Math 660-Lecture 13: Spectral methods: Chebyshev Pseudo-spectral method

1 Polynomial interpolation

If we use Fourier Spectral method to solve equations with non-periodic boundary conditions, we are dealing with non-smooth functions when periodically extended and the spectral accuracy of Fourier method is lost. The so-called Gibbs phenomenon will arise (the fake oscillation due to discontinuity or non-smoothness).

The idea is to use polynomial interpolation. Let's look at 1D problem on interval $[-1, 1]$ (other intervals can be shifted and scaled to be $[-1, 1]$). If we use N points, we should choose the location of the points. One option is to use the equispaced points. Another option, for example, could be the Chebyshev points

$$x_j = \cos(j\pi/N).$$

The density of the Chebyshev points tends to $\rho = \frac{1}{\pi\sqrt{1-x^2}}$.

Example: Consider $u = 1/(1 + 16x^2)$. For N, we use the equispaced and Chebyshev points.

For this example, we find that the uniform sampling is not good while the Chebyshev sampling is good. (Clearly, there are examples where both interpolations work well.)

Theorem 1. *Suppose the density of the interpolation points converge weakly to a density function ρ as $N \to \infty$. Define*

$$\phi(z) = \int_{-1}^{1} \rho(x) \log|z - x| dx,$$

where $z \in \mathbb{C}^2$. Let $\phi_{[-1,1]} = \sup_{x\in[-1,1]} \phi(x)$. For $K > \phi_{[-1,1]}$, if u can be extended analytically into the region $\{z : \phi(z) \le K\}$, then there exists $C_m > 0$ which is independent of N such that

$$\sup_{x\in[-1,1]} |u^{(m)}(x) - p_N^{(m)}(x)| \le C_m e^{-N(K-\phi_{[-1,1]})}.$$

We can see that if we hope the polynomial interpolation to be well behaved, our function u should be nice in the region $\phi(z) \le \phi_{[-1,1]}$.

For $\rho = 1/2$, we have

$$\frac{1}{2}\int \log|z-x|dx = \frac{1}{2}Re\int \log(z-x)dx = \frac{1}{2}x\log|z-x| - \frac{1}{2}Re[\int \frac{x}{x-z}dx]$$

Hence,

$$\phi = \frac{1}{2}\log|z-1| + \frac{1}{2}\log|z+1| - 1 - \frac{1}{2}Re[z\log(x-z)|_{-1}^{1}]$$

Note that $\log(-1) = i\pi$. We have

$$\phi = -1 + \frac{1}{2}Re[\log(z-1)+\log(z+1)] - \frac{1}{2}Re(z\log(z-1) - z\log(z+1))$$

Consider that $\rho = \frac{1}{\pi\sqrt{1-x^2}}$. $\phi = Re(I)$, where

$$I = \frac{1}{\pi}\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}}\log(x-z)dx = \frac{1}{2\pi i}\oint_C \frac{1}{\sqrt{\zeta^2-1}}\log(\zeta-z)d\zeta.$$

where C is the contour enclosing $[-1,1]$, counterclockwise.

In the region where $\log(\zeta - z)$ is analytic, we have

$$I'(z) = \frac{1}{2\pi i}\oint_C \frac{1}{\sqrt{\zeta^2-1}}\frac{-1}{\zeta-z}d\zeta = \frac{1}{2\pi i}\oint_{\tilde{C}} \frac{1}{\sqrt{\zeta^2-1}}\frac{-1}{\zeta-z}d\zeta = -\frac{1}{\sqrt{z^2-1}}$$

where $\tilde{C}$ is a contour enclosing z, counterclockwise.

Hence,

$$I(z) = \log(z-\sqrt{z^2-1}) + C \Rightarrow \phi(z) = \log|z-\sqrt{z^2-1}| + C_1.$$

By Mathematica,

$$C_1 = \phi(0) = \frac{1}{\pi}\int_{-1}^{1}\frac{\log|x|}{\sqrt{1-x^2}}dx = -\log(2).$$

Actually, this integral can be evaluated directly:

$$C_1 = \frac{1}{\pi}\int_0^{\pi}\log|\cos\theta|d\theta = \frac{2}{\pi}\int_0^{\pi/2}\log|\cos\theta|d\theta = \frac{2}{\pi}\int_0^{\pi/2}\log|\sin\theta|d\theta$$
$$= \frac{1}{\pi}\int_0^{\pi/2}\log|\cos\theta\sin\theta|d\theta = \frac{1}{\pi}\int_0^{\pi/2}\log|\sin(2\theta)|d\theta - \frac{1}{2}\log 2 = \frac{C_1}{2} - \frac{1}{2}\log 2.$$

For $\rho = \frac{1}{2}$, the region $\{z : \phi(z) \le \phi_{[-1,1]}\}$ contains, for example, $i/4$. For $\rho = \frac{1}{\pi\sqrt{1-x^2}}$, the region is just $[-1,1]$, which is the possible smallest. Hence, the Chebyshev points are the optimal sampling points.

2 Chebyshev Differentiation matrices

On the points $x_j = \cos(j\pi/N)$, we have a unique polynomial of degree N such that $p(x_j) = u(x_j)$. Then,

$$D_N^{(k)} u = p^{(k)}(x_j).$$

The matrices $D_N^{(k)}$ are independent of u and are called the Chebyshev Differentiation matrices. It turns out that $D_N^{(k)} = D_N^k$. These matrices are singular:

$$r(D_N^k) = N + 1 - k.$$

Clearly, $D_N^{N+1} = 0$ and hence the eigenvalues of D_N are all zero. The degree of the k-th derivative of a polynomial is lower than the degree of the polynomial itself by k.

In the book, there's a formula and a code to construct these matrices.

```
% CHEB  compute D = differentiation matrix, x = Chebyshev grid

  function [D,x] = cheb(N)
  if N==0, D=0; x=1; return, end
  x = cos(pi*(0:N)/N)';
  c = [2; ones(N-1,1); 2].*(-1).^(0:N)';
  X = repmat(x,1,N+1);
  dX = X-X';
  D  = (c*(1./c)')./(dX+(eye(N+1)));      % off-diagonal entries
  D  = D - diag(sum(D'));                 % diagonal entries
```

Code presentation (show cheb.m and the code for solving the problem) Consider the eigenvalue boundary value problem:

$$-u_{xx} = \lambda u, |x| < 1, u(\pm 1) = 0.$$

Idea: D^2 is the Chebyshev differentiation for $\frac{d^2}{dx^2}$. Then, since we have the boundary conditions $u(\pm 1) = 0$, we then don't need the equation at $x = \pm 1$. Further, since they are zero, the first and last columns of the matrix are not needed. Hence, we can only pick out the $(2 : N-1) \times (2 : N-1)$ submatrix.

Note that D^2 is singular and the eigenvalues are all zero, which clearly gives nothing for our problem, but if we have the boundary conditions and only pick out the submatrix, we'll get a nonsingular matrix and the eigenvalues can be computed correctly.

3 Chebyshev series and FFT

In the previous section, we introduced the Chebyshev differentiation matrix, which is a type of pseudo-spectral methods. Here, we provide a new point of view for the Chebyshev differentiation.

We do change of variables $x = \cos\theta$ and then $\theta \in [0, 2\pi]$. Consider the Chebyshev polynomials:

$$T_n(x) = \cos(n\theta(x)).$$

Note that $\cos((n+1)\theta) = 2\cos(n\theta)\cos\theta - \cos((n-1)\theta)$.

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

Direct computation shows that $T_0(x) = 1$ and $T_1(x) = x$. Then, we have

$$\begin{aligned} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_2(x) &= 2x(x) - 1 = 2x^2 - 1, \\ T_3(x) &= 2x(2x^2 - 1) - x = 4x^3 - 3x, \ldots \end{aligned}$$

Clearly, these polynomials are linearly independent. Then, the polynomial $p(x)$ with degree N can be written uniquely as

$$p(x) = \sum_{n=0}^{N} a_n T_n(x) = \sum_{n=0}^{N} a_n \cos(n\theta) = P(\theta).$$

The Chebyshev points x_j then corresponds to equispaced points on $\theta \in [0, 2\pi]$, which then allows us to use DFT for the Chebyshev differentiation. The Chebyshev matrices can be avoided. Imagine that we discretize $[0, 2\pi)$ into $2N$ intervals, and $\theta_j = 2\pi j/N$. Clearly, P is an even function of θ and hence $P(\theta_j) = P(2\pi - \theta_j) = P(-\theta_j) = p(x_j)$. On the frequency side, a_n corresponds to $k = \pm n$. Finally, note that $\frac{d}{dx} = -\frac{1}{\sin\theta}\frac{d}{d\theta} = -\frac{1}{\sqrt{1-x^2}}\frac{d}{d\theta}$. Hence, we have the following algorithm:

- Let $V_j = u_j$ for $j = 0, 1, \ldots, N$ and $V_j = u_{2N-j}$ for $j = N+1, N+2, \ldots, 2N-1$.
- Compute the $d/d\theta$ derivative using FFT: $W = real(ifft(1i * k * \hat{V}))$ where $k = 0, 1, \ldots, N, -N+1, \ldots, -1$, where $\hat{V} = fft(V)$.
- The derivatives for $x_j \neq \pm 1$ are computed using $-\frac{W_j}{\sqrt{1-x_j^2}}$ for $j = 1, 2, \ldots, N-1$ (we don't use the date for $j = N+1, \ldots, 2N-1$). Special care should be taken for the boundary points.