Lecture 4: Spectral Methods

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Outline of the Fourth Lecture

• Introduction

• Recovering exponential accuracy from the Fourier partial sum of a nonperiodic analytic function

• Generalizations: multiple discontinuities and sub-intervals; polynomial spectral methods; collocation methods

• Recovering exponential accuracy from collocation data from functions with end-point singularities

• Concluding remarks
Spectral methods for smooth functions

For a periodic function $f(x)$, we assume the Fourier coefficients

$$\hat{f}(k) = \frac{1}{2} \int_{-1}^{1} f(x) e^{-ik\pi x} dx$$

are given for $-N \leq k \leq N$. 
The partial Fourier sum is defined by

\[ f_N(x) = \sum_{k=-N}^{N} \hat{f}(k) e^{ik\pi x} \]

and it converges very fast to \( f(x) \):

\[ \max_{-1 \leq x \leq 1} |f(x) - f_N(x)| \leq Ce^{-\alpha N} \]

with constants \( C \) and \( \alpha > 0 \) independent of \( N \), provided the periodic function \( f(x) \) is analytic.
If the function is less smooth we still have faster than algebraic convergence

$$\| f - f_N \| \leq \frac{C}{N^p} \| f \|_{H^p}$$

as long as $f$ has its $p$-derivative in $L^2$.

Similar results exist for non-periodic problems using polynomial basis functions (Chebyshev and Legendre spectral methods).
If $f(x)$ is less smooth, the convergence rate degenerates. In particular, if $f(x)$ is discontinuous, then there is no convergence in the maximum norm:

- Away from the shock the convergence rate is $O\left(\frac{1}{N}\right)$;
- Near the shock there are $O(1)$ oscillations.

This is called the Gibbs phenomenon.
Figure 1: The function $f(x) = x$ (solid line); the Fourier partial sum $f_N(x)$ with $N = 4$ (short dashed line) and $N = 8$ (dotted line), and the approximation through the Gegenbauer procedure using $m = \lambda = N/4$ for $N = 4$ (long dashed line).
Traditional approach to overcome the Gibbs phenomenon

A filter is a smooth, even function $\sigma(t)$:

- $\sigma(0) = 1$, $\sigma^{(l)}(0) = 0$, $1 \leq l \leq p - 1$.
- $\sigma(\eta) = 0$, $|\eta| \geq 1$.
- $\sigma(\eta) \in C^{p-1}$, $\eta \in (-\infty, \infty)$.

Then $\sigma^N_k = \sigma\left(\frac{k}{N}\right)$. 

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After filtering:

\[ f_N^\sigma(x) = \sum_{k=-N}^{N} \sigma_k^N \hat{f}(k) e^{ik\pi x} \]

The error can be made exponentially small away from the shock:

\[ \max_{|x - \text{shock}| \geq \delta} |f(x) - f_N^\sigma(x)| \leq Ce^{-\alpha N} \]

where the constants \( C \) and \( \alpha > 0 \) are independent of \( N \) but depend on \( \delta \), when the filter order \( p \) is chosen suitably related to \( N \).

However, the Gibbs phenomenon persists.
SPECTRAL METHOD

Overcoming the Gibbs phenomenon

We consider the following prototype problem: The function \( f(x) \) is analytic in \([-1, 1]\) but is not periodic.

Viewed as a periodic function, this is a piecewise analytic function, with just one discontinuity at the known location \( x = -1 \).

Our goal is to obtain uniform exponential accuracy

\[
\max_{-1 \leq x \leq 1} |f(x) - F_N(x)| \leq Ce^{-\alpha N}
\]

where \( F_N(x) \) is a function obtained from \( f_N(x) \).
Spectral method

This effectively removes the Gibbs phenomenon completely, since it recovers exponential accuracy in the maximum norm over the whole interval including at the discontinuity point (the left and right limits at the discontinuity).

More importantly, our approach is computationally feasible.
Spectral Method

We now describe our approach. We first define Gegenbauer polynomials:

The Gegenbauer polynomials $C^{\lambda}_{n}(x)$ are orthogonal polynomials with the weight function $(1 - x^2)^{\lambda - \frac{1}{2}}$:

$$
\int_{-1}^{1} (1 - x^2)^{\lambda - \frac{1}{2}} C^{\lambda}_{k}(x) C^{\lambda}_{n}(x) dx = 0, \quad k \neq n
$$

One standardization gives:

$$(1 - x^2)^{\lambda - \frac{1}{2}} C^{\lambda}_{n}(x) = G(\lambda, n) \frac{d^n}{dx^n} \left[ (1 - x^2)^{n + \lambda - \frac{1}{2}} \right]$$

where $G(\lambda, n)$ is given by

$$
G(\lambda, n) = \frac{(-1)^n \Gamma(\lambda + \frac{1}{2}) \Gamma(n + 2\lambda)}{2^n n! \Gamma(2\lambda) \Gamma(n + \lambda + \frac{1}{2})}
$$
and

\[ C_n^\lambda(1) = \frac{\Gamma(n + 2\lambda)}{n!\Gamma(2\lambda)} \]

We also have the nice property:

\[ |C_n^\lambda(x)| \leq C_n^\lambda(1), \quad -1 \leq x \leq 1 \]

which is typical for orthogonal polynomials over \([0, 1]\).
SPECTRAL METHOD

For a given function $f(x)$, its Gegenbauer expansion is defined by

$$f(x) = \sum_{l=0}^{\infty} \hat{f}(l) C_l^\lambda(x)$$

where the Gegenbauer coefficients are defined by

$$\hat{f}(l) = \frac{1}{h_l^\lambda} \int_{-1}^{1} (1 - x^2)^{\lambda-\frac{1}{2}} f(x) C_l^\lambda(x) dx$$

with $h_l^\lambda \sim C_l^\lambda(1)$ asymptotically.
There are two steps in our procedure to construct $F_N(x)$:

1. Using $f_N(x)$ to recover the first $m \sim N$ Gegenbauer expansion coefficients with exponential accuracy. This can be achieved for any $L_1$ function, as long as we choose $\lambda$ in the weight function of Gegenbauer polynomials to be proportional to $N$. The error incurred at this stage is called the truncation error.

2. For an analytic function in $[-1, 1]$, proving the exponential convergence of its Gegenbauer expansion, when the parameter $\lambda$ in the weight function is proportional to the number of terms $m$ retained in the expansion. The error at this stage is labeled the regularization error.
Note: When $\lambda$ increases, the truncation error decreases but the regularization error increases. It turns out that both of them can be made exponentially small if we choose $\lambda$ to be proportional to $N$. 
Let us first consider the Regularization Error, i.e.

\[ RE(\lambda, m) = \max_{-1 \leq x \leq 1} |f(x) - f^\lambda_m(x)| \]

where

\[ f^\lambda_m(x) = \sum_{l=0}^{m} \hat{f}(l) C^\lambda_l(x) \]

under the analytic assumption:

\[ \max_{-1 \leq x \leq 1} \left| \frac{d^k f}{dx^k}(x) \right| \leq C'(\rho) \frac{k!}{\rho^k}, \quad \rho \geq 1. \]

For fixed \( \lambda \) the estimate for this Regularization Error is routine. However, we are interested in the situation that \( \lambda \sim m \).
Theorem:

Assume $\lambda = \gamma m$ where $\gamma$ is a constant. If $f(x)$ is analytic in $[-1, 1]$ satisfying the Assumption, then the regularization error can be bounded by

$$RE(\gamma m, m) \leq Aq^m$$

where $q$ is given by

$$q = \frac{(1 + 2\gamma)^{1+2\gamma}}{\rho 2^{1+2\gamma} \gamma \gamma (1 + \gamma)^{1+\gamma}}$$

In particular, if $\gamma = 1$ and $m = \beta N$ where $\beta$ is a positive constant, then

$$RE(\beta N, \beta N) \leq Aq^N, \quad q = \left(\frac{27}{32\rho}\right)^\beta < 1.$$
SPECTRAL METHOD

We now turn our attention to the truncation error.

We use the important formula

$$\frac{1}{h_\lambda^l} \int_{-1}^{1} (1 - x^2)^{\lambda-\frac{1}{2}} e^{in\pi x} C_\lambda^l(x) dx = \Gamma(\lambda) \left( \frac{2}{\pi n} \right)^\lambda i^l(l + \lambda) J_{l + \lambda}(\pi n)$$

We are given

$$f_N(x) = \sum_{k=-N}^{N} \hat{f}(k) e^{ik\pi x}$$

hence we can obtain the approximate Gegenbauer coefficients

$$\hat{g}^\lambda(l) = \frac{1}{h_\lambda^l} \int_{-1}^{1} (1 - x^2)^{\lambda-\frac{1}{2}} f_N(x) C_\lambda^l(x) dx.$$
The truncation error is defined by

\[ TE(\lambda, m, N) = \max_{-1 \leq x \leq 1} \left| \sum_{l=0}^{m} (\hat{f}^{\lambda}(l) - \hat{g}^{\lambda}(l))C_i^{\lambda}(x) \right|. \]

The truncation error cannot be small if \( \lambda \) is fixed. However, if we choose \( \lambda \sim N \) and \( m \sim N \) we have the following theorem:
Theorem:
Let \( f(x) \) be an \( L_1 \) function whose first \( 2N + 1 \) Fourier coefficients \( \hat{f}(k) \) are known. Assume that
\[
\lambda = \alpha N \quad m = \beta N
\]

Then the truncation error is bounded by
\[
TE(\alpha N, \beta N, N) \leq Aq^N,
\]
where
\[
q = \frac{(\beta + 2\alpha)^{\beta+2\alpha}}{(2\pi e)^{\alpha \alpha^\alpha} \beta^\beta}
\]

In particular, if \( \alpha = \beta \approx \frac{1}{4} \), then
\[
q \approx 0.8 < 1.
\]
Figure 2: The function $f(x) = x$ (solid line); the Fourier partial sum $f_N(x)$ with $N = 4$ (short dashed line) and $N = 8$ (dotted line), and the approximation through the Gegenbauer procedure using $m = \lambda = N/4$ for $N = 4$ (long dashed line).
References:


Generalizations in the following aspects have been studied:

- Multiple discontinuities and sub-intervals: Given the spectral partial sum over the whole interval, we can recover spectral accuracy in any sub-interval in which the function is analytic.

This example is two dimensional. We assume that the first $2N + 1$ Fourier coefficients of the function $f(x) = e^{i2.3\pi x + i1.2\pi y}$ are given in each of the four quadrants: $-1 \leq x \leq 0, -1 \leq y \leq 0$; $-1 \leq x \leq 0, 0 \leq y \leq 1$; $0 \leq x \leq 1, -1 \leq y \leq 0$ and $0 \leq x \leq 1, 0 \leq y \leq 1$. Since the function is not periodic in any of the quadrants, we clearly see the Gibbs oscillations in the left figure, which is the contour of plot of the Fourier sum for each quadrant with $N = 32$. The application of the Gegenbauer procedure completely removes these oscillations, see the right figure.
Figure 3: Contour plots of $f(x) = e^{i2.3\pi x + i1.2\pi y}$ using the Fourier partial sum with $N = 32$ in each sub-domain. Left: without the Gegenbauer procedure; Right: with the Gegenbauer procedure.
• Polynomial spectral methods: Given the spectral partial sum of polynomial bases (e.g. Chebyshev or Legendre expansions) over the whole interval, we can recover spectral accuracy in any sub-interval in which the function is analytic.

In this example, we assume that the first $N + 1$ Chebyshev coefficients of

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

are given, where $I_{[-0.5,0.5]}(x)$ is the characteristic function of the interval $[-0.5, 0.5]$, and try to obtain exponentially accurate point values of $f(x)$ in $[-0.5, 0.5]$. 
Figure 4: Errors in log scale, for $f(x) = I_{[-0.5,0.5]}(x) \cdot \sin(\cos(x))$, through the Gegenbauer procedure, with $N = 20, 40, 80, 160$. 

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• Collocation or pseudo-spectral methods: Given the point values of a piecewise analytic function on standard Chebyshev or Legendre collocation points over the whole interval, we can recover spectral accuracy in any sub-interval in which the function is analytic.


In recent years many researchers (e.g. Anne Gelb, Jae-Hun Jung) have performed research both on the theory and on the application of this approach. The application areas include computational fluid dynamics, image processing, etc.
In Chen and Shu, JCAM submitted, we have generalized the Gegenbauer reconstruction procedure to functions with end-point singularities.

We are concerned with functions of the following form

$$f(x) = a(x) + b(x)(1 + x)^s, \quad x \in [-1, 1]$$

(1)

where $s$ is a given fractional constant

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

(2)

where $1 \leq p < q$ and $q > 1$ are relatively prime integers, and $a(x)$ and $b(x)$ are both analytic functions.
Spectral method

- Since we assume that the value of $s$ is known, we are not losing generality by assuming $0 < s < 1$. All functions with end-point singularity at the left end, of the form (1) with arbitrary positive or negative $s$, can be rewritten to the same form with $0 < s < 1$ by multiplying with an analytic function $(1 + x)^k$ with a positive integer $k$, or by absorbing an analytic function $(1 + x)^k$ with a positive integer $k$ into $b(x)$.

- Since we are handling collocation methods and are given values of the original functions at the collocation points, we also have access to the collocation point values of the modified functions which are the original functions multiplied with $(1 + x)^k$. 
Spectral method

- Singularity at the right end or at both ends can be handled in the same fashion.
- The result can be easily generalized to the situation of finitely many singularities (of the form \((x - z_k)^{s_k}\) at finitely many points \(z_k\) inside the interval \([-1, 1]\) with known fractional \(s_k\)), along the lines of Gottlieb and Shu, SINUM 1996; Math Comp 1995 and using the techniques in this work.
We will use the following one to one transformation between $x \in [-1, 1]$ and $y \in [-1, 1]$:

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

where $q$ is defined in (2) (i.e. $s = \frac{p}{q}$).

The function $\bar{f}(y) = f(x(y))$ of the variable $y$ has its usual Gegenbauer expansion under the basis $\{C_l^\lambda(y)\}$:

$$f(x(y)) = \bar{f}(y) = \sum_{l=0}^{\infty} \hat{f}^\lambda(l) C_l^\lambda(y)$$

with the Gegenbauer coefficients $\hat{f}^\lambda(l)$ given by

$$\hat{f}^\lambda(l) = \frac{1}{h_l^\lambda} \int_{-1}^{1} (1 - y^2)^{\lambda - \frac{1}{2}} \bar{f}(y) C_l^\lambda(y) dy.$$  (3)
Our goal is to find a good approximation to the first $m \sim N$ Gegenbauer coefficients $\hat{f}^\lambda(l)$ in (3), denoted as $\hat{g}^\lambda(l)$, from the known point values $\{f(x_i)\}$ at the standard Gaussian collocation points. We will then obtain the approximation of $f(x)$ using these $m \sim N$ terms of its Gegenbauer expansion:

$$f_{N,m,\lambda}^m(x) = \sum_{l=0}^{m} \hat{g}^\lambda(l) C_l^\lambda(y(x))$$

The difficulty is to prove the truncation error is exponentially small. The complication comes from the transformation we used above.
SPECTRAL METHOD

Based on the known point values \( \{ f(x_i) \} \), we define not the usual interpolation polynomial \( I_N f(x) \), but

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

\[
= I_N \left( (1 - y(x)^2)^{\lambda - \frac{1}{2}} (1 + y(x))^{-\frac{q-1}{2}} f(x) \right)
\]

Intuitively, the function being interpolated has about \( \frac{\lambda}{q} \sim N \) continuous derivatives, hence the interpolation would produce nice error estimates.
Our candidate for approximating the Gegenbauer coefficients $\hat{f}^\lambda(l)$ is:

$$
\hat{g}^\lambda(l) = \frac{1}{h_i^\lambda} \int_{-1}^{1} (1 + y)^{\frac{q-1}{2}} (f^\lambda)_N(x(y))C_i^\lambda(y) dy.
$$

(4)

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

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

with

$$
q_T = \frac{(\beta + 2\alpha)^{\beta+2\alpha}}{\beta\beta\alpha^{2\alpha}} \left[ \frac{\alpha}{2q} (1 + \delta) \right]^{\alpha}, \quad \delta = \frac{1}{e} \left( 1 + \frac{1}{2^q A q \rho} \right).
$$
When we choose $\beta = \gamma \alpha$, i.e. $m = \gamma \lambda$, we have

$$q_T = \left( \frac{(\gamma + 2)\gamma + 2}{\gamma^\gamma} \left[ \frac{\alpha}{2q(1 + \delta)} \right] \frac{1}{q} \right)^\alpha.$$ 

If we choose $\alpha$ to satisfy

$$\alpha < \frac{2q}{(1 + \delta)} \left( \frac{\gamma^\gamma}{(2 + \gamma)^{(2+\gamma)}} \right)^q,$$

then $q_T < 1$.

Regularization error is exponentially small using existing results, since the function $f(x(y))$ is analytic with respect to the variable $y$.  

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Example: We take the function

\[ f(x) = \cos(x) + \sin(x)\sqrt{1 + x} \]  

(5)

and try to recover the pointwise values of this function over \([-1, 1]\).

First, we consider the Fourier collocation. We assume the point values \(\{f(x_i)\}\) on the \(2N + 1\) uniform points:

\[ x_i = \frac{2i}{2N + 1}, \quad i = -N, \ldots, N \]  

(6)

are given. The parameters are chosen as

\[ \lambda = 0.2N, \quad m = 0.075N. \]  

(7)
Figure 5: Pointwise errors in the logarithm scale. Fourier case.
SPECTRAL METHOD

Second, we consider the Chebyshev collocation. We assume the point values \( \{ f(x_i) \} \) on the \( N + 1 \) Chebyshev collocation points:

\[
x_i = \cos \left( \frac{\pi (2i + 1)}{2N + 2} \right), \quad i = 0, \ldots, N
\]  

(8) are given. The parameters are chosen as

\[
\lambda = 0.2N, \quad m = 0.1N.
\]  

(9)
Figure 6: Pointwise errors in the logarithm scale. Chebyshev case.
## Table 1: Maximum error table

<table>
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<tr>
<th>N</th>
<th>Fourier case ( \lambda = 0.2N, m = 0.075N )</th>
<th>Chebyshev Case ( \lambda = 0.2N, m = 0.1N )</th>
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<td>( L^\infty ) error</td>
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</tr>
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<td>80</td>
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</tr>
</tbody>
</table>
Concluding remarks

• We have completely overcome the difficulty of Gibbs phenomenon, in the sense that we can recover exponential accuracy from spectral partial sum of discontinuous but piecewise analytic functions, in the maximum norm in any sub-interval of analyticity. We can recover exponential accuracy all the way to the discontinuity (left and right limits) if we know its location.

• The approach is computationally easy to implement, and it works for quite general situations including polynomial spectral methods, collocation methods, etc.
• Recent work generalizes this technique to functions with end-point singularities.

• Applications of this technique are in computational fluid dynamics and image processing.
The End

THANK YOU!