# Introduction to Spectral Collocation

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**The continuous problem**

$\mathcal{L}u(x) = f(x)$

- $\mathcal{L}$: Some linear operator acting on the function $u(x)$
- $u(x)$: Some real-valued function (with some regularity) acting on a point $x \in \Omega \subset \mathbb{R}$
- $f(x)$: Some real-valued function (with possibly different regularity than $u(x)$) acting on the same point $x$

## The discrete problem

$L_N u_N = f_N$

- $L_N$: Some operator taking $N$ pieces of information from $u_N$ and returning $N$ pieces of information in $f_N$, ie. $L_N : \mathbb{R}^N \to \mathbb{R}^N$
- $u_N$: Some set of $N$ pieces of information, ie. $u_N \in \mathbb{R}^N$
- $f_N$: Some set of $N$ pieces of information, ie. $f_N \in \mathbb{R}^N$

By the description of the discrete problem $L_N$ is some matrix of size $N \times N$ and $u_N$ and $f_N$ are both vectors of length $N$. The solution vector $u_N$ is then $u_N = L_N^{-1} f_N$.

We want our solution vector $u_N$ to correspond in some way to the solution function of the continuous problem. That is, we want

$$\lim_{N \to \infty} u_N \equiv u(x)$$

in some sense.

The discrete space may be defined by a set of basis functions (called *trial functions*), $\{\phi_k(x)\}_{k=1}^N$. Our approximation $u_N$ then defines a linear combination of these functions:

$$u_N \equiv \sum_{k=1}^{N} a_k \phi_k(x).$$

We want now that when we apply $\mathcal{L}$ to this linear combination, we'll retrieve an approximation to $f(x)$:

$$\sum_{k=1}^{N} a_k \mathcal{L}\phi_k(x) \approx f(x).$$

More specifically, we want that

$$\left\langle \sum_{k=1}^{N} a_k \mathcal{L}\phi_k(x) - f(x), \psi_j(x) \right\rangle = 0 \ \forall j = 1, ..., N$$

for some inner product defined on the space of functions and for some set of *test functions* $\psi_j(x)$.

This allows us to choose three things:

- the inner product $\langle \cdot, \cdot \rangle$,
- the trial functions $\phi_k(x)$,
- and the test functions $\psi_j(x)$.

Different sets of these choices lead to different classes of methods.

### Finite Element Methods

$\phi_k(x)$ and $\psi_j(x)$ have finite support (locally defined).

### Spectral Methods

$\phi_k(x)$ and $\psi_j(x)$ have infinite support (globally defined).

## Galerkin

The trial functions individually satisfy the boundary conditions.

## Tau

$$\langle \phi_k(x), \psi_j(x) \rangle = \begin{cases} 1 & k = j \\ 0 & k \neq j \end{cases}$$

## Collocation

$$\langle \phi_k(x), \psi_j(x) \rangle = \phi_k(x_j)$$

Galerkin $u_N$ contains the coefficients in the *Galerkin basis*.

Tau $u_N$ also contains coefficients, but for a more general basis.

Collocation $u_N$ contains the values of the approximation at some set of *collocation points*, $u_N(x_j)$.

We will focus on spectral collocation (global basis functions, minimize residual point by point). That is,

$$L_N \begin{bmatrix} u_N(x_1) \\ u_N(x_2) \\ \vdots \\ u_N(x_N) \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{bmatrix}$$

with $L_N$ being a matrix representing the linear operator.

We need to know $L_N$ to solve this system. For that, we need to know the differentiation matrix, $D_N$.

$D_N$ must work perfectly for the trial functions, $\phi_k(x)$:

$$D_N \begin{bmatrix} \phi_k(x_1) \\ \phi_k(x_2) \\ \vdots \\ \phi_k(x_N) \end{bmatrix} = \begin{bmatrix} \phi'_k(x_1) \\ \phi'_k(x_2) \\ \vdots \\ \phi'_k(x_N) \end{bmatrix}$$

for all $k = 1, ..., N$.

$D_N$ is singular since $D_N \begin{bmatrix} 1 & 1 & \dots & 1 \end{bmatrix}^\top = 0$ (nilpotent, actually). The matrix representing second order differentiation is the square of $D_N$. Likewise, $D_N^{(m)} = D_N^m$.

## The continuous operator

$$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{k=1}^{m} p_k(x) u^{(m-k)}(x)$$

## The discrete operator

$$L_N = D_N^m + \sum_{k=1}^{m} P_k D_N^{m-k}$$

where $P_k$ is a $N \times N$ diagonal matrix with entries $p_k(x_j)$.

$L_N$ is singular because $D_N$ and all of its powers are singular. Boundary conditions are needed to make $L_N$ nonsingular. The number of BCs matches the order of the problem, $m$.

BCs may be concatenated so the system is overdetermined or they can be used to replace rows in $L_N$.

What should we choose for $\phi_k(x)$?

- $\phi_k(x)$ span a finite dimensional space
- they should be orthogonal with respect to some inner product (generally a weighted $L_2$ inner product)
- they can be used to approximate functions in the infinite space arbitrarily well

Some candidates:

- Sinusoids (Fourier series)
- Polynomials (Weierstrass approximation theorem)

# Jacobi polynomials

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+\beta+n+1)} \sum_{m=0}^{n} \binom{n}{m} \frac{\Gamma(\alpha+\beta+n+m+1)}{\Gamma(\alpha+m+1)} \left(\frac{x-1}{2}\right)^m$$

Orthogonal with respect to the weight $(1-x)^\alpha(1+x)^\beta$ on $[-1,1]$

# Ultraspherical polynomials

Special cases of the Jacobi polynomials with $\alpha = \beta$

**Legendre polynomials**

$\alpha = \beta = 0$

**Chebyshev polynomials**

$\alpha = \beta = 1/2$

# Sturm-Liouville Theory

The Sturm-Liouville Problem (SLP):

$$\mathcal{L}_{SL}\phi(x) = -\left(p(x)\phi'(x)\right)' + q(x)\phi(x) = \lambda w(x)\phi(x)$$

with $p \in C^1(-1,1)$, $p > 0$, $q, w \geq 0$, $q, w \in C[-1,1]$.

If $\mathcal{L}_{SL}$ is self-adjoint ($\langle \mathcal{L}_{SP} u, v\rangle = \langle u, \mathcal{L}_{SP} v\rangle$) then the SLP has a countable number of eigenvalues ($\lambda$) and the eigenfunctions ($\phi(x)$) form a complete set in $L^2(-1,1)$ and
$L^2_w(-1,1) = \left\{ u \in L^2(-1,1) \middle| \int_{-1}^{1} u^2 w dx < \infty \right\}$.

## Projection of $u(x) \in L^2_w(-1,1)$

$$P_N u(x) = \sum_{k=1}^{N} \hat{u}_k \phi_k(x)$$

where $\hat{u}_k = \int_{-1}^{1} \phi_k(x) u(x) w(x) dx / \lambda_k$

If $p(\pm 1) = 0$ and $u \in C^\infty(-1,1)$ then $|\hat{u}_k| \to 0$ faster than any polynomial power of $1/k$ (known as spectral convergence).

Special cases of SLP: ultraspherical polynomials

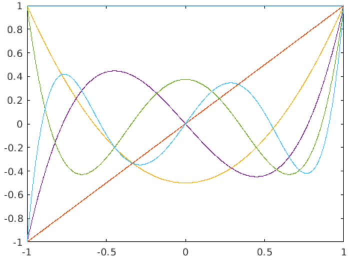
- $p(x) = (1 - x^2)^{\alpha+1}$
- $q(x) = c(1 - x^2)^{\alpha}$
- $w(x) = (1 - x^2)^{\alpha}$

For $\alpha = 0$ the eigenfunctions are the Legendre polynomials. For $\alpha = 1/2$ the eigenfunctions are the Chebyshev polynomials.

# Legendre polynomials

## Rodrigues' formula

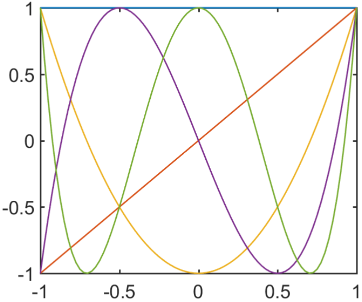
$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$



# Chebyshev polynomials

## Closed form

$$T_n(x) = \cos\left(n \arccos\left(x\right)\right)$$



### Weighted Gaussian quadrature

$$\int_{-1}^{1} f(x)w(x)dx = \sum_{k=1}^{N} w_k f(x_k)$$

We use the points $x_k$ as our collocation points. The weight function $w(x)$ is used in the weighted inner product $\langle \cdot, \cdot \rangle_w$ .

Gauss-Jacobi: $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$

Gauss-Legendre: $w(x) = 1$

Chebyshev-Gauss: $w(x) = \sqrt{1-x^2}$

The corresponding polynomials are orthogonal both with respect to $\langle \cdot, \cdot \rangle_w$ and the quadrature rule.

# A good choice

## Chebyshev polynomials

$$T_n(x) = \cos\left(n \arccos\left(x\right)\right)$$

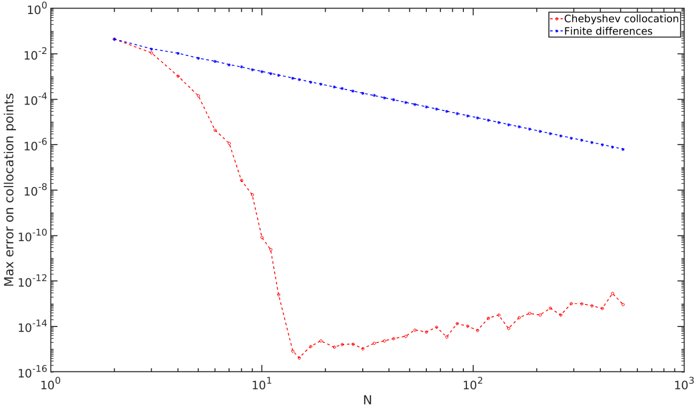
## Chebyshev-Gauss(-Lobatto) quadrature

$$\int_{-1}^{1} f(x)\sqrt{1-x^2}dx = \sum_{k=0}^{N} w_k f\left(\cos\left(\frac{k\pi}{N}\right)\right)$$

So our trial functions are $T_n(x)$, the Chebyshev functions and our collocation points are $x_k = \cos\left(\frac{k\pi}{N}\right)$, the Chebyshev points. The differentiation matrix $D_N$ is then:

| | | |
|---|---|---|
| $\frac{2N^2+1}{6}$ | $2\frac{(-1)^j}{1-x_j}$ | $\frac{1}{2}(-1)^N$ |
| $-\frac{1}{2}\frac{(-1)^i}{1-x_i}$ | $\frac{(-1)^{i+j}}{x_i - x_j}$ <br> $\frac{-x_j}{2(1-x_j^2)}$ <br> $\frac{(-1)^{i+j}}{x_i - x_j}$ | $\frac{1}{2}\frac{(-1)^{N+i}}{1+x_i}$ |
| $-\frac{1}{2}(-1)^N$ | $-2\frac{(-1)^{N+j}}{1+x_j}$ | $-\frac{2N^2+1}{6}$ |

$$u''(x) - u(x) = \cos(\pi x/2),\ u(\pm 1) = 0,$$
$$u(x) = -\cos(\pi x/2)/((\pi/2)^2 + 1)$$



# $L_N L_N^{-1} = I$

Let $R_j$ be the $j$–th column of $L_N^{-1}$.

$$\mathcal{L}R_j(x_i) = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$R_j(x) = \sum_{k=1}^{m} G_{k,j}(x) P_k(x)$$

where $\mathcal{L}P_k(x) = 0$.

## Variation of parameters

$$\sum_{k=1}^{m} G'_{k,j}(x) P_k^{(n)}(x) = 0, \quad n = 0, ..., m-2$$

$$\implies \mathcal{L} R_j(x) = \sum_{k=1}^{m} G'_{k,j}(x) P_k^{(m-1)}(x)$$

$$\implies G'_{k,j}(x_i) = \begin{cases} \beta_{k,j} & i = j \\ 0 & i \neq j \end{cases}$$

$$\implies \sum_{k=1}^{m} \beta_{k,j} P_k^{(n)}(x_j) = \begin{cases} 1 & n = m-1 \\ 0 & n = 0, ..., m-2 \end{cases}$$

$$\implies \begin{bmatrix} P_1(x_j) & \dots & P_m(x_j) \\ \vdots & & \vdots \\ P_1^{(m-1)}(x_j) & \dots & P_m^{(m-1)}(x_j) \end{bmatrix} \begin{bmatrix} \beta_{1,j} \\ \vdots \\ \beta_{m,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

$$P_k^{(n)}(v_k) = \begin{cases} 1 & n = m-1 \\ 0 & n = 0, ..., m-2 \end{cases}$$

$$P_k(x) = \sum_{n=1}^{m} \gamma_{k,n} \hat{P}_n(x)$$

$$\implies \begin{bmatrix} \hat{P}_1(v_k) & \dots & \hat{P}_m(v_k) \\ \vdots & & \vdots \\ \hat{P}_1^{(m-1)}(v_k) & \dots & \hat{P}_m^{(m-1)}(v_k) \end{bmatrix} \begin{bmatrix} \gamma_{k,1} \\ \vdots \\ \gamma_{k,m} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

## Fundamental matrix and Wronskian

$$\det \left( \begin{bmatrix} f_1(x) & \dots & f_m(x) \\ \vdots & & \vdots \\ f_1^{(m-1)}(x) & \dots & f_m^{(m-1)}(x) \end{bmatrix} \right) = W \left( \{f_k\}_{k=1}^m ; x \right)$$

$$\implies \gamma_{k,n} = (-1)^{n+m} \frac{W\left( \left\{ \hat{P}_i \right\}_{i \neq n} ; v_k \right)}{W\left( \left\{ \hat{P}_i \right\}_{i=1}^m ; v_k \right)}$$

$$
\begin{bmatrix} P_1(x) & \dots & P_m(x) \\ \vdots & & \vdots \\ P_1^{(m-1)}(x) & \dots & P_m^{(m-1)}(x) \end{bmatrix}
= \begin{bmatrix} \hat{P}_1(x) & \dots & \hat{P}_m(x) \\ \vdots & & \vdots \\ \hat{P}_1^{(m-1)}(x) & \dots & \hat{P}_m^{(m-1)}(x) \end{bmatrix}
\begin{bmatrix} \gamma_{1,1} & \cdots & \gamma_{m,1} \\ \vdots & & \vdots \\ \gamma_{1,m} & \cdots & \gamma_{m,m} \end{bmatrix}
$$

## Constant coefficient linear operators

$\mathcal{L}u(x) = u^{(m)}(x) + \sum_{k=1}^{m} a_k u^{(m-k)}(x)$

$$\hat{P}_{k,j}(x) = \frac{x^j}{j!} e^{\lambda_k x}$$

where $\lambda_k$ is a root with multiplicity $m_k$ ($\sum m_k = m$) of the polynomial with coefficients $a_k$ and $j = 0, ..., m_k - 1$.

$$u''(x) - u(x) = \cos(\pi x/2),\ u(\pm 1) = 0,$$
$$u(x) = -\cos(\pi x/2)/((\pi/2)^2 + 1)$$