# MAST90026 Computational Differential Equations: Week 2

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# Method of weighted residual

Idea of MWR : $u_N = \sum_{j=0}^{N} c_j \phi_j$

- Basis functions
  - Global basis functions: sin(jx), polynomials
  - Piecewise polynomial functions: hat function
- Determine coefficient
  - Collocation Method : equal to 0 at some points
  - Galerkin method: residual orthogonal to fun space

# Classification of MWR

| Weighted Residual Method | | |
|---|---|---|
| | Global basis | Piecewise polynomial |
| Collocation | Spectral collocation | Spline collocation |
| Galerkin | Spectral Galerkin | Finite element method |

# Idea of spectral collocation

Three step idea:

Step 1: Choose a trial space $V_N$ ($N+1$ dimensional). Write $u_N \in V_N$ as

$$u_N = \sum_{j=0}^{N} c_j b_j(x).$$

Step 2: Choose collocation points $\{x_0, x_1, \dots, x_N\}$.

Step 3: Determine $c_j$ using the collocation condition:

$$Lu_N(x_j) = f(x_j), \quad j = 0, 1, \dots, N.$$

# Choose of trial space and collocation points

Periodic boundary conditions:

- Space of trigonometric functions

$$u_N(x) = \sum_{j=0}^{N} a_j \cos(jx) + \sum_{j=1}^{N} b_j \sin(jx) = \sum_{j=-N}^{N} c_j e^{ijx}.$$

- Collocation points: $x_j = \frac{j\pi}{N}, \quad j = 0, 1, \ldots, 2N.$

Nonperiodic boundary conditions:

- Space of polynomials of degree $N$ (order $N+1$).

$$u_N(x) = p_N(x) \in \mathbb{P}_{N+1}.$$

- Collocation points are roots of orthogonal polynomial of degree $N+1$.

# Definition of orthogonal

**Definition : (Orthogonal)**

Given an open interval $I := (a, b)(-\infty \leq a < b \leq +\infty)$, and a generic weight function $\omega$ such that

$$\omega(x) > 0, \forall x \in I \text{ and } \omega \in L^1(I)$$

two different functions $f$ and $g$ are said to be orthogonal to each other in $L^2_\omega(a, b)$ or orthogonal with respect to $\omega$ if

$$(f, g)_\omega := \int_a^b f(x)g(x)\omega(x)dx = 0$$

# Orthogonal polynomial

**Definition**

A sequence of polynomials $\{p_n\}_{n=0}^{\infty}$ with $\deg(p_n) = n$ is said to be orthogonal in $L^2_\omega(a,b)$ if

$$(p_n, p_m)_\omega = \int_a^b p_n(x) p_m(x) \omega(x) dx = \gamma_n \delta_{mn}$$

where the constant $\gamma_n = \|p_n\|_\infty^2$ is nonzero, and $\delta_{mn}$ is the Kronecker delta.

# Existence and uniqueness of orthogonal polynomial

**Theorem**

For any given positive weight function $\omega \in L^1(a,b)$, there exists a unique sequence of monic orthogonal polynomials $\{\bar{p}_n\}$ with $\deg(\bar{p}_n) = n$, which can be constructed as follows

$$\bar{p}_0 = 1, \bar{p}_1 = x - \alpha_0$$
$$\bar{p}_{n+1} = (x - \alpha_n)\,\bar{p}_n - \beta_n \bar{p}_{n-1}, \quad n \geq 1$$

where

$$\alpha_n = \frac{(x\bar{p}_n, \bar{p}_n)_\omega}{\|\bar{p}_n\|_\omega^2}, \quad n \geq 0,$$
$$\beta_n = \frac{\|\bar{p}_n\|_\omega^2}{\|\bar{p}_{n-1}\|_\omega^2}, \quad n \geq 1.$$

# Example of orthogonal polynomials

Consider $(a, b) = (-1, 1)$ and $\omega = 1$. Legendre polynomials:

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_{n+1}(x) = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x),$$

Consider $(a, b) = (-1, 1)$ and $\omega = (1 - x^2)^{-\frac{1}{2}}$. Chebyshev polynomials of the first kind:

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_{n+1}(x) = 2x P_n(x) - P_{n-1}(x),$$

More general. Consider $(a, b) = (-1, 1)$ and $\omega = (1 - x)^{\alpha}(1 + x)^{\beta}$ with $\alpha, \beta > -1$. The obtained orthogonal polynomials are Jacobi polynomials

# Other definition of Legendre and Chebyshev polynomials

Legendre polynomials:

- Eigenfunciton of

$$-\frac{d}{dx}\left((1-x^2)\frac{d\phi(x)}{dx}\right) = k(k+1)\phi(x)$$

- Rodrigue's formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n.$$

Chebyshev polynomial of the first kind:

- Eigenfunciton of

$$-\frac{d}{dx}\left(\sqrt{(1-x^2)}\frac{d\phi(x)}{dx}\right) = \frac{k^2}{\sqrt{(1-x^2)}}\phi(x)$$

- Explicit formula

$$P_n(x) = \cos(n\theta),\ \text{where } \theta = \arccos(x)$$

# Zeros of orthogonal polynomials

**Theorem**

The zeros of $p_n$ are all real, simple, and lie in the interval $(a, b)$.

# Numerical quadrature

The basis problem is to find quadrature nodes $\{x_j\}$ and weights $\{\omega_j\}$ such that

$$\int_a^b f(x)\omega(x)dx \approx \sum_{j=0}^{N} f(x_j)\omega_j.$$

**Definition**

The quadrature have algebraic accuracy of degree $p$ if

$$\int_a^b p(x)\omega(x)dx = \sum_{j=0}^{N} p(x_j)\omega_j, \quad p(x) \in \mathbb{P}_p.$$

In general, we want choose $\{x_j\}$ and $\{\omega_j\}$ such that we have highest degree of accuracy.

# Gaussian quadrature

**Theorem (Gauss quadrature)**

Let $\{x_j\}_{j=0}^{N}$ be the set of zeros of the orthogonal polynomial $p_{N+1}$. Then there exists a unique set of quadrature weights $\{\omega_j\}_{j=0}^{N}$, defined by (3.36), such that

$$\int_a^b p(x)\omega(x)dx = \sum_{j=0}^{N} p\left(x_j\right)\omega_j, \quad \forall p \in P_{2N+1}$$

Orthogonal Polynomials and Related Approximation Results where the quadrature weights are all positive and given by

$$\omega_j = \frac{k_{N+1}}{k_N}\frac{\|p_N\|_\omega^2}{p_N\left(x_j\right)p_{N+1}'\left(x_j\right)}, \quad 0 \le j \le N,$$

where $k_j$ is the leading coefficient of the polynomial $p_j$.

# Choices of collocation points

We have many different options for collocation points that suit different scenarios

Chebyshev points:

- Chebyshev-Gauss: $x_j = \cos \frac{(2j+1)\pi}{2N+2}, \quad 0 \leq j \leq N.$
- Chebyshev-Gauss-Radau: $x_j = \cos \frac{2j\pi}{2N+1}, \quad 0 \leq j \leq N.$
- Chebyshev-Gauss-Lobatto: $x_j = \cos \frac{j\pi}{N}, \quad 0 \leq j \leq N.$

Legendre points:

- Legendre-Gauss: $x_j$ are the zeros of $P_{N+1}(x)$.
- Legendre-Gauss-Radau: $x_j$ are the zeros of $P_N(x) + P_{N+1}(x)$.
- Legendre-Gauss-Lobatto: $x_0 = -1$, $x_N = 1$, $\{x_j\}_{j=1}^{N}$ are zeros of $P'_{N-1}(x)$.

Question: Why don't we just use equally distributed points?

# Chebyshev-Gauss quadrature

The quadrature rules for Chebyshev points are particularly simple

1. Chebyshev-Gauss:
$$\int_{-1}^{1} \frac{p(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{N+1} \sum_{j=0}^{N} p(x_j), \qquad \forall p \in P_{2N+1}$$
2. Chebyshev-Gauss-Radau:
$$\int_{-1}^{1} \frac{p(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{2N+1} p(1) + \frac{\pi}{N+\frac{1}{2}} \sum_{j=1}^{N} p(x_j), \qquad \forall p \in P_{2N}$$
3. Chebyshev-Gauss-Lobatto:
$$\int_{-1}^{1} \frac{p(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{2N} \Big( p(1) + p(-1) \Big) + \frac{\pi}{N} \sum_{j=1}^{N-1} p(x_j), \qquad \forall p \in P_{2N-1}$$

# Illustration of spectral collocation method

Example: Consider the BVP $u''(x) + p(x)u'(x) + q(x) = r(x)$ over $[a, b]$.

- Map the interval $[a, b]$ to $[-1, 1]$.
  $\rightarrow u''(t) + \bar{p}(t)u'(t) + \bar{q}u(t) = \bar{r}(t)$. Here we still denote the mapped functions as $u(t)$.
- Let

$$u_N(x) = \sum_{j=0}^{N} u_j \ell_j(x),$$

where $\ell_j(x)$ be the Lagrange interpolating polynomials. So,

$$u'_N(x) = \sum_{j=0}^{N} u_j \ell'_j(x),$$

$$u''_N(x) = \sum_{j=0}^{N} u_j \ell''_j(x).$$

# Differentiation matrix

Since we are collocating, we only need to find $u'$ and $u''$ at the collocation points.

$$u_N'(x_k) = \sum_{j=0}^{N} u_j \ell_j'(x_k) = \sum_{j=0}^{N} D_{kj} u_j, \quad \text{and}$$
$$u_N''(x_k) = \sum_{j=0}^{N} u_j \ell_j''(x_k) = \sum_{j=0}^{N} D_{kj}^{(2)} u_j,$$

where $D_{kj} \equiv \frac{d}{dx}\ell_j(x)\Big|_{x_k}$, $D_{kj}^{(2)} = \frac{d^2}{dx^2}\ell_j(x)\Big|_{x_k}$, and $\ell_j$ is the $j$th Lagrange interpolation polynomial.

Note that $D^{(2)} = D^2$ (squared using matrix multiplication).

# How to compute the Differentiation matrix

**Theorem**

The entries of $D$ are determined by

$$d_{kj} = \ell_j'(x_k) = \begin{cases} \frac{Q'(x_k)}{Q'(x_j)} \frac{1}{x_k - x_j}, & \text{if } k \neq j, \\ \frac{Q''(x_k)}{2Q'(x_k)}, & \text{if } k = j, \end{cases}$$

where

$$Q(x) = p_{N+1}(x), (x-a)q_N(x), (x-a)(b-x)z_{N-1}(x)$$

are the quadrature polynomials of the Gauss, Gauss-Radau and Gauss-Lobatto quadrature, respectively. We can write $p_{N+1} = (x-x_0)(x-x_1)\cdots(x-x_N)$, $q_N = (x-x_1)\cdots(x-x_N)$, and $z_{N-1} = (x-x_1)\cdots(x-x_{N-1})$

# How to compute the Differentiation matrix

**Proof**

The Lagrange basis polynomials can be expressed as

$$\ell_j(x) = \frac{Q(x)}{Q'(x_j)(x - x_j)}, \quad 0 \leq j \leq N$$

Differentiating it and using the fact that $Q(x_j) = 0$ leads to

$$d_{kj} = \ell_j'(x_k) = \frac{Q'(x_k)}{Q'(x_j)} \frac{1}{x_k - x_j}, \quad \forall k \neq j.$$

Applying L'Hopital's rule twice yields

$$d_{kk} = \lim_{x \to x_k} \ell_k'(x) = \frac{1}{Q'(x_k)} \lim_{x \to x_k} \frac{Q'(x)(x - x_k) - Q(x)}{(x - x_k)^2} = \frac{Q''(x_k)}{2Q'(x_k)}.$$

This completes the proof.

# Chebyshev differentiation matrix

This code gives the differentiation matrix for Chebyshev-Gauss-Lobatto points using Lagrange basis polynomials

```
% 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
```

# Go back to example

Collocate at the collocation points and

$$u_N''(x_k) + \bar{p}(x_k)u_N'(x_k) + \bar{q}(x_k)u_N(x_k) = \bar{r}(x_k), \quad k = 0, 1, \ldots, N,$$

becomes

$$D^2\vec{u} + \begin{pmatrix} \bar{p}_0 & 0 & \cdots & 0 \\ 0 & \bar{p}_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \bar{p}_N \end{pmatrix} D\vec{u} + \begin{pmatrix} \bar{q}_0 & 0 & \cdots & 0 \\ 0 & \bar{q}_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \bar{q}_N \end{pmatrix} \vec{u} = \begin{pmatrix} \bar{r}_0 \\ \bar{r}_1 \\ \vdots \\ \bar{r}_N \end{pmatrix} = \bar{\vec{r}}.$$

And you can solve this for $\vec{u}$.

# Impose boundary condition

Since we know the value of $u$ at $x = \pm 1$, ($k = 0, N$), we don't need to collocate at these points. So we do not need the first and last rows of $D$ and $D^2$.

So for the rest of our rows we have:

$$\begin{aligned} u'_k &= \sum_{j=0}^{N} D_{kj} u_j \qquad (k = 1, \ldots, N-1) \\ &= \sum_{j=1}^{N-1} D_{kj} u_j + u_0 D_{k0} + u_N D_{kN}. \end{aligned}$$

# Summary of spectral collocation method

Pros and cons

- High-order method, easy to implement
- Superior to spectral-Galerkin method in dealing with variable coefficients and/or nonlinear problems
- Differential matrix is ill-conditioned and full

**End of week 2!**