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 $L_2\,[-1, 1]$

$$
\begin{aligned}
\psi_t(x,t) &= \psi_{xx}(x,t) \\
\psi(x,0) &= \psi_0(x) \\
\psi(\pm 1,t) &= 0
\end{aligned}
$$

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 $\{\phi_m\}$

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

- 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

$$\Delta\,\psi_t \;=\; \left(\mathrm{j}k_x\,(U''(y) \;-\; U(y)\,\Delta) \;+\; \frac{1}{R}\,\Delta^2\right)\psi$$

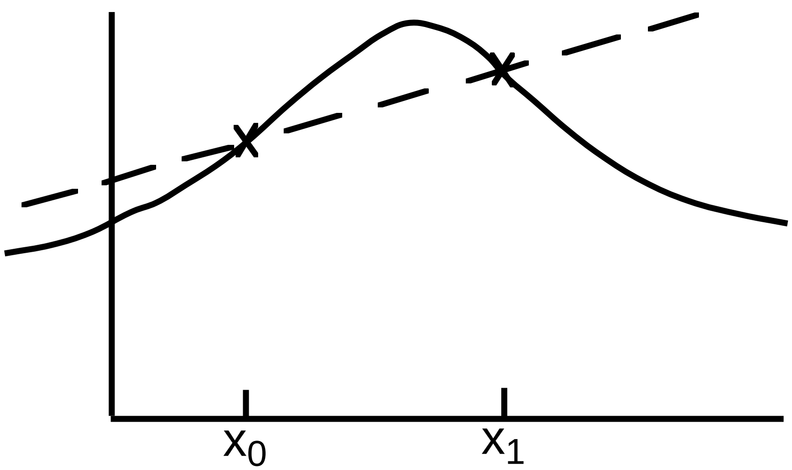
Polynomial interpolation

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

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

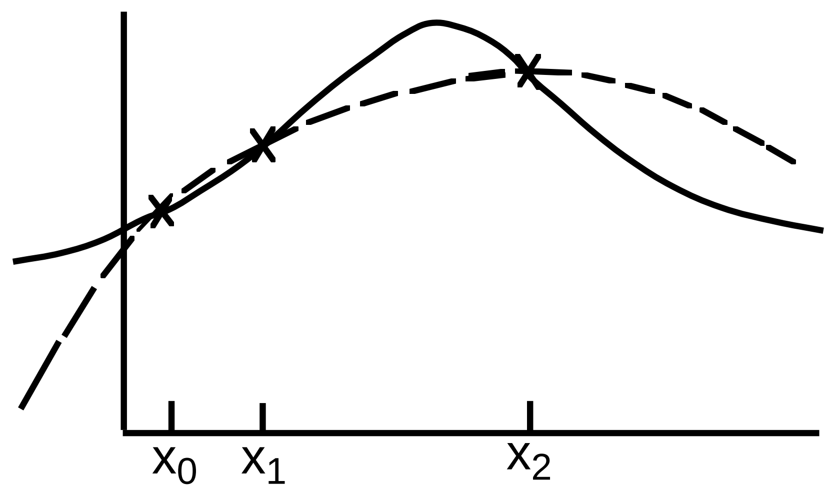
- Examples:

$N = 2 \;\Rightarrow$ Linear Interpolation



$$f(x) \;\approx\; \frac{x - x_1}{x_0 - x_1} f(x_0) \;+\; \frac{x - x_0}{x_1 - x_0} f(x_1)$$

$N = 3 \;\Rightarrow$ Quadratic Interpolation



$$f(x) \;\approx\; \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) \;+\; \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \;+\; \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

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

$$f(x) \;=\; \frac{1}{1 \,+\, x^2}, \quad x \in [-5,\, 5]$$

  - ⋆ Evenly spaced points $\Rightarrow$ convergence for $|x| \;\leq\; 3.63$
    Interactive Demo

Choice of grid points

- Cauchy interpolation error theorem

$$\left.\begin{array}{lll} f & - & \text{has } N+1 \text{ derivatives} \\ p_N & - & \text{interpolant of degree } N \end{array}\right\} \;\Rightarrow\; f(x) - p_N(x) \;=\; \frac{f^{(N+1)}(\xi)}{(N+1)!} \prod_{i=0}^{N} (x - x_i)$$

- 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

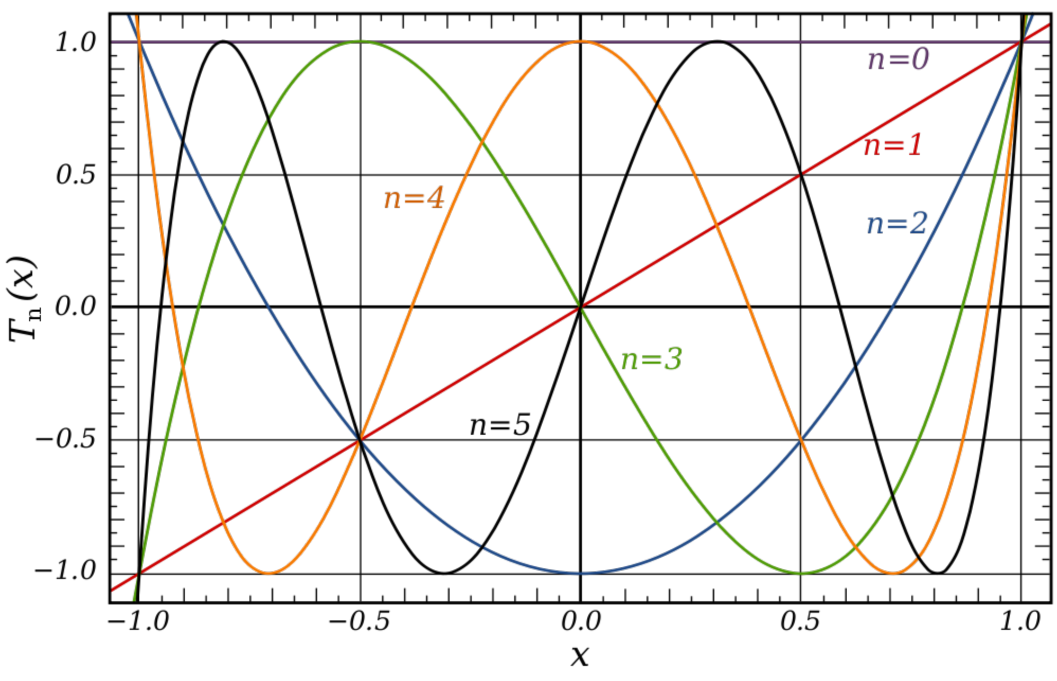
$$(1 - x^2)\, T_n''(x) - x\, T_n'(x) + n^2\, T_n(x) = 0, \;\; x \in [-1,\, 1], \;\; n = 0, 1, \ldots$$

- Three-term recurrence

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

- Alternative definition

$$T_n\,(\cos\,(t)) = \cos\,(n\,t) \;\; \Rightarrow \;\; |T_n(x)| \leq 1, \;\; \text{for all } x \in [-1,\, 1], \; n = 0, 1, \ldots$$



- Inner product

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

- Collocation points

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

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

- Integration

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

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 $p_N(x)$

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \sum_{i\,=\,0}^{N} w_i\, f(x_i)$$

Quadrature weights:

$$w_i \;=\; \int_a^b C_i(x)\,\mathrm{d}x$$

- 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

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

- Good candidates for quadrature points:

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

Interpolation by quadrature

- Orthogonality w.r.t. discrete inner product

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

- 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

$$\begin{aligned}
\alpha_{m,G} &= \langle \phi_m, f \rangle_G \\
&= \left\langle \phi_m, \sum_{n\,=\,0}^{N} \alpha_n \, \phi_n \;+\; E_N \right\rangle_G \\
&= \sum_{n\,=\,0}^{N} \alpha_n \, \langle \phi_m, \phi_n \rangle_G \;+\; \langle \phi_m, E_N \rangle_G \\
&= \alpha_m \;+\; \langle \phi_m, E_N \rangle_G
\end{aligned}$$

Error bound for Chebyshev interpolation

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

  ⋆ $f(x) \; = \; \sum_{n=0}^{\infty} \alpha_n T_n(x)$

  ⋆ $p_N(x)$ – polynomial that interpolates $f(x)$ at Gauss-Lobatto points

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

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

$$C_k(x;h) \;=\; \frac{\sin\left(\dfrac{(x - kh)\,\pi}{h}\right)}{\dfrac{(x - kh)\,\pi}{h}} \;=\; \operatorname{sinc}\left(\frac{x - kh}{h}\right)$$

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

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

$$T_{N+1}(x) = \underbrace{T_{N+1}(x_j)}_{0} + T'_{N+1}(x_j)\,(x - x_j) + \frac{1}{2}T''_{N+1}(x_j)\,(x - x_j)^2 + O\left(|x - x_j|^3\right)$$

Cardinal functions

$$C_j(x) = \frac{T_{N+1}(x)}{T'_{N+1}(x_j)\,(x - x_j)} = 1 + \frac{T''_{N+1}(x_j)\,(x - x_j)}{2T'_{N+1}(x_j)} + O\left(|x - x_j|^2\right)$$

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

Cardinal functions: $C_j(x) = \dfrac{\left(1 - x^2\right)T'_N(x)}{\left((1 - x^2)\,T'_N(x)\right)'\Big|_{x = x_j}(x - x_j)}$

Matlab Differentiation Matrix Suite: A Demo

```
%% number of grid points without boundaries (no \pm 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 \pm 1
[y1,D4] = cheb4c(N+2);

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