Solving PDEs with the method of weighted residuals

MATMEK-4270

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Recap

We have until now considered the approximation of a function $u(x)$ using a function space $V_N = \text{span}\{\psi_j\}_{j=0}^N$

$$u_N(x) \approx u(x), \quad u_N(x) = \sum_{j=0}^N \hat{u}_j \psi_j(x)$$

In order to find the unknowns (degrees of freedom) $\{\hat{u}_j\}_{j=0}^N$ we have considered the error $e = u_N - u$ through various methods

- Variational methods
  - Galerkin
  - Least squares
- Collocation
  - Lagrange polynomials

We will now learn to approximate $u(x)$ by $u_N(x)$ such that it satisfies a linear equation

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

where the generic operator $\mathcal{L}(u)$ can represent anything, like

$$\begin{aligned}
u &= f \\
u' &= f \\
u'' &= f \\
u'' + \alpha u' + \lambda u &= f \\
\frac{d}{dx}\left(\alpha \frac{du}{dx}\right) &= f
\end{aligned}$$

Note

Function approximation is then simply the case $u = f$, such that $u_N \approx f$.

Define a new error measure (the residual) that we ultimately want to be zero

$$\mathcal{R} = \mathcal{L}(u) - f$$

and create a "numerical" residual by inserting for $u = u_N$

$$\mathcal{R}_N = \mathcal{L}(u_N) - f$$

The task now is to minmize $\mathcal{R}_N$ in order to find the unknowns that are still $\{\hat{u}_j\}_{j=0}^N$.

Note

For function approximation $\mathcal{R}_N = e = u_N - f = u_N - u$.

The method of weighted residuals (MWR)

is defined such that the residual (with $u_N \in V_N$) must satisfy

$$(\mathcal{R}_N, v) = 0 \quad \forall \, v \in W$$

for some (possibly different) functionspace W.

This is a generic method, where the choice of V_N and W fully determines the method.

Note the similarity to function approximation

$$(u_N - u, v) = (e, v) = 0$$

Now we have instead the slightly more complicated

$$(\mathcal{L}(u_N) - f, v) = (\mathcal{R}_N, v) = 0$$

The Galerkin method is a MWR with $W = V_N$

Find $u_N \in V_N$ such that

$$(\mathcal{R}_N, v) = (\mathcal{L}(u_N) - f, v) = 0, \quad \forall\, v \in V_N$$

The residual (or error) is orthogonal to all the test functions. We can also write this as

$$(\mathcal{L}(u_N) - f, \psi_j) = 0, \quad j = 0, 1, \ldots, N$$

The least squares method is a MWR with $W = \text{span}\{\frac{\partial \mathcal{R}_N}{\partial \hat{u}_j}\}_{j=0}^N$

since

$$\frac{\partial (\mathcal{R}_N, \mathcal{R}_N)}{\partial \hat{u}_j} = 0, \quad j = 0, 1, \ldots, N$$

can be written as

$$\left(\mathcal{R}_N, \frac{\partial \mathcal{R}_N}{\partial \hat{u}_j}\right) = 0, \quad j = 0, 1, \ldots, N$$

The collocation method is to find

$$\mathcal{R}_N(x_j) = 0, \quad j = 0, 1, \ldots, N$$

for some chosen mesh points $\{x_j\}_{j=0}^N$.

If we write the inner products $(\mathcal{R}_N, v)$ as

$$(\mathcal{R}_N, \psi_j) = 0, \quad j = 0, 1, \ldots, N$$

and use Dirac's delta function as test functions $\psi_j = \delta(x - x_j)$, then

$$(\mathcal{R}_N, \psi_j) = \int_\Omega \mathcal{R}_N(x)\delta(x - x_j)dx = \mathcal{R}_N(x_j)$$

So the collocation method can technically also be considered a MWR!

However, collocation is not a regular variational method since $\delta(x)$ is a distribution and

$$W \neq \text{span}\{\delta(x - x_i)\}_{i=0}^N$$

The MWR is thus

Find $u_N \in V_N$ such that

$$(\mathcal{R}_N, v) = 0, \quad \forall v \in W$$

$N+1$ equations for $N+1$ unknowns!

Find $\{\hat{u}_j\}_{j=0}^N$ by choosing $N+1$ test functions for W. Choose test functions (basis functions for W) using either one of:

- Galerkin
- Least squares
- Collocation

First example - Poisson's equation

$$u''(x) = f(x), \quad x \in (-1, 1)$$
$$u(-1) = u(1) = 0$$

Find $u_N \in V_N$ such that

$$(u_N'' - f, v) = 0, \quad \forall\, v \in W$$

How to choose V_N and W? How do we satisfy the 2 boundary conditions?

If we choose all the trial functions ψ_j such that

$$\psi_j(\pm 1) = 0$$

then, regardless the values of $\{\hat{u}_j\}_{j=0}^N$

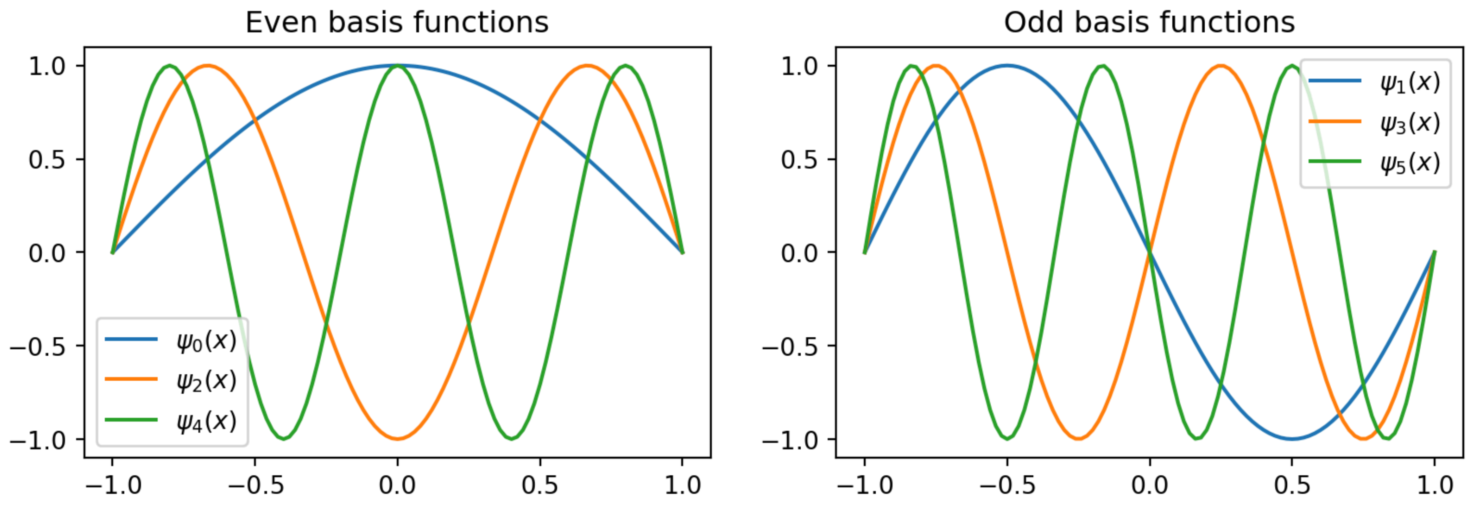
$$u_N(\pm 1) = \sum_{j=0}^{N} \hat{u}_j \psi_j(\pm 1) = 0$$

First choice for trial functions in V_N

The domain is $[-1, 1]$, so a sensible choice for $j \geq 0$ is

$$\psi_j(x) = \sin(\pi(j+1)(x+1)/2)$$

The $(j+1)$ is there because we start at $j = 0$ and $\sin(0) = 0$ is not a basis function.
These sines are also alternating odd/even functions.



In comparison the (unmapped) sine functions $\sin(\pi(j+1)x), x \in [-1, 1]$ are odd for all integer $j \geq 0$

Solve Poisson's equation

Insert for $u_N = \sum_{j=0}^N \hat{u}_j \psi_j$ and $v = \psi_i$ and obtain the linear algebra problem

$$\sum_{j=0}^{N} \left(\psi_j'', \psi_i\right) \hat{u}_j = (f, \psi_i), \quad i = 0, 1, \ldots, N$$

Consider using integration by parts

$$\int_a^b u' v dx = -\int_a^b u v' dx + [uv]_a^b$$

Set $u = u'$ to obtain

$$\int_a^b u'' v dx = -\int_a^b u' v' dx + [u'v]_a^b$$

$$\longrightarrow \left(\psi_j'', \psi_i\right) = -\left(\psi_j', \psi_i'\right) + [\psi_j' \psi_i]_{-1}^{1}$$

Poisson's equation with integration by parts

Since $\psi_j(\pm 1) = 0$ for all $j \ge 0$ we get that

$$(\psi_j'', \psi_i) = -(\psi_j', \psi_i') + \cancel{[\psi_j' \psi_i]_{-1}^{1}}$$

Hence Poisson's equation gets two alternative forms

$$\sum_{j=0}^{N} (\psi_j'', \psi_i) \hat{u}_j = (f, \psi_i), \quad i = 0, 1, \ldots, N \tag{1}$$

$$\sum_{j=0}^{N} (\psi_j', \psi_i') \hat{u}_j = -(f, \psi_i), \quad i = 0, 1, \ldots, N \tag{2}$$

Note

The integration by parts is not really necessary here, as it is actually just as easy to compute $\left(\psi_j'', \psi_i\right)$ as (ψ_j', ψ_i')!

Find the stiffness matrix (ψ_j'', ψ_i)

$$
\begin{aligned}
(\psi_j'', \psi_i) &= \Big((\sin(\pi(j+1)(x+1)/2))'',\, \sin(\pi(i+1)(x+1)/2) \Big) \\
&= -\frac{(j+1)^2\pi^2}{4} \Big(\sin(\pi(j+1)(x+1)/2),\, \sin(\pi(i+1)(x+1)/2) \Big) \\
&= -\frac{(j+1)^2\pi^2}{4} \delta_{ij}
\end{aligned}
$$

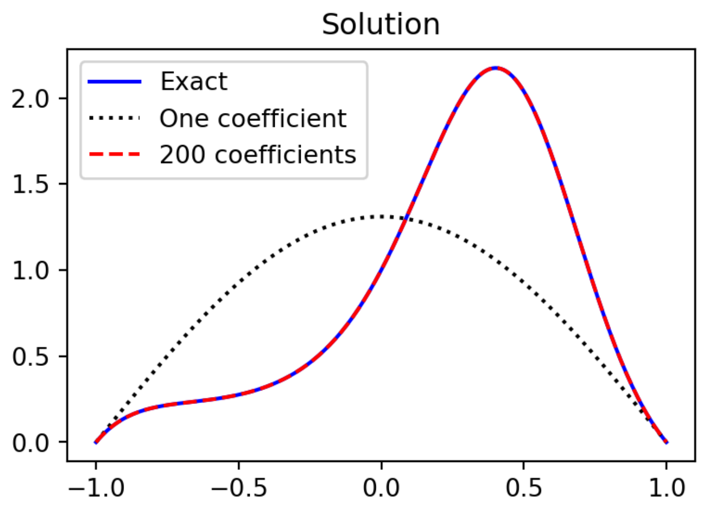
Solve problem

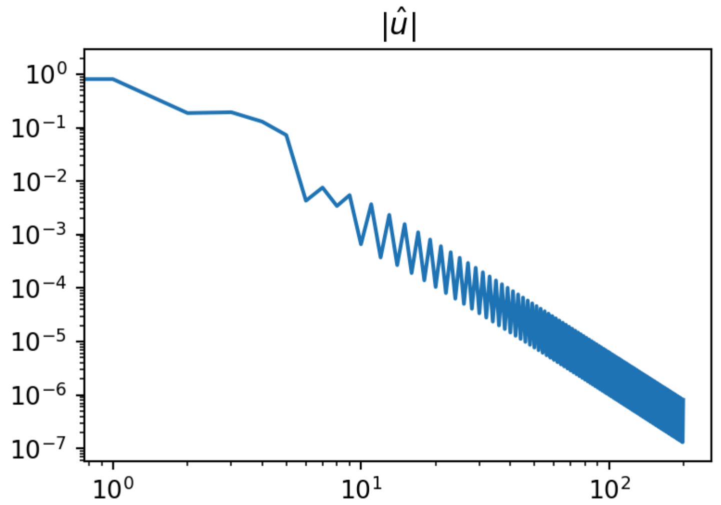
$$
\sum_{j=0}^{N} \big(\psi_j'', \psi_i\big) \hat{u}_j = (f, \psi_i), \quad i = 0, 1, \ldots, N
$$

$$
\longrightarrow \hat{u}_i = \frac{-4}{(i+1)^2\pi^2} \Big(f,\, \sin(\pi(i+1)(x+1)/2) \Big), \quad i = 0, 1, \ldots, N
$$

Implementation using the method of manufactured solution

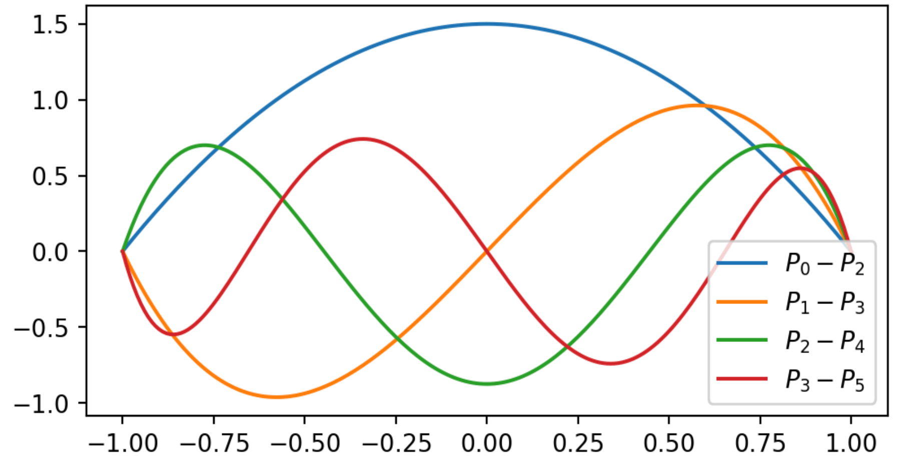
```python
from scipy.integrate import quad
x = sp.Symbol('x')
ue = (1-x**2)*sp.exp(sp.cos(sp.pi*(x-0.5)))
f = ue.diff(x, 2) # manufactured f=u''
uhat = lambda j: -(4/(j+1)**2/np.pi**2)*quad(sp.lambdify(x, f*sp.sin((j+1)*sp.pi*(x+1)/2)), -1, 1)[0]
uh = [uhat(k) for k in range(200)]
xj = np.linspace(-1, 1, 201)
sines = np.sin(np.pi/2*(np.arange(len(uh))[None, :]+1)*(xj[:, None]+1))
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 3))
uej = sp.lambdify(x, ue)(xj)
ax1.plot(xj, uej, 'b', xj, sines[:, :1] @ np.array(uh)[:1], 'k:',
         xj, sines @ np.array(uh), 'r--')
ax2.loglog(abs(np.array(uh)))
ax1.legend(['Exact', 'One coefficient', f'{200} coefficients'])
ax1.set_title('Solution');ax2.set_title(r'$|\hat{u}|$');
```





Another alternating odd/even basis can be created from Legendre polynomials $P_j(x)$

$$\psi_j(x) = P_j(x) - P_{j+2}(x)$$
$$\psi_j(\pm 1) = 0$$



Remember that

$$P_j(-1) = (-1)^j \quad \text{and} \quad P_j(1) = 1.$$

Hence for any j all basis functions are zero

$$P_j(-1) - P_{j+2}(-1) = (-1)^j - (-1)^{j+2} = 0$$
$$P_j(1) - P_{j+2}(1) = 1 - 1 = 0$$

Solve Poisson’s equation with composite Legendre basis

The Legendre polynomials come with a lot of formulas, where two are

$$(P_j, P_i) = \frac{2}{2i+1}\delta_{ij} \quad \text{and} \quad (2i+3)P_{i+1} = P'_{i+2} - P'_i$$

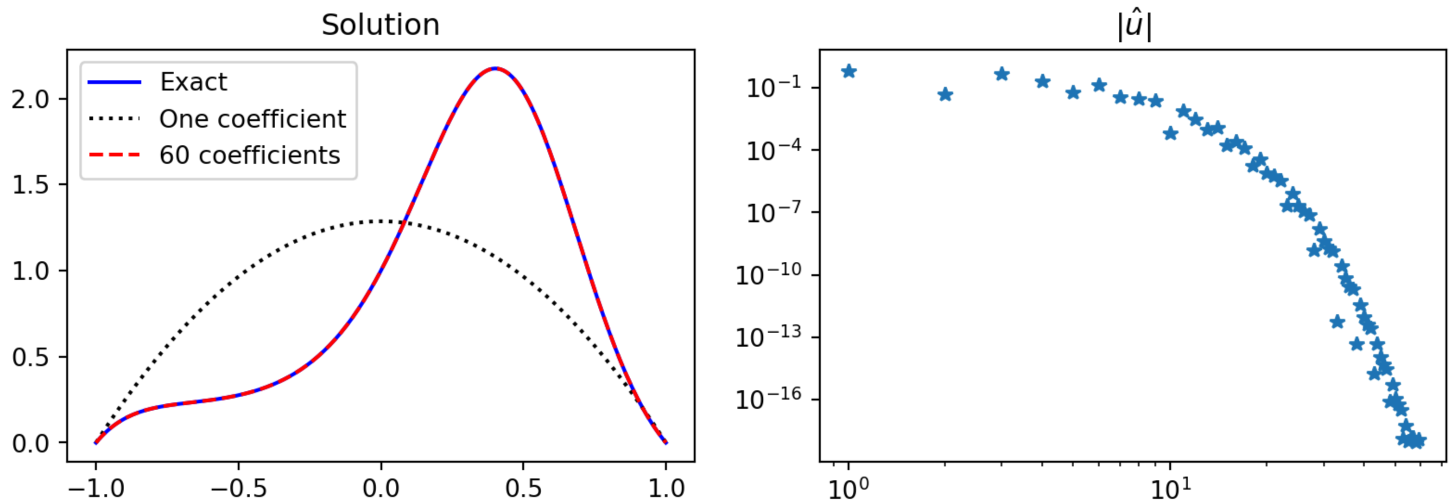
The second is very useful for computing the diagonal (!) stiffness matrix

$$\begin{aligned}
(\psi'_j, \psi'_i) &= (P'_j - P'_{j+2}, P'_i - P'_{i+2}) \\
&= (-(2j+3)P_{j+1}, -(2i+3)P_{i+1}) \\
&= (2i+3)^2(P_{j+1}, P_{i+1}) \\
&= (2i+3)^2 \frac{2}{2(i+1)+1}\delta_{i+1,j+1} \\
&= (4i+6)\delta_{ij}
\end{aligned}$$

$$\text{Solve Poisson's equation: } \longrightarrow \hat{u}_i = \frac{-(f, \psi_i)}{4i+6}$$

Implementation

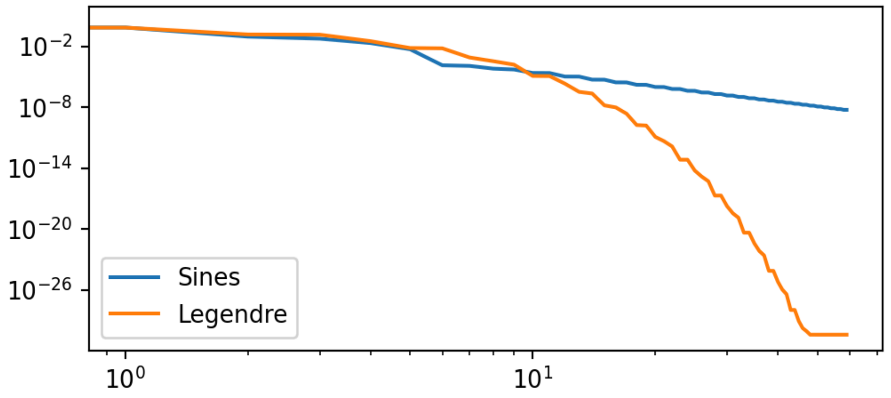
```python
from numpy.polynomial import Legendre as Leg
psi = lambda j: Leg.basis(j)-Leg.basis(j+2)
fl = sp.lambdify(x, f)
def uv(xj, j): return psi(j)(xj) * fl(xj)
uhat = lambda j: (-1/(4*j+6))*quad(uv, -1, 1, args=(j,))[0]
N = 60
uL = [uhat(j) for j in range(N)]
j = sp.Symbol('j', integer=True, positive=True)
V = np.polynomial.legendre.legvander(xj, N+1)
Ps = V[:, :-2] - V[:, 2:]
fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 3))
ax1.plot(xj, uej, 'b',
         xj, Ps[:, :1] @ np.array(uL)[:1], 'k:',
         xj, Ps @ np.array(uL), 'r--')
ax2.loglog(abs(np.array(uL)), '*')
ax1.legend(['Exact', 'One coefficient', f'{N} coefficients'])
ax1.set_title('Solution')
ax2.set_title(r'$|\hat{u}|$');
```



$L^2(\Omega)$ error for sines and Legendre

$$L^2(\Omega) = \sqrt{\int_{-1}^{1} (u-u_e)^2 dx}$$

```python
uh = np.array(uh)
uL = np.array(uL)
error = np.zeros((2, N))
for n in range(N):
    us = sines[:, :n] @ uh[:n]
    ul = Ps[:, :n] @ uL[:n]
    error[0, n] = np.trapz((us-uej)**2, dx=(xj[1]-x
    error[1, n] = np.trapz((ul-uej)**2, dx=(xj[1]-x
plt.figure(figsize=(6, 2.5))
plt.loglog(error.T)
plt.legend(['Sines', 'Legendre'])
```



Why are the Legendre basis functions better than the sines?

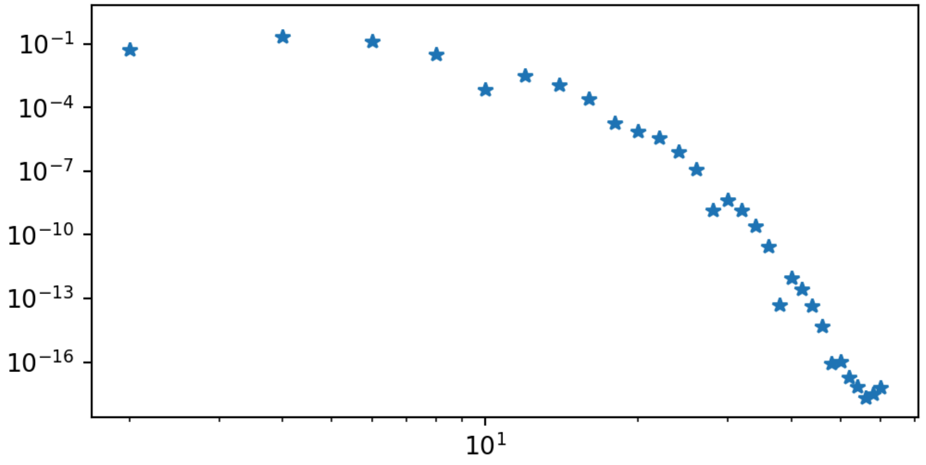
All the sine basis functions $\psi_j = \sin(\pi(j+1)(x+1)/2)$ have even derivatives equal to zero at the boundaries, unlike the chosen manufactured solution…

$$\frac{d^{2n}\psi_j}{dx^{2n}}(\pm 1) = 0 \rightarrow \frac{d^{2n}u_N}{dx^{2n}}(\pm 1) = 0, \quad n = 0, 1, \ldots$$

Implementation using Shenfun

```python
from shenfun import FunctionSpace, TestFunction, TrialFunction, inner, Dx

N = 60
VN = FunctionSpace(N+3, 'L', bc=(0, 0)) # Chooses {P_j-P_{j+2}} basis
u = TrialFunction(VN)
v = TestFunction(VN)
S = inner(Dx(u, 0, 1), Dx(v, 0, 1))
b = inner(-f, v)
uh = S.solve(b.copy())
fig = plt.figure(figsize=(6, 3))
plt.loglog(np.arange(0, N+1, 2), abs(uh[:-2:2]), '*');
```



Inhomogeneous Poisson

$$u''(x) = f(x), \quad x \in (-1,1)$$
$$u(-1) = a, u(1) = b$$

How to handle the inhomogeneous boundary conditions?

Use homogeneous $\tilde{u}_N \in V_N$ and a boundary function $B(x)$

$$u_N(x) = B(x) + \tilde{u}_N(x)$$

where $B(-1) = a$ and $B(1) = b$ such that

$$u_N(-1) = B(-1) = a \quad \text{and} \quad u_N(1) = B(1) = b$$

A function that satisfies this in the current domain is

$$B(x) = \frac{b}{2}(1+x) + \frac{a}{2}(1-x)$$

Solve Poisson

Insert for u_N into $(R_N, v) = 0$:

$$\Big((B(x) + \tilde{u}_N)'' - f, v\Big) = 0$$

Since $B(x)$ is linear $B'' = 0$ and we get the homogeneous problem

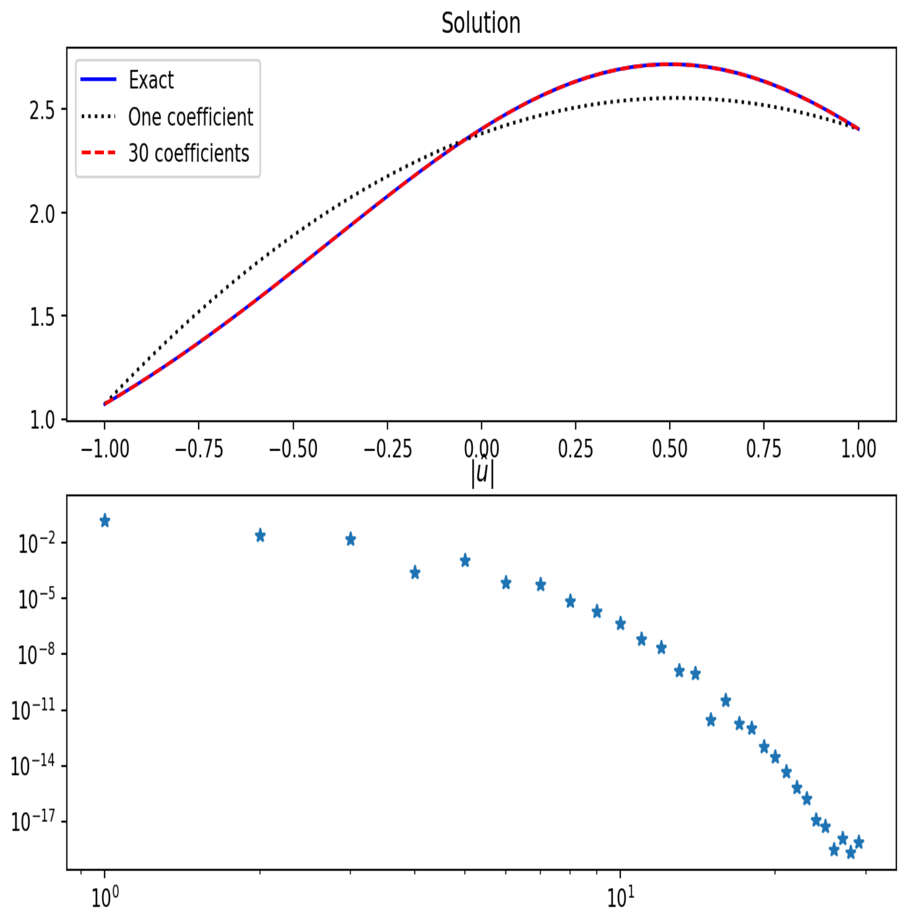
$$\Big(\tilde{u}_N'' - f, v\Big) = 0$$

Solve exactly as before for $\tilde{u}_N$ and the solution will be in the end

$$u_N(x) = B(x) + \tilde{u}_N$$

Implementation

```python
ue = sp.exp(sp.cos(x-0.5))
f = ue.diff(x, 2)
fl = sp.lambdify(x, f)
def uv(xj, j): return psi(j)(xj) * fl(xj)
uhat = lambda j: (-1/(4*j+6))*quad(uv, -1, 1, args=
N = 30
utilde = [uhat(k) for k in range(N)]
a, b = ue.subs(x, -1), ue.subs(x, 1)
B = b*(1+x)/2 + a*(1-x)/2
M = 50
xj = np.linspace(-1, 1, M+1)
V = np.polynomial.legendre.legvander(xj, N+1)
Ps = V[:, :-2] - V[:, 2:]
Bs = sp.lambdify(x, B)(xj)
fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(9, 6)
ax1.plot(xj, sp.lambdify(x, ue)(xj), 'b',
         xj, Ps[:, :1] @ np.array(utilde)[:1] + Bs,
         xj, Ps @ np.array(utilde) + Bs, 'r--')
ax2.loglog(abs(np.array(utilde)), '*')
ax1.legend(['Exact', 'One coefficient', f'{N} coeff
ax1.set_title('Solution')
ax2.set_title(r'$|\hat{u}|$');
```



Neumann boundary conditions

$$\begin{aligned} u''(x) &= f(x), \quad x \in (-1,1) \\ u'(\pm 1) &= 0 \end{aligned}$$

This problem is **ill-defined** because if u is a solution, then $u + c$, where c is a constant, is also a solution!

If $u(x)$ satisfies the above problem, then

$$(u+c)'' = u'' + \cancel{c''} = f \quad \text{and} \quad (u+c)'(\pm 1) = u'(\pm 1) = 0$$

We need an additional constraint! One possibility is then to require

$$(u, 1) = \int_\Omega u(x) dx = c$$

A well-defined Neumann problem

$$\begin{aligned} u''(x) &= f(x), \quad x \in (-1, 1) \\ u'(\pm 1) &= 0 \\ (u, 1) &= c \end{aligned}$$

How about basis functions?

If we choose basis functions ψ_j that satisfy

$$\psi_j'(\pm 1) = 0, \quad j = 0, 1, \dots$$

then

$$u_N'(\pm 1) = \sum_{j=0}^{N} \hat{u}_j \psi_j'(\pm 1) = 0$$

Neumann basis functions

Simplest possibility

$$\psi_j = \cos(\pi j(x+1)/2)$$

Easy to see that $\psi'_j(x) = -j/2\sin(j(x+1)/2)$ and thus $\psi'_j(\pm 1) = 0$. However, we also get that all odd derivatives are zero

$$\frac{d^{2n+1}\psi_j}{dx^{2n+1}}(\pm 1) = 0, \quad n = 0, 1, \ldots$$

Lets try to find a basis function using Legendre polynomials instead

$$\psi_j = P_j + b(j)P_{j+1} + a(j)P_{j+2}$$

and try to find $a(j)$ and $b(j)$ such that $\psi'_j(\pm 1) = 0$.

Composite Legendre Neumann basis

$$\psi_j = P_j + b(j)P_{j+1} + a(j)P_{j+2}$$

Using boundary conditions: $\quad P_j'(-1) = \frac{j(j+1)}{2}(-1)^j \quad \text{and} \quad P_j'(1) = \frac{j(j+1)}{2}$

We have two conditions and two unknowns

$$\begin{aligned}\psi_j'(-1) &= P_j'(-1) + b(j)P_{j+1}'(-1) + a(j)P_{j+2}'(-1) \\ &= \left(\frac{j(j+1)}{2} - b(j)\frac{(j+1)(j+2)}{2} + a(j)\frac{(j+2)(j+3)}{2}\right)(-1)^j = 0\end{aligned}$$

$$\psi_j'(1) = \left(\frac{j(j+1)}{2} + b(j)\frac{(j+1)(j+2)}{2} + a(j)\frac{(j+2)(j+3)}{2}\right) = 0$$

Solve the two equations to find $a(j), b(j)$ and thus the Neumann basis function ψ_j:

$$b(j) = 0,\; a(j) = -\frac{j(j+1)}{(j+2)(j+3)} \longrightarrow \boxed{\psi_j = P_j - \frac{j(j+1)}{(j+2)(j+3)}P_{j+2}}$$

Solve Neumann problem

Use the functionspace

$$V_N = \text{span}\Big\{P_j - \frac{j(j+1)}{(j+2)(j+3)}P_{j+2}\Big\}_{j=0}^{N}$$

and try to find $u_N \in V_N$.

However, we remember also the constraint and that

$$(u, 1) = c \to (u_N, P_0) = c$$

since $\psi_0 = P_0 = 1$. Insert for u_N and use orthogonality of Legendre polynomials to get

$$\Big(\sum_{j=0}^{N} \hat{u}_j (P_j - \frac{j(j+1)}{(j+2)(j+3)}P_{j+2}), P_0\Big) = (P_0, P_0)\hat{u}_0 = 2\hat{u}_0 = c$$

So we already know that $\hat{u}_0 = c/2$ and only have unknowns $\{\hat{u}_j\}_{j=1}^{N}$ left!

Solve Neumann with Galerkin

Define

$$\tilde{V}_N = \text{span}\Big\{P_j - \frac{j(j+1)}{(j+2)(j+3)}P_{j+2}\Big\}_{j=1}^{N} (= V_N \backslash \{P_0\})$$

With Galerkin: Find $\tilde{u}_N \in \tilde{V}_N (= \sum_{j=1}^N \hat{u}_j \psi_j)$ such that

$$(\tilde{u}_N^{''} - f, v) = 0, \quad \forall\, v \in \tilde{V}_N$$

and use in the end

$$u_N = \hat{u}_0 + \tilde{u}_N = \sum_{j=0}^{N} \hat{u}_j \psi_j$$

The linear algebra problem

We need to solve

$$\sum_{j=1}^{N}(\psi_j^{''}, \psi_i)\hat{u}_j = (f, \psi_i), \quad i = 1, 2, \dots, N$$

The stiffness matrix for Neumann

$$(\psi_j^{''}, \psi_i) = -(\psi_j^{'}, \psi_i^{'}) = (\psi_j, \psi_i^{''})$$

is fortunately diagonal (derivation later) and we can easily solve for $\{\hat{u}_i\}_{i=1}^{N}$

$$(\psi_j^{''}, \psi_i) = a(j)(4j+6)\delta_{ij}$$

$$\longrightarrow \hat{u}_i = \frac{(f, \psi_i)}{a(i)(4i+6)}, \quad i = 1, 2, \dots, N$$

Derivation of $(\psi_j^{''}, \psi_i)$

There is a series expansion for the second derivative $P_j^{''}$

$$P_j^{''} = \sum_{\substack{k=0 \\ k+j \text{ even}}}^{j-2} c(k,j)P_k, \text{ where } c(k,j) = (k+1/2)(j(j+1) - k(k+1)) \quad (1)$$

Hence $P_N^{''} + a(N)P_{N+2}^{''}$ is a Legendre series ending at $a(N)c(N-2,N)P_N$. Consider

$$\left(P_j^{''} + a(j)P_{j+2}^{''},\ P_i + a(i)P_{i+2}\right)$$

Based on the orthogonality $(P_i, P_j) = \frac{2}{2j+1}\delta_{ij}$ and (1) we get that

- If $i > j$ then $(P_j^{''} + a(j)P_{j+2}^{''}, P_i + a(i)P_{i+2}) = 0$ since $P_{j+2}^{''} = \sum_{k=0}^{j} c(k,j)P_k$
- If $i < j$ then $(P_j^{''} + a(j)P_{j+2}^{''}, P_i + a(i)P_{j+2}) = 0$ due to symmetry $(\psi_j^{''}, \psi_i) = (\psi_j, \psi_i^{''})$

Hence $\left(P_j^{''} + a(j)P_{j+2}^{''},\ P_i + a(i)P_{i+2}\right)$ is diagonal!

Compute $(\psi_i^{''}, \psi_i)$

Using again the expression $P_i^{''} = \sum_{k=0}^{i-2} c(k,i) P_k$

$$\left(P_i^{''} + a(i)P_{i+2}^{''}, P_i + a(i)P_{i+2}\right) =$$

$$\cancel{(P_i^{''}, P_i)} + \cancel{a(i)(P_i^{''}, P_{i+2})} + a(i)(P_{i+2}^{''}, P_i) + \cancel{a^2(i)(P_{i+2}^{''}, P_{i+2})}$$

All cancellations because of orthogonality and $P_i^{''} = \sum_{k=0}^{i-2}(\cdots)P_k$

$$\begin{aligned} a(i)(P_{i+2}^{''}, P_i) &= a(i) \sum_{\substack{k=0 \\ k+i \text{ even}}}^{i} \left((k+1/2)((i+2)(i+3)-k(k+1))P_k,\ P_i\right) \\ &= a(i)(i+1/2)((i+2)(i+3)-i(i+1))(P_i, P_i) \\ &= a(i)(4i+6) \end{aligned}$$

Hence we get the stiffness matrix

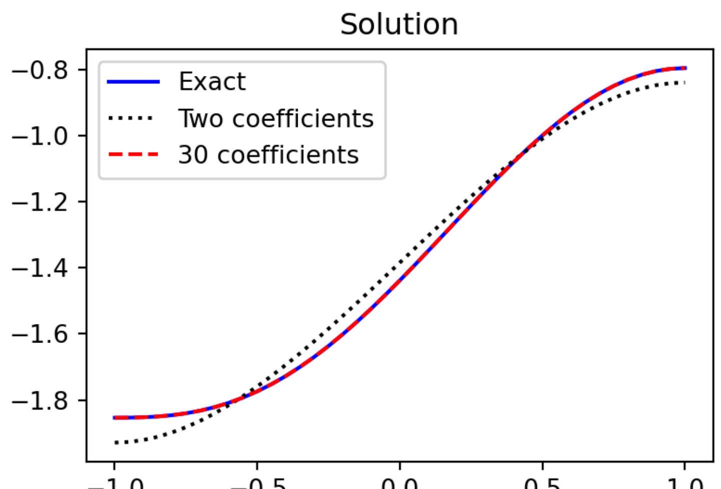
$$(\psi_j^{''}, \psi_i) = a(i)(4i+6)\delta_{ij}$$

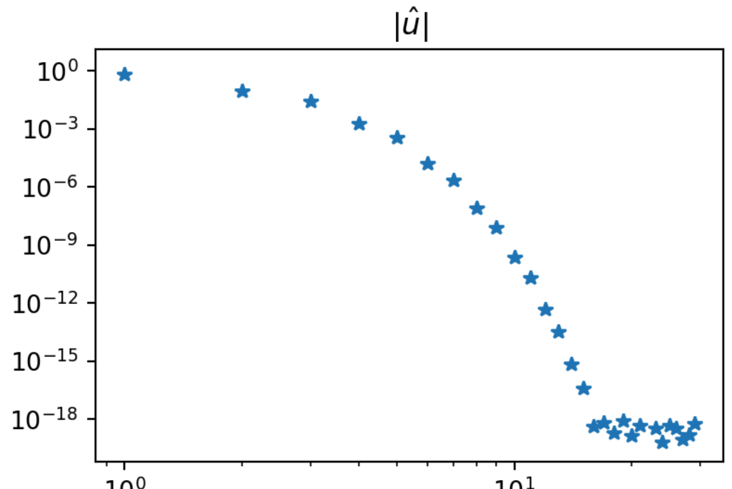
Implementation

Use manufactured solution that we know satisfies the boundary conditions

$$u(x) = \int (1 - x^2) \cos(x - 1/2) dx$$

```python
ue = sp.integrate((1-x**2)*sp.cos(x-sp.S.Half), x)
f = ue.diff(x, 2) # manufactured f
c = sp.integrate(ue, (x, -1, 1)).n() # constraint c
psi = lambda j: Leg.basis(j)-j*(j+1)/((j+2)*(j+3))*Leg.basis(j+2)
fj = sp.lambdify(x, f)
def uv(xj, j): return psi(j)(xj) * fj(xj)
def a(j): return -j*(j+1)/((j+2)*(j+3))
uhat = lambda j: 1/(a(j)*(4*j+6))*quad(uv, -1, 1, args=(j,))[0]
N = 30; uh = np.zeros(N); uh[0] = c/2
uh[1:] = [uhat(k) for k in range(1, N)]
```





More about Neumann boundary conditions

We have used basis functions that satisfied

$$\psi_j^{'}(\pm 1) = 0$$

However, this was not strictly necessary! Neumann boundary conditions are often called **natural** conditions and we can implement them directly in the variational form:

$$(\psi_j^{''}, \psi_i) = -(\psi_j^{'}, \psi'_i) + [\psi_j^{'}\psi_i]_{-1}^{1}$$

Enforce boundary conditions weakly using $\psi_j^{'}(-1) = a, \psi_j^{'}(1) = b$:

$$(\psi_j^{''}, \psi_i) = -(\psi_j^{'}, \psi'_i) + b\psi_i(1) - a\psi_i(-1)$$

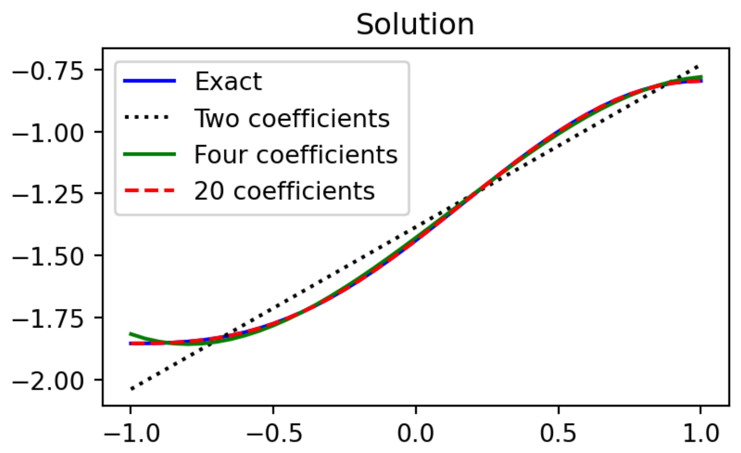
Homogeneous Neumann ($a = b = 0$):

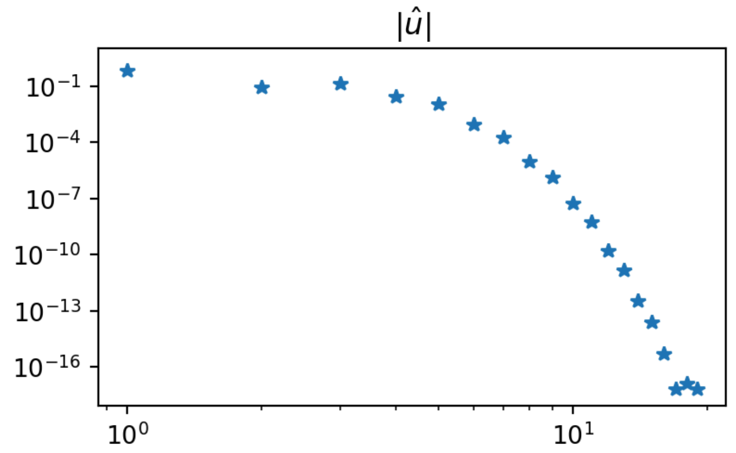
$$(\psi_j^{''}, \psi_i) = -(\psi_j^{'}, \psi'_i)$$

Implementation

Using basis function $\psi_j(x) = P_j(x)$ that have $\psi_j'(\pm 1) \neq 0$

```python
psi = lambda j: Leg.basis(j)
def uf(xj, j): return psi(j)(xj) * fj(xj)
def uv(xj, i, j): return -psi(i).deriv(1)(xj) * psi(j).deriv(1)(xj)
fhat = lambda j: quad(uf, -1, 1, args=(j,))[0]
N = 20
# Compute the stiffness matrix (not diagonal)
S = np.zeros((N, N))
for i in range(1, N):
    for j in range(i, N):
        S[i, j] = quad(uv, -1, 1, args=(i, j))[0]
        S[j, i] = S[i, j]
S[0, 0] = 1 # To fix constraint uh[0] = c/2
fh = np.zeros(N); fh[0] = c/2
fh[1:] = [fhat(k) for k in range(1, N)]
fh = np.array(fh, dtype=float)
uh = np.linalg.solve(S, fh)
```

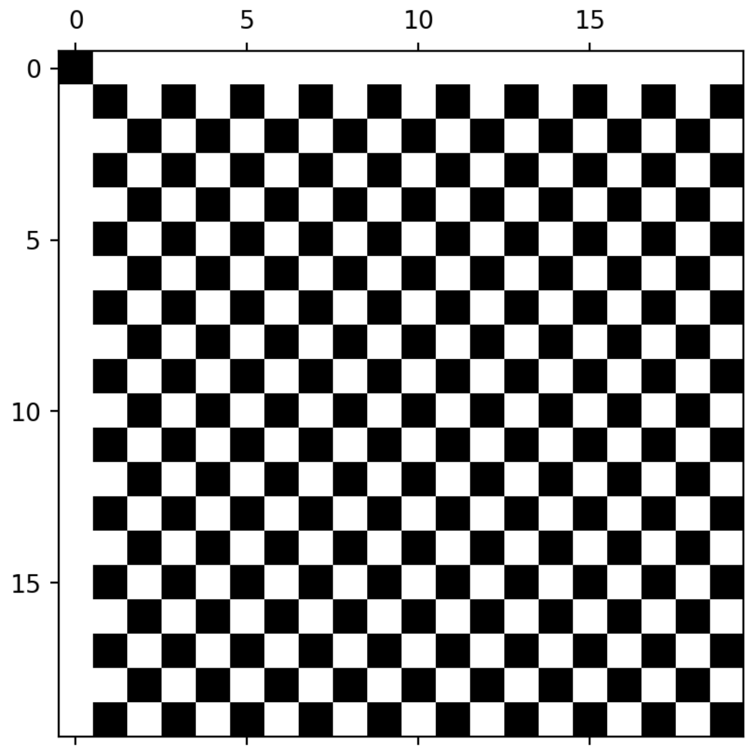




Dense stiffness matrix (ψ'_j, ψ'_i)

Using basis function $\psi_j = P_j$ leads to a dense stiffness matrix

```
plt.spy(S)
```



and thus the need for the linear algebra solve $\hat{\boldsymbol{u}} = S^{-1}\boldsymbol{f}$

```
uh = np.linalg.solve(S, fh)
```

Chebyshev basis functions

- Exactly the same approach as for Legendre, only with a weighted inner product

$$(u, v)_\omega = \int_{-1}^{1} \frac{uv}{\sqrt{1-x^2}} dx$$

- For Dirichlet boundary conditions: Find $u_N \in V_N = \text{span}\{T_i - T_{i+2}\}_{i=0}^N$ such that

$$(\mathcal{R}_N, v)_\omega = 0, \quad \forall\, v \in V_N$$

  The basis functions $\psi_i = T_i - T_{i+2}$ satisfy $\psi_i(\pm 1) = 0$.

- For Neumann boundary conditions, the basis functions are slightly different since

$$T_k'(-1) = (-1)^{k+1} k^2 \quad \text{and} \quad T_k'(1) = k^2$$

  The basis functions $\phi_k = T_k - \left(\frac{k}{k+2}\right)^2 T_{k+2}$ satisfy $\phi_k'(\pm 1) = 0$.

- Inhomogeneous boundary conditions are handled like for Legendre with the same boundary function $B(x)$.

Collocation

Consider the Dirichlet problem

$$u''(x) = f(x), \quad x \in (-1, 1)$$
$$u(-1) = a \quad \text{and} \quad u(1) = b$$

To solve this problem with collocation we use a mesh $\boldsymbol{x} = \{x_i\}_{i=0}^{N}$, where $x_0 = -1$ and $x_N = 1$. The solution, using Lagrange polynomials, is

$$u_N(x) = \sum_{i=0}^{N} \hat{u}_i \ell_i(x)$$

We then require that the following $N+1$ equations are satisfied

$$\mathcal{R}_N(x_i) = 0, \quad i = 1, 2, \ldots, N-1$$
$$u(x_0) = a \quad \text{and} \quad u(x_N) = b$$

where $\mathcal{R}_N(x) = u_N^{''}(x) - f(x)$.

Solve by inserting for u_N in $\mathcal{R}_N$

We get the $N-1$ equations for $\{\hat{u}_j\}_{j=1}^{N-1}$

$$\sum_{j=0}^{N} \hat{u}_j \ell_j''(x_i) = f(x_i), \quad i = 1, 2, \ldots, N-1$$

in addition to the boundary conditions: $\hat{u}_0 = u_N(x_0) = a$ and $\hat{u}_N = u_N(x_N) = b$.

The matrix $D^{(2)} = (d_{ij}^{(2)}) = (\ell_j''(x_i))_{i,j=0}^{N}$ is dense. How do we compute it?

Note

Using the Sympy Lagrange functions is numerically unstable

Another useful form of the Lagrange polynomials

$$\ell_j(x) = \prod_{\substack{0\le m\le N\\ m\ne j}} \frac{x - x_m}{x_j - x_m}$$

A small rearrangement leads to

$$\ell_j(x) = \ell(x)\frac{w_j}{x - x_j},$$

where

$$\ell(x) = \prod_{i=0}^{N}(x - x_i) \quad \text{and} \quad w_j = \frac{1}{\ell'(x_j)} = \frac{1}{\prod_{\substack{i=0\\ i\ne j}}^{N}(x_j - x_i)}$$

Here $(w_j)_{j=0}^{N}$ are the **barycentric weights**. Scipy will give you these weights: `from scipy.interpolate import BarycentricInterpolator`

The main advantage of the Barycentric approach is numerical stability

And we can obtain the derivative matrix $d_{ij} = \ell'_j(x_i)$ as

$$d_{ij} = \frac{w_j}{w_i(x_i - x_j)}, \quad i \neq j,$$

$$d_{ii} = -\sum_{\substack{j=0 \\ j\neq i}}^{N} d_{ij}.$$

```python
from scipy.interpolate import BarycentricInterpolat
def Derivative(xj):
    w = BarycentricInterpolator(xj).wi
    W = w[None, :] / w[:, None]
    X = xj[:, None]-xj[None, :]
    np.fill_diagonal(X, 1)
    D = W / X
    np.fill_diagonal(D, 0)
    np.fill_diagonal(D, -np.sum(D, axis=1))
    return D
```

Numpy broadcasting!

`W` is the matrix with items w_j/w_i. w_i varies along the first axis and is thus `w[:, None]`. w_j varies along the second axis and is `w[None, :]`. Likewise x_i is `xj[:, None]` and x_j is `xj[None, :]`

Higher order derivative matrices $d^n_{ij} = \ell_j^{(n)}(x_i)$ can be computed recursively

$$d_{ij}^{(n)} = \frac{n}{x_i - x_j}\left(\frac{w_j}{w_i} d_{ii}^{(n-1)} - d_{ij}^{(n-1)}\right)$$

$$d_{ii}^{(n)} = -\sum_{\substack{j=0 \\ j\neq i}}^{N} d_{ij}^{(n)}$$

```python
def PolyDerivative(xj, m):
    w = BarycentricInterpolator(xj).wi * (2*(len(xj)-1))
    W = w[None, :] / w[:, None]
    X = xj[:, None]-xj[None, :]
    np.fill_diagonal(X, 1)
    D = W / X
    np.fill_diagonal(D, 0)
    np.fill_diagonal(D, -np.sum(D, axis=1))
    if m == 1: return D
    D2 = np.zeros_like(D)
    for k in range(2, m+1):
        D2[:] = k / X * (W * D.diagonal()[:, None] - D)
        np.fill_diagonal(D2, 0)
        np.fill_diagonal(D2, -np.sum(D2, axis=1))
        D[:] = D2
    return D2
```

Use Chebyshev points for spectral accuracy

$$x_i = \cos(i\pi/N)$$

The barycentric weights are then simply

$$w_i = (-1)^i c_i, \quad c_i = \begin{cases} 0.5 & i = 0 \text{ or } i = N \\ 1 & \text{otherwise} \end{cases} \tag{1}$$

```python
N = 8
xj = np.cos(np.arange(N+1)*np.pi/N)
w = BarycentricInterpolator(xj).wi * 2*N
w
```

```
array([ 0.5, -1. ,  1. , -1. ,  1. , -1. ,  1. , -1. ,  0.5])
```

Note

The weights are only relative, so we have here scaled by $2N$ to get (1)

And then we solve any equation by replacing the ordinary derivatives with derivative matrices

$$u''(x) = f(x), \quad x \in (-1, 1)$$
$$u(-1) = a \quad \text{and} \quad u(1) = b$$

Let $d_{ij}^{(2)} = \ell_j''(x_i)$ for all $i = 1, \ldots, N-1$, ident the first and last rows of $D^{(2)}$ and set $f_0 = a$ and $f_N = b$. Solve

$$\sum_{j=0}^{N} d_{ij}^{(2)} \hat{u}_j = f_i, \quad i = 0, 1, \ldots, N$$

Matrix form using $\hat{\boldsymbol{u}} = (\hat{u}_j)_{j=0}^N$ and $\boldsymbol{f} = (f_j)_{j=0}^N$

$$D^{(2)} \hat{\boldsymbol{u}} = \boldsymbol{f}$$

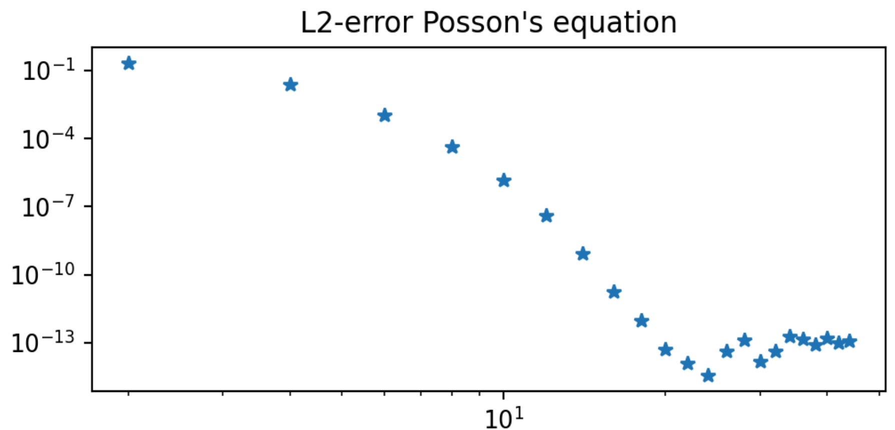
$$\hat{\boldsymbol{u}} = (D^{(2)})^{-1} \boldsymbol{f}$$

Implementation for Poisson’s equation

```python
def poisson_coll(N, f, bc=(0, 0)):
    xj = np.cos(np.arange(N+1)*np.pi/N)[::-1]
    D2 = PolyDerivative(xj, 2)      # Get second derivative matrix
    D2[0, 0] = 1; D2[0, 1:] = 0      # ident first row
    D2[-1, -1] = 1; D2[-1, :-1] = 0  # ident last row
    fh = np.zeros(N+1)
    fh[1:-1] = sp.lambdify(x, f)(xj[1:-1])
    fh[0], fh[-1] = bc              # Fix boundary conditions
    uh = np.linalg.solve(D2, fh)
    return uh, D2

def l2_error(uh, ue):
    uj = sp.lambdify(x, ue)
    N = len(uh)-1
    xj = np.cos(np.arange(N+1)*np.pi/N)[::-1]
    L = BarycentricInterpolator(np.cos(np.arange(N+1)*np.pi/N)[::-1], yi=uh)
    N = 4*len(uh) # Use denser mesh to compute L2-error
    xj = np.linspace(-1, 1, N+1)
    return np.sqrt(np.trapz((uj(xj)-L(xj).astype(float))**2, dx=2./N))
```

```python
ue = sp.exp(sp.cos(x-0.5))
f = ue.diff(x, 2)
bc = ue.subs(x, -1), ue.subs(x, 1)
err = []
for N in range(2, 46, 2):
    uh, D = poisson_coll(N, f, bc=bc)
    err.append(l2_error(uh, ue))
fig = plt.figure(figsize=(6, 2.5))
plt.loglog(np.arange(2, 46, 2), err, '*')
plt.title("L2-error Posson's equation");
```



Summary

- Find $u_N \in V_N$ such that

$$(\mathcal{L}(u_N) - f, v) = (\mathcal{R}_N, v) = 0 \quad \forall v \in W$$

- Differential equations are solved using the method of weighted residuals
  - Galerkin ($W = V_N$)
  - Least squares ($W = \text{span}\{\frac{\partial \mathcal{R}_N}{\partial \hat{u}_i}\}_{i=0}^N$)
  - Collocation ($v = \delta(x - x_i)$)
- Same approach as function approximation, but assembling matrices is more work!
- Basis functions chosen to satisfy homogeneous boundary conditions (either Dirichlet or Neumann) and then a lifting function $B(x)$ handles nonzero conditions

$$u_N(x) = \sum_{i=0}^{N} \hat{u}_i \psi_i(x) + B(x)$$