| \bar{f}(y) - \sum_{k=0}^{m} \hat{f}_k^\lambda C_k^\lambda(y) \right|$$

- Truncation error:

$$TE(\lambda, m, N) = \max_{-1\leq y\leq 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right|$$

Main Theorem

Consider a function in the form of $f(x) = a(x) + b(x)(1+x)^s$, with given fractional constant $0 < s = \frac{p}{q} < 1$.

Theorem(Removal of the Gibbs Phenomenon)

For $\lambda = \alpha N$ and $m = \gamma\lambda$ with $\alpha < \frac{2q}{(1+\delta)}\left(\frac{\gamma^\gamma}{(2+\gamma)^{(2+\gamma)}}\right)^q$ and $\delta = \frac{1}{e}\left(1 + \frac{1}{2^q A q \rho}\right)$

$$\max_{-1\leq x\leq 1}\left|f(x) - \sum_{k=0}^{m} \hat{g}_k^\lambda C_k^\lambda(y(x))\right| \leq C\left(q_T^N + q_R^N\right), \qquad 0 < q_T, q_R < 1$$

‖Chen, Z. and C.-W. Shu (JCAM2014)

Numerical example

Example 1:

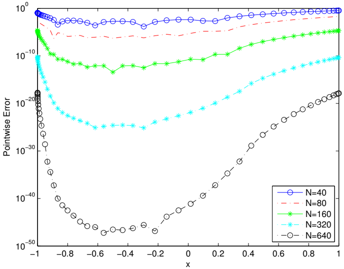
$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1, 1]$$

Fourier Case:

Given $f(x_i)$ at the $2N+1$ uniform points

$$x_i = \frac{2i}{2N+1}, \qquad -N \le i \le N,$$

with $N = 40, 80, 160, 320, 640$ and $\lambda = 0.2N$, $m = 0.075N$.



Pointwise errors in log scales, Gegenbauer reconstruction, Fourier case

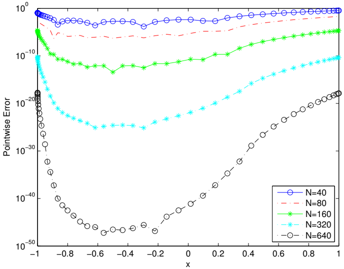
Numerical example

Example 1:

$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order
40	3.46E-01	
80	2.01E-02	4.11
160	2.19E-05	9.84
320	5.93E-11	18.49
640	1.82E-18	24.96



Pointwise errors in log scales, Gegenbauer reconstruction, Fourier case

Numerical example

Example 1:

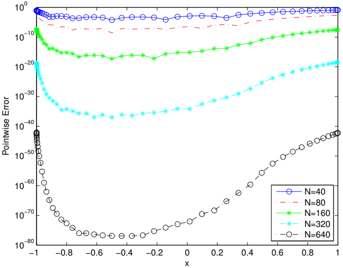
$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1,1]$$

Chebyshev Case:

Given $f(x_i)$ at the $N+1$ Chebyshev collocation points

$$x_i = \cos\left(\frac{\pi(2i+1)}{2N+2}\right), \qquad 0 \le i \le N,$$

with $N = 40, 80, 160, 320, 640$ and $\lambda = 0.2N$, $m = 0.1N$.



Pointwise errors in log scales, Gegenbauer reconstruction, Chebyshev case

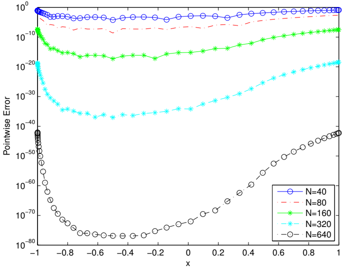
Numerical example

Example 1:

$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order
40	1.34E-01	
80	2.49E-03	5.75
160	5.17E-08	15.56
320	3.58E-19	37.07
640	8.48E-43	78.48



Pointwise errors in log scales, Gegenbauer reconstruction, Chebyshev case

Outline

Reconstruction from Fourier partial sums

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^{\lambda} C_k^{\lambda}(y(x)) \sim \sum_{k=0}^{m} \hat{f}_k^{\lambda} C_k^{\lambda}(y(x)) = f_q^{\lambda,m}(x)$$

with

$$\hat{f}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1 - y^2)^{\lambda - \frac{1}{2}} f(x(y)) C_k^{\lambda}(y) dy$$

Reconstruction from Fourier partial sums

Reconstruction

$$f(x) = \sum_{k=0}^{\infty} \hat{f}_k^{\lambda} C_k^{\lambda}(y(x)) \sim \sum_{k=0}^{m} \hat{g}_k^{\lambda} C_k^{\lambda}(y(x)) = f_{N,q}^{\lambda,m}(x)$$

with

$$\hat{f}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} f(x(y)) C_k^{\lambda}(y) dy$$

$$\hat{g}_k^{\lambda} = \frac{1}{h_k^{\lambda}} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} f_N(x(y)) C_k^{\lambda}(y) dy$$

Error

$$\left\| f - f_{N,q}^{\lambda,m} \right\|_{L_\infty} \leq \underbrace{\left\| f - f_q^{\lambda,m} \right\|_{L_\infty}}_{Regularization} + \underbrace{\left\| f_q^{\lambda,m} - f_{N,q}^{\lambda,m} \right\|_{L_\infty}}_{Truncation}$$

Main Theorem

Consider a function in the form of $f(x) = a(x) + b(x)(1+x)^s$, with given fractional constant $0 < s = \frac{p}{q} < 1$.

Theorem(Removal of the Gibbs Phenomenon)

For $\lambda = \alpha N$ and $m = \gamma \lambda$ with $\alpha < \frac{\pi}{A}\left(\frac{2\gamma^{\gamma}(1+\gamma)^{1-\frac{1}{q}}}{e^{\gamma}(2+\gamma)^{2+\gamma}}\right)^{q}$

$$\max_{-1\leq x\leq 1}\left|f(x) - \sum_{k=0}^{m} \hat{g}_k^{\lambda} C_k^{\lambda}(y(x))\right| \leq C\left(q_T^N + q_R^N\right), \qquad 0 < q_T, q_R < 1$$

‖Chen, Z. and C.-W. Shu (2014b)

Numerical example

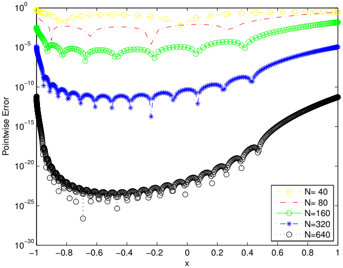
Example 1:

$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1, 1]$$

Recover point values over $[-1, 1]$ with exponential accuracy from the first $2N+1$ Fourier coefficients $\tilde{f}_n$, $-N \leq n \leq N$, with

$$\lambda = \frac{1}{16}N, \qquad m = \frac{3}{80}N$$

and $N = 40, 80, 160, 320, 640$.



Pointwise errors in log scales, Gegenbauer reconstruction

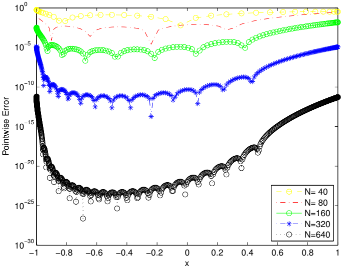
Numerical example

Example 1:

$$f(x) = \cos(x) + \sin(x)\sqrt{1+x}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order	λ	m
40	5.91E-001		2	1
80	2.95E-001	1.00	5	3
160	1.56E-002	4.25	10	6
320	1.33E-005	10.19	20	12
640	6.46E-012	20.98	40	24



Pointwise errors in log scales, Gegenbauer reconstruction

Numerical example: Tolerance with noises

Example 1:

Table 3 Maximum error with different levels of noise in data (linear choice)

N	L^∞ (no noise)	L^∞	Noise	L^∞	Noise	L^∞	Noise
40	5.91E−01	6.07E−01	1.00E−02	5.53E−01	1.00E−01	8.54E−01	1.00E+00
80	2.95E−01	1.82E−01	1.00E−02	3.25E−01	1.00E−01	8.59E+00	1.00E+00
160	1.56E−02	1.53E−02	1.00E−05	8.16E−03	1.00E−04	9.44E−02	1.00E−03
320	1.33E−05	1.36E−05	1.00E−11	1.12E−05	1.00E−10	8.37E−05	1.00E−09

Application

Example 2: For linear transport equations with variable coefficients:

$$\begin{cases} u_t - xu_x = 0, & x \in [-1,1], \quad t > 0 \\ u(x,0) = g(x) = \sqrt{1+x}, & x \in [-1,1] \end{cases}$$

with periodic boundary condition.

The exact solution is

$$u(x,t) = \sqrt{1 + xe^t \pmod 2}$$

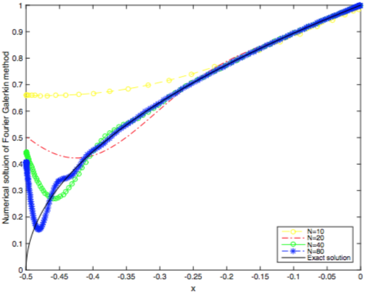
At $T = \log 2$, it has two deformed "copies" of the initial condition, and has singularities at ± 0.5.

We would like to recover it on subinterval $[-0.5, 0]$, on whose left end it behaves like square root:

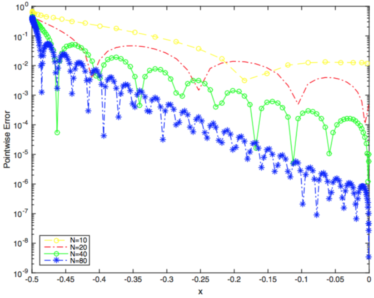
$$u(x, \log 2) = \sqrt{1+2x}, \qquad x \in [-0.5, 0].$$

Example 2:

The filtered Fourier Galerkin method with Runge-Kutta time stepping provides solutions with poor accuracy and oscillations near the singularities.
$N = 10, 20, 40, 80$



Numerical and exact solutions (in black)



Pointwise errors in log scales

Application

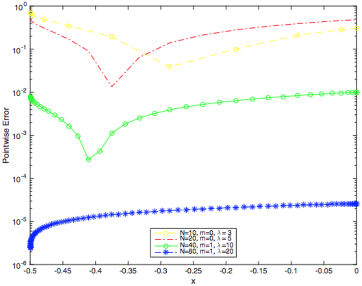
Example 2:

Apply the new Gegenbauer reconstruction ⇐ spectral convergence of moments**

$$\lambda = \frac{1}{80}N, m = \frac{1}{4}N$$

Table: Maximum error table

N	L^∞ error	order	λ	m
10	6.93E-01		0	3
20	5.13E-01	0.43	0	5
40	1.01E-02	5.67	1	10
80	2.61E-05	8.60	1	20



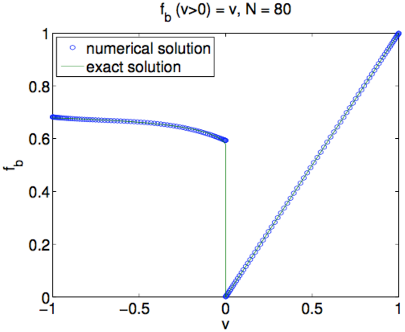
Pointwise errors in log scales

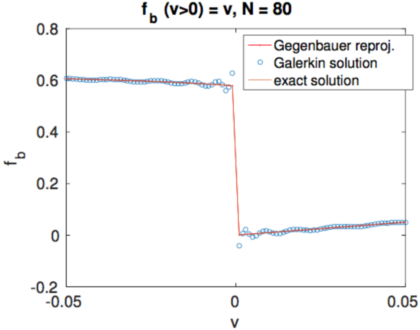
** S. Abarbanel, D. Gottlieb, and E. Tadmor (1985). "Spectral methods for discontinuous problems". In: J. Zudrop and J. S. Hesthaven (2015). "Accuracy of high order and spectral methods for hyperbolic conservation laws with discontinuous solutions". In: *SIAM Journal on Numerical Analysis* 53.4, pp. 1857–1875

Applications in isotropic neutron transport equation

Galerkin methods with other orthogonal bases (e.g. Hermite) should also work with the reconstruction methods, with a modified analysis, even with different types of singularities.

Example: Use Legendre polynomials for half-space isotropic neutron transport equation, whose solution has a "logarithmic" singularity near 0, e.g. $x \ln(x)$ on $[0, 1]$. $\Longleftarrow$ NEW transformation + "overlapping" technique





** J. Li Q.and Lu and W. Sun (2014). "A convergent method for linear half-space kinetic equations". In: *arXiv preprint arXiv:1408.6630*

Summary

- Gibbs phenomenon: non-periodic functions
- Gegenbauer reconstruction: provide a post-processing method to recover the piecewise analytic functions with exponential accuracy in the maximum norm.
- Extended methods: reconstruct piecewise smooth functions with unbounded derivative singularities from the first $2N + 1$ Fourier coefficients or N standard collocation point values, achieving exponential accuracy uniformly.

Future work:

- Reconstruction in higher dimension
- Applications in improving numerical methods on Partial Differential Equations, such as nonlinear PDEs
- Analysis for more complex singularities
- New techniques free of "s"

Thank you! Any questions?

Spectral Methods

- A class of techniques used in applied mathematics and scientific computing to numerically solve certain differential equations.
- A global approach: basis functions are nonzero over the whole domain.
- Excellent error properties: "exponential convergence" - the fastest possible for smooth solutions
- Less expensive than finite element methods.
- Fourier series methods for periodic geometry problems, polynomial spectral methods for finite and unbounded geometry problems, pseudo spectral methods for highly nonlinear problems, and spectral iteration methods for fast solution of steady state problems ...
- Less accurate for problems with complex geometries and discontinuous coefficients. $\leftarrow$ Gibbs phenomenon

Analyticity Assumption

Let us assume that the function $f(x)$ is analytic in $[-1, 1]$ and satisfies the following

Analyticity Assumption

There exists a constant $\rho \geq 1$ and $C(\rho)$ such that, for every $k \geq 0$,

$$\max_{-1 \leq x \leq 1} \left| \frac{d^k f}{dx^k}(x) \right| \leq C(\rho) \frac{k!}{\rho^k}.$$

Truncation Error - Collocation case

$$
\begin{aligned}
TE(\lambda, m, N) &\leq \sum_{k=0}^{m} |(\hat{f}_k^\lambda - \hat{g}_k^\lambda)| C_k^\lambda(1) \\
&= C \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \int_{-1}^{1} \sqrt{\frac{dx}{dy}} \left[\alpha(x)f(x) - I_N\left(\alpha(x)f(x)\right)\right] C_k^\lambda(y) dy \right| \\
&\leq C \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \int_{-1}^{1} \sqrt{\frac{dx}{dy}} \left|\alpha(x)f(x) - I_N\left(\alpha(x)f(x)\right)\right| dy \\
C - S \rightarrow \quad &\leq C \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \left(\int_{-1}^{1} \omega(x) \frac{dx}{dy} \left(\alpha(x)f(x) - I_N\left(\alpha(x)f(x)\right)\right)^2 dy \right)^{\frac{1}{2}} \\
&\quad \cdot \left(\int_{-1}^{1} \frac{1}{\omega(x)} dx \right)^{\frac{1}{2}} \\
&= C \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \left\|\alpha(x)f(x) - I_N\left(\alpha(x)f(x)\right)\right\|_{L^2_\omega}
\end{aligned}
$$

Truncation Error - Collocation case

$$TE(\lambda, m, N) \quad \leq \quad C \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \|\alpha(x)f(x) - I_N\left(\alpha(x)f(x)\right)\|_{L_\omega^2}$$

Lemma (Interpolation)

If $f(x)$ has m continuous derivatives in $[-1, 1]$, then we have the following estimate for the interpolation polynomial $I_N f(x)$:

$$\|f - I_N f\|_{L_\omega^2} \leq \frac{C}{N^m} \left\| f^{(m)} \right\|_{L^\infty},$$

where, C is a constant independent of N and m.

Lemma (Regularity)

The function

$$\alpha(x)f(x) = (1 - y(x)^2)^{\lambda - \frac{q}{2}} (1 - y(x))^{\frac{q-1}{2}} f(x)$$

has up to t-th derivatives in x, where $t = \lfloor \frac{\lambda}{q} \rfloor - 1 \leq \frac{\lambda}{q}$, the largest integer below $\frac{\lambda}{q} - 1$.

Truncation Error - Collocation case

$$TE(\lambda, m, N) \leq C^{\dagger\dagger} \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \|\alpha(x)f(x) - I_N(\alpha(x)f(x))\|_{L^2_\omega}$$

interpolation $\rightarrow$
$$\leq C \sum_{k=0}^{m} \frac{\left(C_k^\lambda(1)\right)^2}{h_k^\lambda} \frac{1}{N^t} \left\| \frac{d^t}{dx^t}[\alpha(x)f(x)] \right\|_{L^\infty}$$

Lemma (Derivative estimate)

$$\left\| \frac{d^t}{dx^t}[\alpha(x)f(x)] \right\|_{L^\infty} \leq C\left(2^q A\lambda(1+\delta)\right)^t$$

where, C and δ are constants, independent of t.

††Here C is a generic constant

Truncation Error - Collocation case

$$
\begin{aligned}
TE(\lambda, m, N) \quad &\leq \quad \sum_{k=0}^{m} |(\hat{f}_k^\lambda - \hat{g}_k^\lambda)| C_k^\lambda(1) \\
\textit{derivative estimate} \rightarrow \quad &\leq \quad C\frac{(m+1)(m+\lambda)\Gamma(m+2\lambda)}{\sqrt{\lambda}m!\Gamma(2\lambda)}\left(\frac{2^q A\lambda(1+\delta)}{N}\right)^t
\end{aligned}
$$

Let $\lambda = \alpha N$ and $m = \beta N$ with $0 < \alpha, \beta < 1$, then

$$
TE(\alpha N, \beta N, N) \leq Aq_T^N
$$

with

$$
q_T = \frac{(2\alpha+\beta)^{(2\alpha+\beta)}}{\alpha^{2\alpha}\beta^\beta} \cdot \left(\frac{\alpha}{2q}(1+\delta)\right)^{\frac{\alpha}{q}}
$$

If $\beta = \gamma\alpha$ with $\alpha < \frac{2q}{(1+\delta)}\left(\frac{\gamma^\gamma}{(2+\gamma)^{(2+\gamma)}}\right)^q$, then $q_T < 1$.

Numerical example(cont'd)

Example 2:

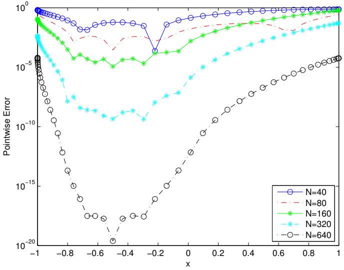
$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1, 1]$$

Fourier Case:

Recover point values over $[-1, 1]$ with exponential accuracy from the point values $f(x_i)$ at the $2N+1$ uniform points

$$x_i = \frac{2i}{2N+1}, \qquad -N \le i \le N,$$

with $N = 40, 80, 160, 320, 640$ and $\lambda = 0.2N$, $m = 0.025N$.



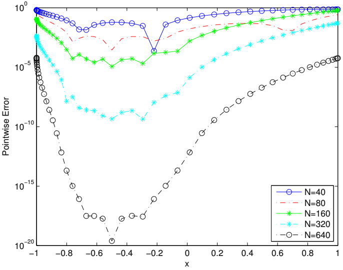
Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ in Fourier case with $\lambda = 0.2N$, $m = 0.025N$.

Example 2:

$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order
40	7.56E-01	
80	3.96E-01	0.93
160	6.00E-01	-0.60
320	5.16E-02	3.54
640	6.36E-05	9.66



Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ in Fourier case with $\lambda = 0.2N, m = 0.025N$.

Numerical example(cont'd)

Example 2:

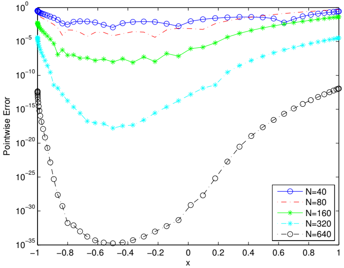
$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1, 1]$$

Chebyshev Case:

Recover point values over $[-1, 1]$ with exponential accuracy from the point values $f(x_i)$ at the $N+1$ Chebyshev collocation points

$$x_i = \cos\left(\frac{\pi(2i+1)}{2N+2}\right), \qquad 0 \le i \le N,$$

with $N = 40, 80, 160, 320, 640$ and $\lambda = 0.2N, m = 0.05N$.



Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ in Chebyshev case with $\lambda = 0.2N, m = 0.05N$.

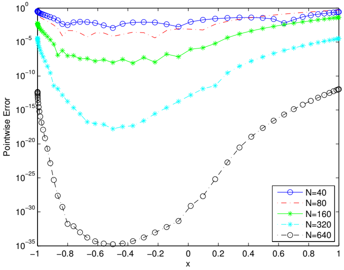
Numerical example(cont'd)

Example 2:

$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order
40	3.49E-01	
80	5.25E-01	-0.59
160	4.25E-02	3.63
320	3.95E-05	10.07
640	1.15E-12	25.03



Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ in Chebyshev case with $\lambda = 0.2N$, $m = 0.05N$.

Truncation Error - Fourier Series

$$
\begin{aligned}
TE(\lambda, m, N) &= \max_{-1\le y\le 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right| \\
&= \max_{-1\le y\le 1} \left| \sum_{k=0}^{m} \frac{C_k^\lambda(y)}{h_k^\lambda} \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} (f - f_N) C_k^\lambda(y) dy \right| \\
&\le \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} (f - f_N) C_k^\lambda(y) dy \right| \\
&= \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \int_{-1}^{1} (1-y^2)^{\lambda-\frac{1}{2}} \sum_{|n|>N} \tilde{f}_n e^{in\pi x} C_k^\lambda(y) dy \right| \\
&= \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \sum_{|n|>N} \tilde{f}_n \int_{-1}^{1} e^{in\pi x} \left[(1-y^2)^{\lambda-\frac{1}{2}} C_k^\lambda(y) \frac{dy}{dx} \right] dx \right|
\end{aligned}
$$

Truncation Error - Fourier Series

$$
\begin{aligned}
TE(\lambda, m, N) &= \max_{-1\le y\le 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right| \\
&= \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \sum_{|n|>N} \tilde{f}_n \int_{-1}^{1} e^{in\pi x} \left[(1-y^2)^{\lambda-\frac{1}{2}} C_k^\lambda(y) \frac{dy}{dx} \right] dx \right|
\end{aligned}
$$

Lemma (Regularity)

The function

$$
M(y) = (1-y^2)^{\lambda-\frac{1}{2}} C_k^\lambda(y) \frac{dy}{dx} = \frac{d^k}{dy^k} (1-y^2)^{k+\lambda-\frac{1}{2}} \frac{dy}{dx}
$$

has up to t-th derivatives in x, where $t = \lfloor \frac{\lambda+\frac{1}{2}}{q} \rfloor - 1$, the largest integer below $\frac{\lambda+\frac{1}{2}}{q} - 1$. And for $0 \le i \le t-1$, we have

$$
\frac{d^i}{dx^i} M(\pm 1) = 0.
$$

Truncation Error - Fourier Series

$$
\begin{aligned}
TE(\lambda, m, N) &= \max_{-1\le y\le 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right| \\
&= \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \sum_{|n|>N} \tilde{f}_n \int_{-1}^{1} e^{in\pi x} \left[(1-y^2)^{\lambda-\frac{1}{2}} C_k^\lambda(y) \frac{dy}{dx} \right] dx \right| \\
\textcolor{red}{t \text{ times } IBP \rightarrow} \quad &= \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left| \sum_{|n|>N} \frac{\tilde{f}_n}{(in\pi)^t} \int_{-1}^{1} e^{in\pi x} \frac{d^t}{dx^t} M(y) dx \right| \\
&\le C \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \sum_{|n|>N} \frac{1}{(n\pi)^t} \left\| \frac{d^t}{dx^t} M(y) \right\|_{L^\infty} \\
&\le \frac{C}{(N\pi)^{t-1}} \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left\| \frac{d^t}{dx^t} M(y) \right\|_{L^\infty}
\end{aligned}
$$

Truncation Error - Fourier Series

$$
\begin{aligned}
TE(\lambda, m, N) &= \max_{-1\le y\le 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right| \\
&\le \frac{C}{(N\pi)^{t-1}} \sum_{k=0}^{m} \frac{C_k^\lambda(1)}{h_k^\lambda} \left\| \frac{d^t}{dx^t} M(y) \right\|_{L^\infty}
\end{aligned}
$$

Derivative estimate

For $0 \le k \le m$,

$$
\begin{aligned}
\left\| \frac{d^t}{dx^t} M(y) \right\|_{L^\infty} &= \left\| \frac{d^t}{dx^t} \left[\frac{d^k}{dy^k} (1-y^2)^{k+\lambda-\frac{1}{2}} \frac{dy}{dx} \right] \right\|_{L^\infty} \\
&\le CA^t 2^{k+\lambda} (k+\lambda)^{k+t}
\end{aligned}
$$

$$
\begin{aligned}
TE(\lambda, m, N) &= \max_{-1\leq y\leq 1} \left| \sum_{k=0}^{m} (\hat{f}_k^\lambda - \hat{g}_k^\lambda) C_k^\lambda(y) \right| \\
&\leq C \frac{A^t 2^\lambda \Gamma(\lambda)(m+1)\Gamma(m+2\lambda)(m+\lambda)^{m+t+1}}{m!\Gamma(2\lambda)\Gamma(m+\lambda+\frac{1}{2})(N\pi)^{t-1}}
\end{aligned}
$$

Let $\lambda = \alpha N$ and $m = \beta N$ with $0 < \alpha, \beta < 1$, then

$$TE(\alpha N, \beta N, N) \leq C q_T^N$$

with

$$q_T = \frac{A^{\frac{\alpha}{q}} e^\beta (2\alpha+\beta)^{2\alpha+\beta}}{\pi^{\frac{\alpha}{q}} (2\alpha)^\alpha \beta^\beta (\alpha+\beta)^{(1-\frac{1}{q})\alpha}}$$

If $\beta = \gamma\alpha$ with $\alpha < \frac{\pi}{A} \left(\frac{2\gamma^\gamma (1+\gamma)^{1-\frac{1}{q}}}{e^\gamma (2+\gamma)^{2+\gamma}} \right)^q$, then $q_T < 1$.

Numerical example(cont'd)

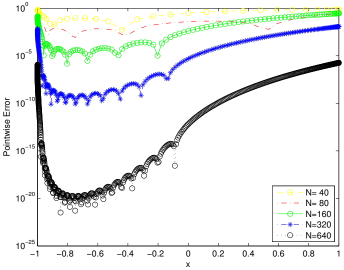
Example 2:

$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1,1]$$

Recover point values over $[-1,1]$ with exponential accuracy from the first $2N+1$ Fourier coefficients $\tilde{f}_n$, $-N \le n \le N$, with

$$\lambda = \frac{1}{8}N, \qquad m = \frac{1}{32}N$$

and $N = 40, 80, 160, 320, 640$.



Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ with $\lambda = \frac{1}{8}N, m = \frac{1}{32}N$.

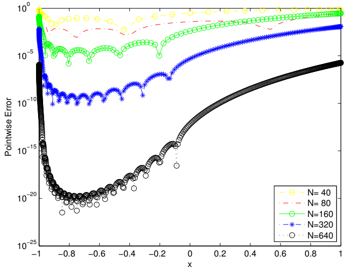
Numerical example(cont'd)

Example 2:

$$f(x) = \cos(x) + \sin(x)(1+x)^{\frac{1}{3}}, \qquad x \in [-1, 1]$$

Table: Maximum error table

N	L^∞ error	order	λ	m
40	7.13E-001		5	1
80	3.64E-001	0.97	10	2
160	2.91E-001	0.33	20	5
320	1.17E-002	4.64	40	10
640	1.83E-006	12.64	80	20



Pointwise errors in log scales, for Gegenbauer reconstruction of $f(x)$ with $\lambda = \frac{1}{8}N, m = \frac{1}{32}N$.

Numerical example: Tolerance with noises

Example 1:

Table 3 Maximum error with different levels of noise in data (linear choice)

N	L^∞ (no noise)	L^∞	Noise	L^∞	Noise	L^∞	Noise
40	5.91E−01	6.07E−01	1.00E−02	5.53E−01	1.00E−01	8.54E−01	1.00E+00
80	2.95E−01	1.82E−01	1.00E−02	3.25E−01	1.00E−01	8.59E+00	1.00E+00
160	1.56E−02	1.53E−02	1.00E−05	8.16E−03	1.00E−04	9.44E−02	1.00E−03
320	1.33E−05	1.36E−05	1.00E−11	1.12E−05	1.00E−10	8.37E−05	1.00E−09

Example 2:

Table 5 Maximum error with different levels of noise in data (linear choice)

N	L^∞ (no noise)	L^∞	Noise	L^∞	Noise	L^∞	Noise
40	7.13E−01	6.82E−01	1.00E−02	7.21E−01	1.00E−01	1.25E+00	1.00E+00
80	3.64E−01	3.43E−01	1.00E−02	8.04E−01	1.00E−01	8.30E+00	1.00E+00
160	2.91E−01	2.81E−01	1.00E−04	8.87E−01	1.00E−03	6.06E+00	1.00E−02
320	1.17E−02	1.65E−02	1.00E−08	4.93E−02	1.00E−07	1.13E+00	1.00E−06