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 (λ) 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 $u(x) \in L_w^2(-1,1)$

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

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

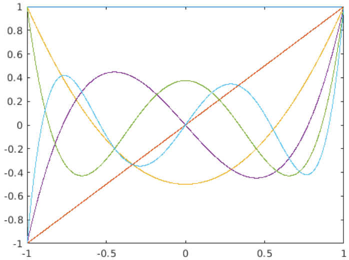
- $p(x) = (1 - x^2)^{\alpha+1}$
- $q(x) = c(1 - x^2)^{\alpha}$
- $w(x) = (1 - x^2)^{\alpha}$

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

Legendre polynomials

Rodrigues' formula

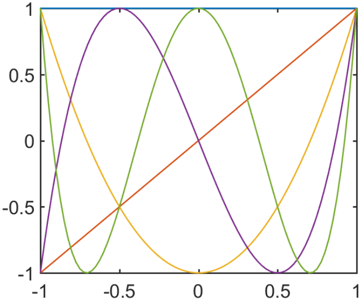
$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$



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

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

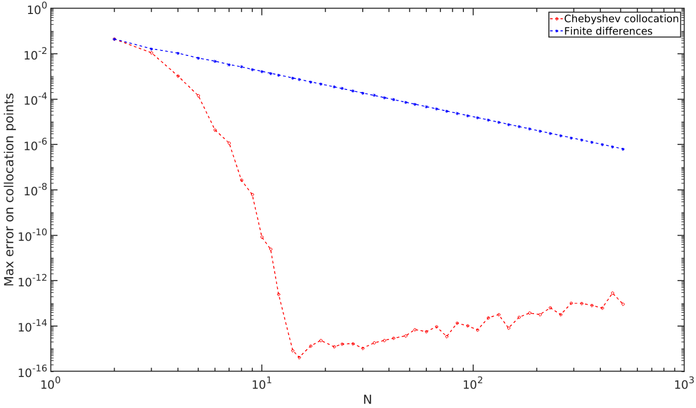
Chebyshev-Gauss(-Lobatto) quadrature

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

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:

$\frac{2N^2+1}{6}$	$2\frac{(-1)^j}{1-x_j}$	$\frac{1}{2}(-1)^N$
$-\frac{1}{2}\frac{(-1)^i}{1-x_i}$	above diagonal: $\frac{(-1)^{i+j}}{x_i-x_j}$; diagonal: $\frac{-x_j}{2(1-x_j^2)}$; below diagonal: $\frac{(-1)^{i+j}}{x_i-x_j}$	$\frac{1}{2}\frac{(-1)^{N+i}}{1+x_i}$
$-\frac{1}{2}(-1)^N$	$-2\frac{(-1)^{N+j}}{1+x_j}$	$-\frac{2N^2+1}{6}$

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



$L_N L_N^{-1} = I$

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

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