Lectures 17 & 18: Numerical methods

- Spectral (Galerkin) method
  - Basis function expansion
  - Compute inner products to determine equation for spectral coefficients

- Pseudo-spectral method
  - Satisfy equation at the set of "collocation" points
  - Connection to polynomial interpolation

- Chebyshev polynomials
  - Why they should be used
  - Basic properties
Online resources

- Freely available books/papers
  - Jonh P. Boyd
    Chebyshev and Fourier Spectral Methods
  - Lloyd N. Trefethen
    Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations
  - Weideman and Reddy
    A Matlab Differentiation Matrix Suite

- Publicly available software
  - A Matlab Differentiation Matrix Suite
    http://dip.sun.ac.za/~weideman/research/differ.html
  - Chebfun
    http://www2.maths.ox.ac.uk/chebfun/
Diffusion equation on $L_2[-1, 1]$

\[ \psi_t(x, t) = \psi_{xx}(x, t) \]

\[ \psi(x, 0) = \psi_0(x) \]

\[ \psi(\pm 1, t) = 0 \]

Basis function expansion

\[ \psi(x, t) = \sum_{n=1}^{\infty} \alpha_n(t) \phi_n(x) \]

$\alpha_n(t)$ — (unknown) spectral coefficients

$\phi_n(x)$ — (known) basis functions
Galerkin method

- Approximate solution by

\[ \psi(x, t) \approx \sum_{n=1}^{N} \alpha_n(t) \phi_n(x) = \begin{bmatrix} \phi_1(x) & \cdots & \phi_N(x) \end{bmatrix} \begin{bmatrix} \alpha_1(t) \\ \vdots \\ \alpha_N(t) \end{bmatrix} \]

substitute into the equation and take an inner product with \( \{\phi_m\} \)

\[
\begin{bmatrix}
\langle \phi_1, \phi_1 \rangle & \cdots & \langle \phi_1, \phi_N \rangle \\
\vdots & \ddots & \vdots \\
\langle \phi_N, \phi_1 \rangle & \cdots & \langle \phi_N, \phi_N \rangle
\end{bmatrix}
\begin{bmatrix}
\dot{\alpha}_1(t) \\
\vdots \\
\dot{\alpha}_N(t)
\end{bmatrix}
=
\begin{bmatrix}
\langle \phi_1, \phi''_1 \rangle & \cdots & \langle \phi_1, \phi''_N \rangle \\
\vdots & \ddots & \vdots \\
\langle \phi_N, \phi''_1 \rangle & \cdots & \langle \phi_N, \phi''_N \rangle
\end{bmatrix}
\begin{bmatrix}
\alpha_1(t) \\
\vdots \\
\alpha_N(t)
\end{bmatrix}
\]

- Done if basis functions satisfy BCs

Otherwise, need additional conditions on spectral coefficients

\[
\begin{bmatrix}
0 \\
0
\end{bmatrix}
= \begin{bmatrix}
\phi_1(-1) & \cdots & \phi_N(-1) \\
\phi_1(+1) & \cdots & \phi_N(+1)
\end{bmatrix}
\begin{bmatrix}
\alpha_1(t) \\
\vdots \\
\alpha_N(t)
\end{bmatrix}
\]
Pros and cons

- Advantage: superior convergence
  (if basis functions selected properly)

- Problem: requires integration
  - Cumbersome in spatially-varying and nonlinear systems

Example: Orr-Sommerfeld equation in fluid mechanics

\[ \Delta \psi_t = \left( jk_x (U''(y) \ - \ U(y) \Delta) \ + \ \frac{1}{R} \Delta^2 \right) \psi \]
Polynomial interpolation

- Approximate $f(x)$ by a polynomial that matches $f(x)$ at interpolation points

$$p_{N-1}(x_i) = f(x_i), \quad i = \{1, \ldots, N\}$$

- Examples:

  $\begin{align*}
  N = 2 & \Rightarrow \text{Linear Interpolation} \\
  N = 3 & \Rightarrow \text{Quadratic Interpolation}
  \end{align*}$

  $\begin{align*}
  f(x) & \approx \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \\
  f(x) & \approx \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \\
  & \quad \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \\
  & \quad \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)
  \end{align*}$
Lagrange interpolation formula

\[ p_N(x) = \sum_{i=0}^{N} f(x_i) C_i(x) \]

\[ C_i(x) = \prod_{j=0, j\neq i}^{N} \frac{x - x_j}{x_i - x_j} \]

- Cardinal functions \( C_i(x_j) = \delta_{ij} \)
  - Not efficient for computations
  - Suitable for theoretical arguments

- Runge Phenomenon
  \[ f(x) = \frac{1}{1 + x^2}, \ x \in [-5, 5] \]

  - Evenly spaced points \( \Rightarrow \) convergence for \( |x| \leq 3.63 \)

Interactive Demo
Choice of grid points

- Cauchy interpolation error theorem

\[
\begin{align*}
  f & \quad \text{has } N + 1 \text{ derivatives} \\
  p_N & \quad \text{interpolant of degree } N
\end{align*}
\Rightarrow
f(x) - p_N(x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} \prod_{i=0}^{N} (x - x_i)
\]

- Chebyshev minimal amplitude theorem

★ Among all polynomials \( q_N(x) \) of degree \( N \), with leading coefficient 1,

\[
\frac{T_N(x)}{2^{N-1}} = \frac{N \text{th Chebyshev polynomial}}{2^{N-1}}
\]

has the smallest \( L_\infty[-1, 1] \) norm

\[
\sup_{x \in [-1, 1]} |q_N(x)| \geq \sup_{x \in [-1, 1]} \left| \frac{T_N(x)}{2^{N-1}} \right| = \frac{1}{2^{N-1}}, \quad \text{for all } q_N(x)
\]
Optimal interpolation points

• Select polynomial part of \( f(x) - p_N(x) \) as

\[
\prod_{i=0}^{N} (x - x_i) = \frac{T_{N+1}(x)}{2^N}
\]

• Optimal interpolation points: roots of \( T_{N+1}(x) \)

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

- Solutions to Sturm-Liouville Problem

\[(1 - x^2) T_n''(x) - x T_n'(x) + n^2 T_n(x) = 0, \quad x \in [-1, 1], \quad n = 0, 1, \ldots\]

- Three-term recurrence

\[\{T_0 = 1; \quad T_1(x) = x; \quad T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x), \quad n \geq 1\}\]

- Alternative definition

\[T_n(\cos(t)) = \cos(nt) \Rightarrow |T_n(x)| \leq 1, \quad \text{for all } x \in [-1, 1], \quad n = 0, 1, \ldots\]
• Inner product

$$\langle T_m, T_n \rangle_w = \int_{-1}^{1} \frac{T_m(x) T_n(x)}{\sqrt{1 - x^2}} \, dx = \begin{cases} 0 & m \neq n \\ \pi & m = n = 0 \\ \frac{\pi}{2} & m = n \neq 0 \end{cases}$$

• Collocation points

Gauss-Chebyshev: $x_i = \cos\left(\frac{(2i - 1) \pi}{2N}\right)$, $i = \{1, \ldots, N\}$

Gauss-Lobatto: $x_i = \cos\left(\frac{\pi i}{N - 1}\right)$, $i = \{0, \ldots, N - 1\}$

• Integration

$$\int_{-1}^{x} T_n(\xi) \, d\xi = \frac{T_{n+1}(x)}{2(n + 1)} + \frac{T_{n-1}(x)}{2(n - 1)}, \quad n \geq 2$$
Gaussian integration

- Approximate \( f(x) \) by a polynomial that matches \( f(x) \) at interpolation points

\[
p_N(x_i) = f(x_i), \quad i = \{0, \ldots, N\}
\]

\[
f(x) \approx p_N(x) = \sum_{i=0}^{N} f(x_i) C_i(x)
\]

- Evaluate integral of \( f(x) \) by integrating \( p_N(x) \)

\[
\int_a^b f(x) \, dx \approx \sum_{i=0}^{N} w_i f(x_i)
\]

Quadrature weights:

\[
w_i = \int_a^b C_i(x) \, dx
\]

- Gaussian integration: exact if integrand is a polynomial of degree \( N \)
• Can be made exact for polynomials of degree $2N + 1$ by optimal selection of
  ★ interpolation points $\{x_i\}$
  ★ weights $\{w_i\}$

• Gauss-Jacobi integration
  ★ orthogonal polynomials w.r.t. the inner product with weight function $\rho(x)$
  ★ interpolation points: zeros of $p_{N+1}(x)$
  ★ quadrature formula: exact for polynomials of degree $2N + 1$ or smaller

$$\int_a^b f(x) \rho(x) \, dx = \sum_{i=0}^{N} w_i f(x_i)$$

• Good candidates for quadrature points:

  Gauss-Lobatto: $x_i = \cos \left( \frac{\pi i}{N} \right)$, $i = \{0, \ldots, N\}$
Interpolation by quadrature

• Orthogonality w.r.t. discrete inner product

\[ \langle \phi_i, \phi_j \rangle = \delta_{ij} \Rightarrow \langle \phi_i, \phi_j \rangle_G = \sum_{m=0}^{N} w_m \phi_i(x_m) \phi_j(x_m) = \delta_{ij} \]

• Basis function expansion

\[ f(x) = \sum_{n=0}^{\infty} \alpha_n \phi_n(x) = \sum_{n=0}^{N} \alpha_n \phi_n(x) + E_N(x) \]

• Discrete vs. exact spectral coefficients

\[ \alpha_{m,G} = \langle \phi_m, f \rangle_G \]
\[ = \langle \phi_m, \sum_{n=0}^{N} \alpha_n \phi_n + E_N \rangle_G \]
\[ = \sum_{n=0}^{N} \alpha_n \langle \phi_m, \phi_n \rangle_G + \langle \phi_m, E_N \rangle_G \]
\[ = \alpha_m + \langle \phi_m, E_N \rangle_G \]
Error bound for Chebyshev interpolation

- Error between Galerkin and Pseudo-spectral
  
  twice the sum of absolute values of neglected spectral coefficients

\[
\star \quad f(x) = \sum_{n=0}^{\infty} \alpha_n T_n(x)
\]

\[
\star \quad p_N(x) \text{ – polynomial that interpolates } f(x) \text{ at Gauss-Lobatto points}
\]

\[
|f(x) - p_N(x)| \leq 2 \sum_{n=N+1}^{\infty} |\alpha_n|, \text{ for all } N \text{ and all } x \in [-1, 1]
\]
Back to cardinal functions

- Lagrange interpolation

\[ p_N(x) = \sum_{i=0}^{N} f(x_i) C_i(x) \]

\[ C_i(x) = \prod_{j=0, j \neq i}^{N} \frac{x - x_j}{x_i - x_j} \]

Cardinal functions \( C_i(x_j) = \delta_{ij} \)

- Sinc functions

\[ C_k(x; h) = \frac{\sin \left( \frac{(x - kh) \pi}{h} \right)}{(x - kh) \pi} = \text{sinc} \left( \frac{x - kh}{h} \right) \]

\( \{x_j = jh; j \in \mathbb{Z}\} \Rightarrow C_k(x_j; h) = \delta_{jk} \)

Approximate \( f \) by

\[ f(x) = \sum_{j=-\infty}^{\infty} f(x_j) C_j(x; h) \]
Cardinal functions for Chebyshev polynomials

- Gauss-Chebyshev points: zeros of \( T_{N+1}(x) \)
  - Taylor series expansion around \( x_j \)

\[
T_{N+1}(x) = \underbrace{T_{N+1}(x_j)}_0 + T'_{N+1}(x_j)(x-x_j) + \frac{1}{2} T''_{N+1}(x_j)(x-x_j)^2 + \mathcal{O}(|x-x_j|^3)
\]

Cardinal functions:

\[
C_j(x) = \frac{T_{N+1}(x)}{T'_{N+1}(x_j)(x-x_j)} = 1 + \frac{T''_{N+1}(x_j)(x-x_j)}{2T'_{N+1}(x_j)} + \mathcal{O}(|x-x_j|^2)
\]

- Gauss-Lobatto points: zeros of \((1-x^2)T'_N(x)\)

Cardinal functions:

\[
C_j(x) = \frac{(1-x^2)T'_N(x)}{((1-x^2)T'_N(x))'\big|_{x=x_j}(x-x_j)}
\]
Matlab Differentiation Matrix Suite: A Demo

%% number of grid points without boundaries (no ±1)
N = 50

%% 1st & 2nd order differentiation matrices
[yT,DM] = chebdif(N+2,2);
y = yT(2:end-1);

%% 1st & 2nd derivatives wrt y on a total grid (no BCs)
DT1 = DM(:,:,1);
DT2 = DM(:,:,2);

%% implement homogeneous Dirichlet BCs
%% ammounts to deleting 1st rows and columns of DT1 & DT2
D1 = DT1(2:N+1,2:N+1);
D2 = DT2(2:N+1,2:N+1);

%% 4th derivative with Dirichlet & Neumann BCs at both ends
%% D4 - obtained on a grid without ±1
[y1,D4] = cheb4c(N+2);

%% e-value decomposition of D2 with Dirichlet BCs
[Vh,Dh] = eig(D2);  % compare with analytical results