Study guide: Computing with variational forms

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We shall apply least squares, Galerkin/projection, and collocation to differential equation models

Our aim is to extend the ideas for approximating f by u, or solving

$$u = f$$

to real, *spatial* differential equations like

$$-u'' + bu = f, \quad u(0) = C,\ u'(L) = D$$

$\boxed{\text{Emphasis will be on the Galerkin/projection method}}$

Abstract differential equation

$$\mathcal{L}(u) = 0, \quad x \in \Omega$$

Examples (1D problems):

$$\begin{aligned}
\mathcal{L}(u) &= \frac{d^2u}{dx^2} - f(x),\\
\mathcal{L}(u) &= \frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) + f(x),\\
\mathcal{L}(u) &= \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) - au + f(x),\\
\mathcal{L}(u) &= \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) + f(u,x)
\end{aligned}$$

Abstract boundary conditions

$$\mathcal{B}_0(u) = 0,\ x = 0, \quad \mathcal{B}_1(u) = 0,\ x = L$$

Examples:

$$\begin{aligned}
\mathcal{B}_i(u) &= u - g, && \text{Dirichlet condition}\\
\mathcal{B}_i(u) &= -\alpha\frac{du}{dx} - g, && \text{Neumann condition}\\
\mathcal{B}_i(u) &= -\alpha\frac{du}{dx} - h(u - g), && \text{Robin condition}
\end{aligned}$$

Reminder about notation

- $u_e(x)$ is the symbol for the *exact* solution of $\mathcal{L}(u_e) = 0$ and $\mathcal{B}_i(u_e) = 0$
- $u(x)$ denotes an *approximate* solution
- $V = \text{span}\{\psi_0(x), \ldots, \psi_N(x)\}$, V has basis $\{\psi_i\}_{i\in\mathcal{I}_s}$
- We seek $u \in V$
- $\mathcal{I}_s = \{0, \ldots, N\}$ is an index set
- $u(x) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)$
- Inner product: $(u, v) = \int_\Omega uv\,\mathrm{d}x$
- Norm: $||u|| = \sqrt{(u, u)}$

New topics: variational formulation and boundary conditions

Much is similar to approximating a function (solving $u = f$), but two new topics are needed:

- Variational formulation of the differential equation problem (including integration by parts)
- Handling of boundary conditions

Residual-minimizing principles

- When solving $u = f$ we knew the error $e = f - u$ and could use principles for minimizing the error
- When solving $\mathcal{L}(u_e) = 0$ we do not know u_e and cannot work with the error $e = u_e - u$
- We can only know the *error in the equation*: the residual R

Inserting $u = \sum_j c_j\psi_j$ in $\mathcal{L} = 0$ gives a residual R

$$\mathcal{L}(u) = \mathcal{L}(\sum_j c_j\psi_j) = R \neq 0$$

Goal: minimize R with respect to $\{c_i\}_{i\in\mathcal{I}_s}$ (and hope it makes a small e too)

$$R = R(c_0, \ldots, c_N; x)$$

The least squares method

Idea: minimize

$$E = ||R||^2 = (R, R) = \int_\Omega R^2\, dx$$

Minimization wrt $\{c_i\}_{i\in\mathcal{I}_s}$ implies

$$\frac{\partial E}{\partial c_i} = \int_\Omega 2R\frac{\partial R}{\partial c_i}dx = 0 \quad \Leftrightarrow \quad (R, \frac{\partial R}{\partial c_i}) = 0, \quad i \in \mathcal{I}_s$$

$N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i\in\mathcal{I}_s}$

The Galerkin method

Idea: make R orthogonal to V,

$$(R, v) = 0, \quad \forall v \in V$$

This implies

$$(R, \psi_i) = 0, \quad i \in \mathcal{I}_s$$

$N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i\in\mathcal{I}_s}$

The Method of Weighted Residuals

Generalization of the Galerkin method: demand R orthogonal to some space W, possibly $W \neq V$:

$$(R, v) = 0, \quad \forall v \in W$$

If $\{w_0, \ldots, w_N\}$ is a basis for W:

$$(R, w_i) = 0, \quad i \in \mathcal{I}_s$$

- $N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i\in\mathcal{I}_s}$
- Weighted residual with $w_i = \partial R/\partial c_i$ gives least squares

New terminology: test and trial functions

- ψ_j used in $\sum_j c_j\psi_j$ is called *trial function*
- ψ_i or w_i used as weight in Galerkin's method is called *test function*

The collocation method

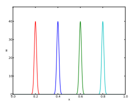
Idea: demand $R = 0$ at $N + 1$ points in space

$$R(x_i; c_0, \ldots, c_N) = 0, \quad i \in \mathcal{I}_s$$

The collocation method is a weighted residual method with delta functions as weights

$$0 = \int_\Omega R(x; c_0, \ldots, c_N)\delta(x - x_i)\,\mathrm{d}x = R(x_i; c_0, \ldots, c_N)$$

$$\text{property of } \delta(x): \quad \int_\Omega f(x)\delta(x - x_i)dx = f(x_i), \quad x_i \in \Omega$$



Examples on using the principles

Goal

Exemplify the least squares, Galerkin, and collocation methods in a simple 1D problem with global basis functions.

The first model problem

$$-u''(x) = f(x), \quad x \in \Omega = [0, L], \quad u(0) = 0,\ u(L) = 0$$

Basis functions:

$$\psi_i(x) = \sin\left((i+1)\pi\frac{x}{L}\right), \quad i \in \mathcal{I}_s$$

Residual:

$$\begin{aligned} R(x; c_0, \ldots, c_N) &= u''(x) + f(x), \\ &= \frac{d^2}{dx^2}\left(\sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\right) + f(x), \\ &= \sum_{j\in\mathcal{I}_s} c_j\psi_j''(x) + f(x) \end{aligned}$$

Boundary conditions

Since $u(0) = u(L) = 0$ we must ensure that all $\psi_i(0) = \psi_i(L) = 0$, because then

$$u(0) = \sum_j c_j\psi_j(0) = 0, \quad u(L) = \sum_j c_j\psi_j(L) = 0$$

- u known: Dirichlet boundary condition
- u' known: Neumann boundary condition
- Must have $\psi_i = 0$ where Dirichlet conditions apply

The least squares method; principle

$$(R, \frac{\partial R}{\partial c_i}) = 0, \quad i \in \mathcal{I}_s$$

$$\frac{\partial R}{\partial c_i} = \frac{\partial}{\partial c_i}\left(\sum_{j\in\mathcal{I}_s} c_j\psi_j''(x) + f(x)\right) = \psi_i''(x)$$

Because:

$$\frac{\partial}{\partial c_i}\left(c_0\psi_0'' + c_1\psi_1'' + \cdots + c_{i-1}\psi_{i-1}'' + c_i\psi_i'' + c_{i+1}\psi_{i+1}'' + \cdots + c_N\psi_N''\right) =$$

The least squares method; equation system

$$(\sum_j c_j\psi_j'' + f, \psi_i'') = 0, \quad i \in \mathcal{I}_s$$

Rearrangement:

$$\sum_{j\in\mathcal{I}_s}(\psi_i'', \psi_j'')c_j = -(f, \psi_i''), \quad i \in \mathcal{I}_s$$

This is a linear system

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i, \quad i \in \mathcal{I}_s$$

The least squares method; matrix and right-hand side expressions

$$\begin{aligned} A_{i,j} &= (\psi_i'', \psi_j'') \\ &= \pi^4(i+1)^2(j+1)^2L^{-4}\int_0^L \sin\left((i+1)\pi\frac{x}{L}\right)\sin\left((j+1)\pi\frac{x}{L}\right)\, dx \\ &= \begin{cases} \frac{1}{2}L^{-3}\pi^4(i+1)^4 & i = j \\ 0, & i \neq j \end{cases} \end{aligned}$$

$$b_i = -(f, \psi_i'') = (i+1)^2\pi^2L^{-2}\int_0^L f(x)\sin\left((i+1)\pi\frac{x}{L}\right)\, dx$$

Orthogonality of the basis functions gives diagonal matrix

Useful property of the chosen basis functions:

$$\int_0^L \sin\left((i+1)\pi\frac{x}{L}\right)\sin\left((j+1)\pi\frac{x}{L}\right)\,dx = \delta_{ij}, \qquad \delta_{ij} = \begin{cases} \frac{1}{2}L & i=j \\ 0, & i \neq j \end{cases}$$

$\Rightarrow$ $(\psi_i'', \psi_j'') = \delta_{ij}$, i.e., diagonal $A_{i,j}$, and we can easily solve for c_i:

$$c_i = \frac{2L}{\pi^2(i+1)^2}\int_0^L f(x)\sin\left((i+1)\pi\frac{x}{L}\right)\,dx$$

Least squares method; solution

Let sympy do the work ($f(x) = 2$):

```
from sympy import *
import sys

i, j = symbols('i j', integer=True)
x, L = symbols('x L')
f = 2
a = 2*L/(pi**2*(i+1)**2)
c_i = a*integrate(f*sin((i+1)*pi*x/L), (x, 0, L))
c_i = simplify(c_i)
print c_i
```

$$c_i = 4\frac{L^2\left((-1)^i + 1\right)}{\pi^3\left(i^3 + 3i^2 + 3i + 1\right)}, \quad u(x) = \sum_{k=0}^{N/2}\frac{8L^2}{\pi^3(2k+1)^3}\sin\left((2k+1)\pi\frac{x}{L}\right)$$

Fast decay: $c_2 = c_0/27$, $c_4 = c_0/125$ - only one term might be good enough:

$$u(x) \approx \frac{8L^2}{}\sin\left(\pi\frac{x}{}\right)$$

The Galerkin method; principle

$R = u'' + f$:

$$(u'' + f, v) = 0, \quad \forall v \in V,$$

or rearranged,

$$(u'', v) = -(f, v), \quad \forall v \in V$$

This is a *variational formulation* of the differential equation problem.

$\forall v \in V$ is equivalent with $\forall v \in \psi_i$, $i \in \mathcal{I}_s$, resulting in

$$(\sum_{j\in\mathcal{I}_s} c_j\psi_j'', \psi_i) = -(f, \psi_i), \quad i \in \mathcal{I}_s$$

$$\sum_{j\in\mathcal{I}_s}(\psi_j'', \psi_i)c_j = -(f, \psi_i), \quad i \in \mathcal{I}_s$$

The Galerkin method; solution

Since $\psi_i'' \propto -\psi_i$, Galerkin's method gives the same linear system and the same solution as the least squares method (in this particular example).

The collocation method

$R = 0$ (i.e.,the differential equation) must be satisfied at $N+1$ points:

$$-\sum_{j\in\mathcal{I}_s} c_j\psi_j''(x_i) = f(x_i), \quad i \in \mathcal{I}_s$$

This is a linear system $\sum_j A_{i,j} = b_i$ with entries

$$A_{i,j} = -\psi_j''(x_i) = (j+1)^2\pi^2L^{-2}\sin\left((j+1)\pi\frac{x_i}{L}\right), \quad b_i = 2$$

Choose: $N = 0$, $x_0 = L/2$

$$c_0 = 2L^2/\pi^2$$

Comparison of the methods

- Exact solution: $u(x) = x(L-x)$
- Galerkin or least squares ($N = 0$): $u(x) = 8L^2\pi^{-3}\sin(\pi x/L)$
- Collocation method ($N = 0$): $u(x) = 2L^2\pi^{-2}\sin(\pi x/L)$.

```
>>> import sympy as sym
>>> # Computing with Dirichlet conditions: -u''=2 and sines
>>> x, L = sym.symbols('x L')
>>> e_Galerkin = x*(L-x) - 8*L**2*sym.pi**(-3)*sym.sin(sym.pi*x/L)
>>> e_colloc = x*(L-x) - 2*L**2*sym.pi**(-2)*sym.sin(sym.pi*x/L)

>>> # Verify max error for x=L/2
>>> dedx_Galerkin = sym.diff(e_Galerkin, x)
>>> dedx_Galerkin.subs(x, L/2)
0
>>> dedx_colloc = sym.diff(e_colloc, x)
>>> dedx_colloc.subs(x, L/2)
0

# Compute max error: x=L/2, evaluate numerical, and simplify
>>> sym.simplify(e_Galerkin.subs(x, L/2).evalf(n=3))
-0.00812*L**2
>>> sym.simplify(e_colloc.subs(x, L/2).evalf(n=3))
0.0473*L**2
```

Integration by parts has many advantages

Second-order derivatives will hereafter be integrated by parts

$$\begin{aligned}\int_0^L u''(x)v(x)dx &= -\int_0^L u'(x)v'(x)dx + [vu']_0^L\\ &= -\int_0^L u'(x)v'(x)dx + u'(L)v(L) - u'(0)v(0)\end{aligned}$$

Motivation:

- Lowers the order of derivatives
- Gives more symmetric forms (incl. matrices)
- Enables easy handling of Neumann boundary conditions
- Finite element basis functions φ_i have discontinuous derivatives (at cell boundaries) and are not suited for terms with φ_i''

We use a boundary function to deal with non-zero Dirichlet boundary conditions

- What about nonzero Dirichlet conditions? Say $u(L) = D$
- We always require $\psi_i(L) = 0$ (i.e., $\psi_i = 0$ where Dirichlet conditions applies)
- Problem: $u(L) = \sum_j c_j\psi_j(L) = \sum_j c_j \cdot 0 = 0 \neq D$ - always!
- Solution: $u(x) = B(x) + \sum_j c_j\psi_j(x)$
- $B(x)$: user-constructed boundary function that fulfills the Dirichlet conditions
- If $u(L) = D$, make sure $B(L) = D$
- No restrictions of how $B(x)$ varies in the interior of Ω

Example on constructing a boundary function for two Dirichlet conditions

Dirichlet conditions: $u(0) = C$ and $u(L) = D$. Choose for example

$$B(x) = \frac{1}{L}(C(L-x) + Dx): \qquad B(0) = C,\ B(L) = D$$

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x),$$

$$u(0) = B(0) = C, \quad u(L) = B(L) = D$$

Example on constructing a boundary function for one Dirichlet condition

Dirichlet condition: $u(L) = D$. Choose for example

$$B(x) = D: \qquad B(L) = D$$

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x),$$

$$u(L) = B(L) = D$$

With a $B(x)$, $u \notin V$, but $\sum_j c_j\psi_j \in V$

- $\{\psi_i\}_{i\in\mathcal{I}_s}$ is a basis for V
- $\sum_{j\in\mathcal{I}_s} c_j\psi_j(x) \in V$
- But $u \notin V$!
- Reason: say $u(0) = C$ and $u \in V$; any $v \in V$ has $v(0) = C$, then $2u \notin V$ because $2u(0) = 2C$ (wrong value)
- When $u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)$, $B \notin V$ (in general) and $u \notin V$, but $(u - B) \in V$ since $\sum_j c_j\psi_j \in V$

Abstract notation for variational formulations

The finite element literature (and much FEniCS documentation) applies an abstract notation for the variational formulation:

Find $(u - B) \in V$ such that

$$a(u, v) = L(v) \quad \forall v \in V$$

Example on abstract notation

$$-u'' = f,\quad u'(0) = C,\ u(L) = D,\quad u = D + \sum_j c_j\psi_j$$

Variational formulation:

$$\int_\Omega u'v'dx = \int_\Omega fvdx - v(0)C \quad\text{or}\quad (u',v') = (f,v) - v(0)C \quad \forall v\in V$$

Abstract formulation: find $(u-B)\in V$ such that

$$a(u,v) = L(v)\quad \forall v\in V$$

We identify

$$a(u,v) = (u',v'),\quad L(v) = (f,v) - v(0)C$$

Bilinear and linear forms

- $a(u,v)$ is a *bilinear form*
- $L(v)$ is a *linear form*

Linear form means

$$L(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 L(v_1) + \alpha_2 L(v_2),$$

Bilinear form means

$$a(\alpha_1 u_1 + \alpha_2 u_2, v) = \alpha_1 a(u_1,v) + \alpha_2 a(u_2,v),$$
$$a(u, \alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 a(u,v_1) + \alpha_2 a(u,v_2)$$

In nonlinear problems: Find $(u-B)\in V$ such that $F(u;v) = 0\ \forall v\in V$

The linear system associated with the abstract form

$$a(u,v) = L(v)\quad \forall v\in V \quad\Leftrightarrow\quad a(u,\psi_i) = L(\psi_i)\quad i\in\mathcal{I}_s$$

We can now derive the corresponding linear system once and for all by inserting $u = B + \sum_j c_j\psi_j$:

$$a(B + \sum_{j\in\mathcal{I}_s} c_j\psi_j, \psi_i) = L(\psi_i)\quad i\in\mathcal{I}_s$$

Because of linearity,

$$\sum_{j\in\mathcal{I}_s} \underbrace{a(\psi_j,\psi_i)}_{A_{i,j}} c_j = \underbrace{L(\psi_i) - a(B,\psi_i)}_{b_i}\quad i\in\mathcal{I}_s$$

Equivalence with minimization problem

If a is symmetric: $a(u,v) = a(v,u)$,

$$a(u,v) = L(v)\quad \forall v\in V$$

is equivalent to minimizing the functional

$$F(v) = \frac{1}{2}a(v,v) - L(v)$$

over all functions $v\in V$. That is,

$$F(u) \le F(v)\quad \forall v\in V$$

- Much used in the early days of finite elements
- Still much used in structural analysis and elasticity
- Not as general as Galerkin's method (since we require $a(u,v) = a(v,u)$)

Examples on variational formulations

Goal

Derive variational formulations for some prototype differential equations in 1D that include

- variable coefficients
- mixed Dirichlet and Neumann conditions
- nonlinear coefficients

Variable coefficient; problem

$$-\frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) = f(x),\quad x\in\Omega = [0,L],\ u(0) = C,\ u(L) = D$$

- Variable coefficient $\alpha(x)$
- $V = \text{span}\{\psi_0,\ldots,\psi_N\}$
- *Nonzero* Dirichlet conditions at $x = 0$ *and* $x = L$
- Must have $\psi_i(0) = \psi_i(L) = 0$
- Any $v\in V$ has then $v(0) = v(L) = 0$
- $B(x) = C + \frac{1}{L}(D-C)x$

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_i(x),$$

Variable coefficient; Galerkin principle

$$R = -\frac{d}{dx}\left(a\frac{du}{dx}\right) - f$$

Galerkin's method:

$$(R, v) = 0,\quad \forall v \in V$$

or with integrals:

$$\int_\Omega \left(-\frac{d}{dx}\left(\alpha\frac{du}{dx}\right) - f\right) v\,\mathrm{d}x = 0,\quad \forall v \in V$$

Variable coefficient; integration by parts

$$-\int_\Omega \frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) v\,\mathrm{d}x = \int_\Omega \alpha(x)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x - \left[\alpha\frac{du}{dx}v\right]_0^L$$

Boundary terms vanish since $v(0) = v(L) = 0$

Variable coefficient; variational formulation

Variational formulation

Find $(u - B) \in V$ such that

$$\int_\Omega \alpha(x)\frac{du}{dx}\frac{dv}{dx}dx = \int_\Omega f(x)v dx,\quad \forall v \in V$$

Compact notation:

$$\underbrace{(\alpha u', v')}_{a(u,v)} = \underbrace{(f, v)}_{L(v)},\quad \forall v \in V$$

Variable coefficient; linear system (the easy way)

With

$$a(u, v) = (\alpha u', v'),\quad L(v) = (f, v)$$

we can just use the formula for the linear system:

$$A_{i,j} = a(\psi_j, \psi_i) = (\alpha\psi_j', \psi_i') = \int_\Omega \alpha\psi_j'\psi_i'\,\mathrm{d}x = \int_\Omega \psi_i'\alpha\psi_j'\,\mathrm{d}x \quad (= a(\psi_i, \psi_j)$$

$$b_i = (f, \psi_i) - (\alpha B', \psi_i') = \int_\Omega (f\psi_i - \alpha L^{-1}(D - C)\psi_i')\,\mathrm{d}x$$

Variable coefficient; linear system (full derivation)

$v = \psi_i$ and $u = B + \sum_j c_j\psi_j$:

$$(\alpha B' + \alpha\sum_{j\in\mathcal{I}_s} c_j\psi_j', \psi_i') = (f, \psi_i),\quad i \in \mathcal{I}_s$$

Reorder to form linear system:

$$\sum_{j\in\mathcal{I}_s}(\alpha\psi_j', \psi_i')c_j = (f, \psi_i) - (aL^{-1}(D - C), \psi_i'),\quad i \in \mathcal{I}_s$$

This is $\sum_j A_{i,j}c_j = b_i$ with

$$A_{i,j} = (a\psi_j', \psi_i') = \int_\Omega \alpha(x)\psi_j'(x)\psi_i'(x)\,\mathrm{d}x$$

$$b_i = (f, \psi_i) - (aL^{-1}(D - C), \psi_i') = \int_\Omega \left(f\psi_i - \alpha\frac{D - C}{L}\psi_i'\right)\,\mathrm{d}x$$

First-order derivative in the equation and boundary condition; problem

$$-u''(x) + bu'(x) = f(x),\quad x \in \Omega = [0, L],\ u(0) = C,\ u'(L) = E$$

New features:

- first-order derivative u' in the equation
- boundary condition with u': $u'(L) = E$

Initial steps:

- Must force $\psi_i(0) = 0$ because of Dirichlet condition at $x = 0$
- Boundary function: $B(x) = C(L - x)/L$ or just $B(x) = C$
- No requirements on $\psi_i(L)$ (no Dirichlet condition at $x = L$)

First-order derivative in the equation and boundary condition; details

$$u = C + \sum_{j\in\mathcal{I}_s} c_j\psi_i(x)$$

Galerkin's method: multiply by v, integrate over Ω, integrate by parts.

$$(-u'' + bu' - f, v) = 0,\quad \forall v\in V$$

$$(u', v') + (bu', v) = (f, v) + [u'v]_0^L,\quad \forall v\in V$$

$[u'v]_0^L = u'(L)v(L) - u'(0)v(0) = Ev(L)$ since $v(0) = 0$ and $u'(L) = E$

$$(u', v') + (bu', v) = (f, v) + Ev(L),\quad \forall v\in V$$

First-order derivative in the equation and boundary condition; observations

$$(u', v') + (bu', v) = (f, v) + Ev(L),\quad \forall v\in V$$

Important observations:

- The boundary term can be used to implement Neumann conditions
- Forgetting the boundary term implies the condition $u' = 0$ (!)
- Such conditions are called *natural boundary conditions*

First-order derivative in the equation and boundary condition; abstract notation (optional)

Abstract notation:

$$a(u, v) = L(v)\quad \forall v\in V$$

With

$$(u', v') + (bu', v) = (f, v) + Ev(L),\quad \forall v\in V$$

we have

$$a(u, v) = (u', v') + (bu', v)$$
$$L(v) = (f, v) + Ev(L)$$

First-order derivative in the equation and boundary condition; linear system

Insert $u = C + \sum_j c_j\psi_j$ and $v = \psi_i$ in

$$(u', v') + (bu', v) = (f, v) + Ev(L),\quad \forall v\in V$$

and manipulate to get

$$\sum_{j\in\mathcal{I}_s}\underbrace{((\psi_j', \psi_i') + (b\psi_j', \psi_i))}_{A_{i,j}} c_j = \underbrace{(f, \psi_i) + E\psi_i(L)}_{b_i},\quad i\in\mathcal{I}_s$$

Observation: $A_{i,j}$ is not symmetric because of the term

$$(b\psi_j', \psi_i) = \int_\Omega b\psi_j'\psi_i dx \neq \int_\Omega b\psi_i'\psi_j dx = (\psi_i', b\psi_j)$$

Terminology: natural and essential boundary conditions

$$(u', v') + (bu', v) = (f, v) + u'(L)v(L) - u'(0)v(0)$$

- Note: forgetting the boundary terms implies $u'(L) = u'(0) = 0$ (unless prescribe a Dirichlet condition)
- Conditions on u' are simply inserted in the variational form and called *natural conditions*
- Conditions on u at $x = 0$ requires modifying V (through $\psi_i(0) = 0$) and are known as *essential conditions*

Lesson learned

It is easy to forget the boundary term when integrating by parts. That mistake may prescribe a condition on u'!

Nonlinear coefficient; problem

Problem:

$$-(\alpha(u)u')' = f(u),\quad x\in[0, L],\ u(0) = 0,\ u'(L) = E$$

- V: basis $\{\psi_i\}_{i\in\mathcal{I}_s}$ with $\psi_i(0) = 0$ because of $u(0) = 0$
- How do the nonlinear coefficients $\alpha(u)$ and $f(u)$ impact the variational formulation?
  (Not much!)

Nonlinear coefficient; variational formulation

Galerkin: multiply by v, integrate, integrate by parts

$$\int_0^L \alpha(u)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x + [\alpha(u)vu']_0^L \quad \forall v\in V$$

- $\alpha(u(0))v(0)u'(0) = 0$ since $v(0)$
- $\alpha(u(L))v(L)u'(L) = \alpha(u(L))v(L)E$ since $u'(L) = E$

$$\int_0^L \alpha(u)\frac{du}{dx}\frac{dv}{dx}v\,\mathrm{d}x = \int_0^L f(u)v\,\mathrm{d}x + \alpha(u(L))v(L)E \quad \forall v\in V$$

or

$$(\alpha(u)u', v') = (f(u), v) + \alpha(u(L))v(L)E \quad \forall v\in V$$

Nonlinear coefficient; where does the nonlinearity cause challenges?

- Abstract notation: no $a(u,v)$ and $L(v)$ because a and L get nonlinear
- Abstract notation for nonlinear problems: $F(u;v) = 0\ \forall v\in V$
- What about forming a linear system? We get a *nonlinear* system of algebraic equations
- Must use methods like Picard iteration or Newton's method to solve nonlinear algebraic equations
- But: the variational formulation was not much affected by nonlinearities

Dirichlet and Neumann conditions; problem

$$-u''(x) = f(x),\quad x\in\Omega=[0,1],\quad u'(0) = C,\ u(1) = D$$

- Use a *global* polynomial basis $\psi_i \sim x^i$ on $[0,1]$
- Because of $u(1) = D$: $\psi_i(1) = 0$
- Basis: $\psi_i(x) = (1-x)^{i+1},\quad i\in\mathcal{I}_s$
- Boundary function: $B(x) = Dx$
- $u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j = Dx + \sum_{j\in\mathcal{I}_s} c_j(1-x)^{j+1}$

Variational formulation: find $(u-B)\in V$ such that

$$(u', \psi_i') = (f, \psi_i) - C\psi_i(0),\ i\in\mathcal{I}_s$$

Dirichlet and Neumann conditions; linear system

Insert $u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j$ and derive

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i,\quad i\in\mathcal{I}_s$$

with

$$A_{i,j} = (\psi_j', \psi_i')$$
$$b_i = (f,\psi_i) - (D,\psi_i') - C\psi_i(0)$$

Dirichlet and Neumann conditions; integration

$$A_{i,j} = (\psi_j', \psi_i') = \int_0^1 \psi_i'(x)\psi_j'(x)dx = \int_0^1 (i+1)(j+1)(1-x)^{i+j}dx$$

Choose $f(x) = 2$:

$$\begin{aligned} b_i &= (2,\psi_i) - (D,\psi_i') - C\psi_i(0) \\ &= \int_0^1 \left(2(1-x)^{i+1} - D(i+1)(1-x)^i\right)dx - C\psi_i(0) \end{aligned}$$

Dirichlet and Neumann conditions; 2×2 system

Can easily do the integrals with sympy. $N = 1$ and $\mathcal{I}_s = \{0,1\}$:

$$\begin{pmatrix} 1 & 1 \\ 1 & 4/3 \end{pmatrix}\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} -C+D+1 \\ 2/3-C+D \end{pmatrix}$$

$$c_0 = -C + D + 2,\quad c_1 = -1,$$

$$u(x) = 1 - x^2 + D + C(x-1)\quad \text{(exact solution)}$$

When the numerical method is exact?

Assume that apart from boundary conditions, u_e lies in the same space V as where we seek u:

$$
\begin{aligned}
u &= B + F, \quad F \in V\\
a(B+F, v) &= L(v), \quad \forall v \in V\\
u_e &= B + E, \quad E \in V\\
a(B+E, v) &= L(v), \quad \forall v \in V
\end{aligned}
$$

Subtract: $a(F-E, v) = 0 \ \Rightarrow\ E = F$ and $u = u_e$

Computing with finite elements

Tasks:

- Address the model problem $-u''(x) = 2$, $u(0) = u(L) = 0$
- Uniform finite element mesh with P1 elements
- Show all finite element computations in detail

Variational formulation

$$-u''(x) = 2, \quad x \in (0, L),\ u(0) = u(L) = 0,$$

Variational formulation:

$$(u', v') = (2, v) \quad \forall v \in V$$

How to deal with the boundary conditions?

Since $u(0) = 0$ and $u(L) = 0$, we must force

$$v(0) = v(L) = 0, \quad \psi_i(0) = \psi_i(L) = 0$$

Let's choose the obvious finite element basis: $\psi_i = \varphi_i$, $i = 0, \ldots, N_n - 1$

Problem: $\varphi_0(0) \neq 0$ and $\varphi_{N_n-1}(L) \neq 0$

Solution: we just exclude φ_0 and φ_{N_n-1} from the basis and work with

$$\psi_i = \varphi_{i+1}, \quad i = 0, \ldots, N = N_n - 3$$

Introduce index mapping $\nu(i)$: $\psi_i = \varphi_{\nu(i)}$

$$u = \sum_{j \in \mathcal{I}_s} c_j \varphi_{\nu(j)}, \quad i = 0, \ldots, N, \quad \nu(j) = j + 1$$

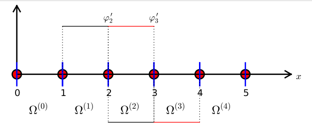
Computation in the global physical domain; formulas

$$A_{i,j} = \int_0^L \varphi_{i+1}'(x)\varphi_{j+1}'(x) dx, \quad b_i = \int_0^L 2\varphi_{i+1}(x) dx$$

Many will prefer to change indices to obtain a $\varphi_i'\varphi_j'$ product: $i+1 \rightarrow i$, $j+1 \rightarrow j$

$$A_{i-1,j-1} = \int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x, \quad b_{i-1} = \int_0^L 2\varphi_i(x)\,\mathrm{d}x$$

Computation in the global physical domain; details



$$\varphi_i' \sim \pm h^{-1}$$

$$A_{i-1,i-1} = h^{-2}2h = 2h^{-1}, \quad A_{i-1,i-2} = h^{-1}(-h^{-1})h = -h^{-1}$$

and $A_{i-1,i} = A_{i-1,i-2}$

$$b_{i-1} = 2(\frac{1}{2}h + \frac{1}{2}h) = 2h$$

Computation in the global physical domain; linear system

$$\frac{1}{h}\begin{pmatrix}
2 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0\\
-1 & 2 & -1 & \ddots & & & & & \vdots\\
0 & -1 & 2 & -1 & \ddots & & & & \vdots\\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots\\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots\\
\vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots\\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0\\
\vdots & & & & & \ddots & \ddots & \ddots & -1\\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 2
\end{pmatrix}
\begin{pmatrix} c_0\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ c_N \end{pmatrix}
=
\begin{pmatrix} 2h\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ 2h \end{pmatrix}$$

Write out the corresponding difference equation

General equation at node i:

$$-\frac{1}{h}c_{i-1} + \frac{2}{h}c_i - \frac{1}{h}c_{i+1} = 2h$$

Now, $c_i = u(x_{i+1}) \equiv u_{i+1}$. Writing out the equation at node $i-1$,

$$-\frac{1}{h}c_{i-2} + \frac{2}{h}c_{i-1} - \frac{1}{h}c_i = 2h$$

translates directly to

$$-\frac{1}{h}u_{i-1} + \frac{2}{h}u_i - \frac{1}{h}u_{i+1} = 2h$$

Comparison with a finite difference discretization

The standard finite difference method for $-u'' = 2$ is

$$-\frac{1}{h^2}u_{i-1} + \frac{2}{h^2}u_i - \frac{1}{h^2}u_{i+1} = 2$$

Multiply by h!

The finite element method and the finite difference method are identical *in this example*.

(Remains to study the equations at the end points, which involve boundary values - but these are also the same for the two methods)

Cellwise computations; formulas

- Repeat the previous example, but apply the cellwise algorithm
- Work with one cell at a time
- Transform physical cell to reference cell $X \in [-1, 1]$

$$A^{(e)}_{i-1,j-1} = \int_{\Omega^{(e)}} \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x = \int_{-1}^{1} \frac{d}{dx}\tilde\varphi_r(X)\frac{d}{dx}\tilde\varphi_s(X)\frac{h}{2}\,\mathrm{d}X,$$

$$\tilde\varphi_0(X) = \frac{1}{2}(1-X), \quad \tilde\varphi_1(X) = \frac{1}{2}(1+X)$$

$$\frac{d\tilde\varphi_0}{dX} = -\frac{1}{2}, \quad \frac{d\tilde\varphi_1}{dX} = \frac{1}{2}$$

From the chain rule

$$\frac{d\tilde\varphi_r}{dx} = \frac{d\tilde\varphi_r}{dX}\frac{dX}{dx} = \frac{2}{h}\frac{d\tilde\varphi_r}{dX}$$

Cellwise computations; details

$$A^{(e)}_{i-1,j-1} = \int_{\Omega^{(e)}} \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x = \int_{-1}^{1} \frac{2}{h}\frac{d\tilde\varphi_r}{dX}\frac{2}{h}\frac{d\tilde\varphi_s}{dX}\frac{h}{2}\,\mathrm{d}X = \tilde A^{(e)}_{r,s}$$

$$b^{(e)}_{i-1} = \int_{\Omega^{(e)}} 2\varphi_i(x)\,\mathrm{d}x = \int_{-1}^{1} 2\tilde\varphi_r(X)\frac{h}{2}\,\mathrm{d}X = \tilde b^{(e)}_r, \quad i = q(e,r),\ r = 0,1$$

Must run through all $r, s = 0, 1$ and $r = 0, 1$ and compute each entry in the element matrix and vector:

$$\tilde A^{(e)} = \frac{1}{h}\begin{pmatrix} 1 & -1\\ -1 & 1\end{pmatrix}, \quad \tilde b^{(e)} = h\begin{pmatrix} 1\\ 1\end{pmatrix}$$

Example:

$$\tilde A^{(e)}_{0,1} = \int_{-1}^{1} \frac{2}{h}\frac{d\tilde\varphi_0}{dX}\frac{2}{h}\frac{d\tilde\varphi_1}{dX}\frac{h}{2}\,\mathrm{d}X = \frac{2}{h}(-\frac{1}{2})\frac{2}{h}\frac{1}{2}\frac{h}{2}\int_{-1}^{1}\mathrm{d}X = -\frac{1}{h}$$

Cellwise computations; details of boundary cells

- The boundary cells involve only one unknown
- $\Omega^{(0)}$: left node value known, only a contribution from right node
- $\Omega^{(N_e)}$: right node value known, only a contribution from left node

For $e = 0$ and $= N_e$:

$$\tilde A^{(e)} = \frac{1}{h}\begin{pmatrix} 1 \end{pmatrix}, \quad \tilde b^{(e)} = h\begin{pmatrix} 1 \end{pmatrix}$$

Only one degree of freedom ("node") in these cells ($r = 0$ counts the only dof)

Cellwise computations; assembly

4 P1 elements:

```
vertices = [0, 0.5, 1, 1.5, 2]
cells = [[0, 1], [1, 2], [2, 3], [3, 4]]
dof_map = [[0], [0, 1], [1, 2], [2]]       # only 1 dof in elm 0, 3
```

Python code for the assembly algorithm:

```
# Ae[e][r,s]: element matrix, be[e][r]: element vector
# A[i,j]: coefficient matrix, b[i]: right-hand side

for e in range(len(Ae)):
    for r in range(Ae[e].shape[0]):
        for s in range(Ae[e].shape[1]):
            A[dof_map[e,r],dof_map[e,s]] += Ae[e][i,j]
        b[dof_map[e,r]] += be[e][i,j]
```

Result: same linear system as arose from computations in the physical domain

General construction of a boundary function

- Now we address *nonzero Dirichlet conditions*
- $B(x)$ is not always easy to construct (i.e., extend to the interior of Ω), especially not in 2D and 3D
- With finite element basis functions, φ_i, $B(x)$ can be constructed in a completely general way (!)

Define

- I_b: set of indices with nodes where u is known
- U_i: Dirichlet value of u at node i, $i \in I_b$

The general formula for B is now

$$B(x) = \sum_{j\in I_b} U_j\varphi_j(x)$$

Explanation

Suppose we have a Dirichlet condition $u(x_k) = U_k$, $k \in I_b$:

$$u(x_k) = \sum_{j\in I_b} U_j \underbrace{\varphi_j(x_k)}_{\neq 0 \text{ only for } j=k} + \sum_{j\in\mathcal{I}_s} c_j \underbrace{\varphi_{\nu(j)}(x_k)}_{=0,\ k\not\in\mathcal{I}_s} = U_k$$

Example with two *nonzero* Dirichlet values; variational formulation

$$-u'' = 2, \quad u(0) = C,\ u(L) = D$$

$$\int_0^L u'v'\,\mathrm{d}x = \int_0^L 2v\,\mathrm{d}x \quad \forall v \in V$$

$$(u', v') = (2, v) \quad \forall v \in V$$

Example with two Dirichlet values; boundary function

$$B(x) = \sum_{j\in I_b} U_j\varphi_j(x)$$

Here $I_b = \{0, N_n - 1\}$, $U_0 = C$, $U_{N_n-1} = D$; ψ_i are the internal φ_i functions:

$$\psi_i = \varphi_{\nu(i)}, \quad \nu(i) = i+1, \quad i \in \mathcal{I}_s = \{0, \ldots, N = N_n - 3\}$$

$$\begin{aligned} u(x) &= \underbrace{C\varphi_0 + D\varphi_{N_n-1}}_{B(x)} + \sum_{j\in\mathcal{I}_s} c_j\varphi_{j+1} \\ &= C\varphi_0 + D\varphi_{N_n-1} + c_0\varphi_1 + c_1\varphi_2 + \cdots + c_N\varphi_{N_n-2} \end{aligned}$$

Example with two Dirichlet values; details

Insert $u = B + \sum_j c_j\psi_j$ in variational formulation:

$$(u', v') = (2, v) \quad \Rightarrow \quad (\sum_j c_j\psi_j', \psi_i') = (2, \psi_i) - (B', \psi_i') \quad \forall v \in V$$

$$\begin{aligned} A_{i-1,j-1} &= \int_0^L \varphi_i'(x)\varphi_j'(x)\,\mathrm{d}x \\ b_{i-1} &= \int_0^L (f(x)\varphi_i(x) - B'(x)\varphi_i'(x))\,\mathrm{d}x, \quad B'(x) = C\varphi_0'(x) + D\varphi_{N_n-}' \end{aligned}$$

for $i, j = 1, \ldots, N+1 = N_n - 2$.

New boundary terms from $-\int B'\varphi_i'\,\mathrm{d}x$: add C/h to b_0 and D/h to b_N

Example with two Dirichlet values; cellwise computations

- All element matrices are as in the previous example
- New element vector in the first and last cell

From the first cell:

$$\tilde{b}_0^{(1)} = \int_{-1}^{1} \left(f\tilde{\varphi}_1 - C\frac{2}{h}\frac{d\tilde{\varphi}_0}{dX}\frac{2}{h}\frac{d\tilde{\varphi}_1}{dX} \right) \frac{h}{2}\,\mathrm{d}X = \frac{h}{2}2\int_{-1}^{1} \tilde{\varphi}_1\,\mathrm{d}X - C\frac{2}{h}(-\frac{1}{2})\frac{2}{h}\frac{1}{2}$$

From the last cell:

$$\tilde{b}_0^{(N_e)} = \int_{-1}^{1} \left(f\tilde{\varphi}_0 - D\frac{2}{h}\frac{d\tilde{\varphi}_1}{dX}\frac{2}{h}\frac{d\tilde{\varphi}_0}{dX} \right) \frac{h}{2}\,\mathrm{d}X = \frac{h}{2}2\int_{-1}^{1} \tilde{\varphi}_0\,\mathrm{d}X - D\frac{2}{h}\frac{1}{2}\frac{2}{h}(-\frac{1}{2}$$

Modification of the linear system; ideas

- Method 1: incorporate Dirichlet values through a $B(x)$ function and demand $\psi_i = 0$ where Dirichlet values apply
- Method 2: drop $B(x)$, drop demands to ψ_i, just assemble as if there were no Dirichlet conditions, and modify the linear system instead

Method 2: always choose $\psi_i = \varphi_i$ for all $i \in \mathcal{I}_s$ and set

$$u(x) = \sum_{j\in\mathcal{I}_s} c_j\varphi_j(x), \quad \mathcal{I}_s = \{0,\ldots,N = N_n - 1\}$$

Attractive way of incorporating Dirichlet conditions

u is treated as unknown at all boundaries when computing entries in the linear system

Modification of the linear system; original system

$$-u'' = 2, \quad u(0) = 0,\ u(L) = D$$

Assemble as if there were no Dirichlet conditions:

$$\frac{1}{h}\begin{pmatrix}
1 & -1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & 2 & -1 & \ddots & & & & & \vdots \\
0 & -1 & 2 & -1 & \ddots & & & & \vdots \\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & & & & & \ddots & \ddots & \ddots & -1 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & -1 & 1
\end{pmatrix}
\begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix}
=
\begin{pmatrix} h \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h \\ h \end{pmatrix}$$

Modification of the linear system; row replacement

- Dirichlet condition $u(x_k) = U_k$ means $c_k = U_k$ (since $c_k = u(x_k)$)
- Replace first row by $c_0 = 0$
- Replace last row by $c_N = D$

$$\frac{1}{h}\begin{pmatrix}
h & 0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
-1 & 2 & -1 & \ddots & & & & & \vdots \\
0 & -1 & 2 & -1 & \ddots & & & & \vdots \\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & & & & & \ddots & \ddots & \ddots & -1 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & h
\end{pmatrix}
\begin{pmatrix} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{pmatrix}
=
\begin{pmatrix} 0 \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h \\ D \end{pmatrix}$$

Modification of the linear system; element matrix/vector

In cell 0 we know u for local node (degree of freedom) $r = 0$. Replace the first cell equation by $\tilde{c}_0 = 0$:

$$\tilde{A}^{(0)} = A = \frac{1}{h}\begin{pmatrix} h & 0 \\ -1 & 1 \end{pmatrix}, \quad \tilde{b}^{(0)} = \begin{pmatrix} 0 \\ h \end{pmatrix}$$

In cell N_e we know u for local node $r = 1$. Replace the last equation in the cell system by $\tilde{c}_1 = D$:

$$\tilde{A}^{(N_e)} = A = \frac{1}{h}\begin{pmatrix} 1 & -1 \\ 0 & h \end{pmatrix}, \quad \tilde{b}^{(N_e)} = \begin{pmatrix} h \\ D \end{pmatrix}$$

Symmetric modification of the linear system; algorithm

- The modification above destroys symmetry of the matrix: e.g., $A_{0,1} \neq A_{1,0}$
- Symmetry is often important in 2D and 3D (faster computations, less storage)
- A more complex modification can preserve symmetry!

Algorithm for incorporating $c_i = U_i$ in a symmetric way:

1. Subtract column i times U_i from the right-hand side
2. Zero out column and row no i
3. Place 1 on the diagonal
4. Set $b_i = U_i$

Symmetric modification of the linear system; example

$$
\frac{1}{h}\left(\begin{array}{ccccccccc}
h & 0 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
0 & 2 & -1 & \ddots & & & & & \vdots \\
0 & -1 & 2 & -1 & \ddots & & & & \vdots \\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & 0 & -1 & 2 & -1 & \ddots & \vdots \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & & & & & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 0 & h
\end{array}\right)
\left(\begin{array}{c} c_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_N \end{array}\right)
=
\left(\begin{array}{c} 0 \\ 2h \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 2h + \frac{D}{h} \\ D \end{array}\right)
$$

Symmetric modification of the linear system; element level

Symmetric modification applied to $\tilde{A}^{(N_e)}$:

$$
\tilde{A}^{(N_e)} = A = \frac{1}{h}\left(\begin{array}{cc} 1 & 0 \\ 0 & h \end{array}\right), \quad \tilde{b}^{(N_e)} = \left(\begin{array}{c} h + D/h \\ D \end{array}\right)
$$

Boundary conditions: specified derivative

Neumann conditions

How can we incorporate $u'(0) = C$ with finite elements?

$$
-u'' = f, \quad u'(0) = C, \ u(L) = D
$$

- $\psi_i(L) = 0$ because of Dirichlet condition $u(L) = D$ (or no demand and modify linear system)
- No demand to $\psi_i(0)$
- The condition $u'(0) = C$ will be handled (as usual) through a boundary term arising from integration by parts

The variational formulation

Galerkin's method:

$$
\int_0^L (u''(x) + f(x))\psi_i(x)dx = 0, \quad i \in \mathcal{I}_s
$$

Integration of $u''\psi_i$ by parts:

$$
\int_0^L u'(x)\psi_i'(x)\,\mathrm{d}x - (u'(L)\psi_i(L) - u'(0)\psi_i(0)) - \int_0^L f(x)\psi_i(x)\,\mathrm{d}x = 0
$$

- $u'(L)\psi_i(L) = 0$ since $\psi_i(L) = 0$
- $u'(0)\psi_i(0) = C\psi_i(0)$ since $u'(0) = C$

Method 1: Boundary function and exclusion of Dirichlet degrees of freedom

- $\psi_i = \varphi_i$, $i \in \mathcal{I}_s = \{0, \ldots, N = N_n - 2\}$
- $B(x) = D\varphi_{N_n-1}(x)$, $u = B + \sum_{j=0}^{N} c_j\varphi_j$

$$
\int_0^L u'(x)\varphi_i'(x)dx = \int_0^L f(x)\varphi_i(x)dx - C\varphi_i(0), \quad i \in \mathcal{I}_s
$$

$$
\sum_{j=0}^{N}\left(\int_0^L \varphi_i'\varphi_j' dx\right)c_j = \int_0^L \left(f\varphi_i - D\varphi_N'\varphi_i\right)dx - C\varphi_i(0)
$$

for $i = 0, \ldots, N = N_n - 2$.

Method 2: Use all φ_i and insert the Dirichlet condition in the linear system

- Now $\psi_i = \varphi_i$, $i = 0, \ldots, N = N_n - 1$ (all nodes)
- $\varphi_N(L) \neq 0$, so $u'(L)\varphi_N(L) \neq 0$
- However, the term $u'(L)\varphi_N(L)$ in b_N *will be erased* when we insert the Dirichlet value in $b_N = D$

We can therefore forget about the term $u'(L)\varphi_i(L)$!

Boundary terms $u'\varphi_i$ at points x_i where Dirichlet values apply can always be forgotten.

$$
u(x) = \sum_{j=0}^{N=N_n-1} c_j\varphi_j(x)
$$

$$
\sum_{j=0}^{N=N_n-1}\left(\int_0^L \varphi_i'(x)\varphi_j'(x)dx\right)c_j = \int_0^L f(x)\varphi_i(x)dx - C\varphi_i(0)
$$

How the Neumann condition impacts the element matrix and vector

The extra term $C\varphi_0(0)$ affects only the element vector from the first cell since $\varphi_0 = 0$ on all other cells.

$$\tilde{A}^{(0)} = A = \frac{1}{h}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \tilde{b}^{(0)} = \begin{pmatrix} h - C \\ h \end{pmatrix}$$

The finite element algorithm

The differential equation problem defines the integrals in the variational formulation.

Request these functions from the user:

```
integrand_lhs(phi, r, s, x)
boundary_lhs(phi, r, s, x)
integrand_rhs(phi, r, x)
boundary_rhs(phi, r, x)
```

Must also have a mesh with `vertices`, `cells`, and `dof_map`

Python pseudo code; the element matrix and vector

```
<Declare global matrix, global rhs: A, b>

# Loop over all cells
for e in range(len(cells)):

    # Compute element matrix and vector
    n = len(dof_map[e])  # no of dofs in this element
    h = vertices[cells[e][1]] - vertices[cells[e][0]]
    <Declare element matrix, element vector: A_e, b_e>

    # Integrate over the reference cell
    points, weights = <numerical integration rule>
    for X, w in zip(points, weights):
        phi = <basis functions + derivatives at X>
        detJ = h/2
        x = <affine mapping from X>
        for r in range(n):
            for s in range(n):
                A_e[r,s] += integrand_lhs(phi, r, s, x)*detJ*w
            b_e[r] += integrand_rhs(phi, r, x)*detJ*w

    # Add boundary terms
    for r in range(n):
        for s in range(n):
            A_e[r,s] += boundary_lhs(phi, r, s, x)*detJ*w
        b_e[r] += boundary_rhs(phi, r, x)*detJ*w
```

Python pseudo code; boundary conditions and assembly

```
for e in range(len(cells)):
    ...

    # Incorporate essential boundary conditions
    for r in range(n):
        global_dof = dof_map[e][r]
        if global_dof in essbc_dofs:
            # dof r is subject to an essential condition
            value = essbc_docs[global_dof]
            # Symmetric modification
            b_e -= value*A_e[:,r]
            A_e[r,:] = 0
            A_e[:,r] = 0
            A_e[r,r] = 1
            b_e[r] = value

    # Assemble
    for r in range(n):
        for s in range(n):
            A[dof_map[e][r], dof_map[e][r]] += A_e[r,s]
        b[dof_map[e][r] += b_e[r]

<solve linear system>
```

Variational formulations in 2D and 3D

Major differences when going from 1D to 2D/3D

- The integration by part formula is different
- Cells have different geometry

Integration by parts

Rule for multi-dimensional integration by parts

$$-\int_\Omega \nabla\cdot(\alpha(\boldsymbol{x})\nabla u)v\,\mathrm{d}x = \int_\Omega \alpha(\boldsymbol{x})\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega} a\frac{\partial u}{\partial n}v\,\mathrm{d}s$$

- $\int_\Omega ()\,\mathrm{d}x$: area (2D) or volume (3D) integral
- $\int_{\partial\Omega} ()\,\mathrm{d}s$: line(2D) or surface (3D) integral

- $\partial\Omega_N$: Neumann conditions $-a\frac{\partial u}{\partial n} = g$
- $\partial\Omega_D$: Dirichlet conditions $u = u_0$
- $v \in V$ must vanish on $\partial\Omega_D$ (in method 1)

Example on integration by parts; problem

$$
\begin{aligned}
\boldsymbol{v}\cdot\nabla u + \beta u &= \nabla\cdot(\alpha\nabla u) + f, &\quad \boldsymbol{x}\in\Omega\\
u &= u_0, &\quad \boldsymbol{x}\in\partial\Omega_D\\
-\alpha\frac{\partial u}{\partial n} &= g, &\quad \boldsymbol{x}\in\partial\Omega_N
\end{aligned}
$$

- Known: α, β, f, u_0, and g.
- Second-order PDE: must have *exactly one boundary condition at each point of the boundary*

Method 1 with boundary function and $\psi_i = 0$ on $\partial\Omega_D$ (ensures $u = u_0$ condition):

$$u(\boldsymbol{x}) = B(\boldsymbol{x}) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(\boldsymbol{x}),\quad B(\boldsymbol{x}) = u_0(\boldsymbol{x})$$

Example on integration by parts in 1D/2D/3D

Galerkin's method: multiply by $v\in V$ and integrate over Ω,

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \beta u)v\,\mathrm{d}x = \int_\Omega \nabla\cdot(\alpha\nabla u)\,v\,\mathrm{d}x + \int_\Omega fv\,\mathrm{d}x$$

Integrate the second-order term by parts according to the formula:

$$\int_\Omega \nabla\cdot(\alpha\nabla u)\,v\,\mathrm{d}x = -\int_\Omega \alpha\nabla u\cdot\nabla v\,\mathrm{d}x + \int_{\partial\Omega}\alpha\frac{\partial u}{\partial n}v\,\mathrm{d}s,$$

Galerkin's method then gives

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \beta u)v\,\mathrm{d}x = -\int_\Omega \alpha\nabla u\cdot\nabla v\,\mathrm{d}x + \int_{\partial\Omega}\alpha\frac{\partial u}{\partial n}v\,\mathrm{d}s + \int_\Omega fv\,\mathrm{d}x$$

Incorporation of the Neumann condition in the variational formulation

Note: $v\neq 0$ only on $\partial\Omega_N$ (since $v=0$ on $\partial\Omega_D$):

$$\int_{\partial\Omega}\alpha\frac{\partial u}{\partial n}v\,\mathrm{d}s = \int_{\partial\Omega_N}\underbrace{\alpha\frac{\partial u}{\partial n}}_{-g}v\,\mathrm{d}s = -\int_{\partial\Omega_N} gv\,\mathrm{d}s$$

The final variational form:

$$\int_\Omega(\boldsymbol{v}\cdot\nabla u + \beta u)v\,\mathrm{d}x = -\int_\Omega \alpha\nabla u\cdot\nabla v\,\mathrm{d}x - \int_{\partial\Omega_N} gv\,\mathrm{d}s + \int_\Omega fv\,\mathrm{d}x$$

Or with inner product notation:

$$(\boldsymbol{v}\cdot\nabla u, v) + (\beta u, v) = -(\alpha\nabla u, \nabla v) - (g, v)_N + (f, v)$$

$(g, v)_N$: line or surface integral over $\partial\Omega_N$.

Derivation of the linear system

- $\forall v\in V$ is replaced by for all ψ_i, $i\in\mathcal{I}_s$
- Insert $u = B + \sum_{j\in\mathcal{I}_s} c_j\psi_j$, $B = u_0$, in the variational form
- Identify i,j terms (matrix) and i terms (right-hand side)
- Write on form $\sum_{i\in\mathcal{I}_s} A_{i,j}c_j = b_i$, $i\in\mathcal{I}_s$

$$A_{i,j} = (\boldsymbol{v}\cdot\nabla\psi_j, \psi_i) + (\beta\psi_j, \psi_i) + (\alpha\nabla\psi_j, \nabla\psi_i)$$

$$b_i = (g, \psi_i)_N + (f, \psi_i) - (\boldsymbol{v}\cdot\nabla u_0, \psi_i) + (\beta u_0, \psi_i) + (\alpha\nabla u_0, \nabla\psi_i)$$

Transformation to a reference cell in 2D/3D (1)

We want to compute an integral in the physical domain by integrating over the reference cell.

$$\int_{\Omega^{(e)}}\alpha(\boldsymbol{x})\nabla\varphi_i\cdot\nabla\varphi_j\,\mathrm{d}x$$

Mapping from reference to physical coordinates:

$$\boldsymbol{x}(\boldsymbol{X})$$

with Jacobian J,

$$J_{i,j} = \frac{\partial x_j}{\partial X_i}$$

Transformation to a reference cell in 2D/3D (2)

- $\mathrm{d}x \rightarrow \det J\,\mathrm{d}X$.
- Must express $\nabla\varphi_i$ by an expression with $\tilde{\varphi}_r$, $i = q(e,r)$: $\nabla\tilde{\varphi}_r(\boldsymbol{X})$
- We want $\nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X})$ (derivatives wrt $\boldsymbol{x}$)
- What we readily have is $\nabla_{\boldsymbol{X}}\tilde{\varphi}_r(\boldsymbol{X})$ (derivative wrt $\boldsymbol{X}$)
- Need to transform $\nabla_{\boldsymbol{X}}\tilde{\varphi}_r(\boldsymbol{X})$ to $\nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X})$

Transformation to a reference cell in 2D/3D (3)

Can derive

$$\begin{aligned}\nabla_{\boldsymbol{X}}\tilde{\varphi}_r &= J\cdot\nabla_{\boldsymbol{x}}\varphi_i\\ \nabla_{\boldsymbol{x}}\varphi_i &= \nabla_{\boldsymbol{x}}\tilde{\varphi}_r(\boldsymbol{X}) = J^{-1}\cdot\nabla_{\boldsymbol{X}}\tilde{\varphi}_r(\boldsymbol{X})\end{aligned}$$

Integral transformation from physical to reference coordinates:

$$\int_{\Omega^{(e)}}\alpha(\boldsymbol{x})\nabla_{\boldsymbol{x}}\varphi_i\cdot\nabla_{\boldsymbol{x}}\varphi_j\,\mathrm{d}x = \int_{\tilde{\Omega}^r}\alpha(\boldsymbol{x}(\boldsymbol{X}))(J^{-1}\cdot\nabla_{\boldsymbol{X}}\tilde{\varphi}_r)\cdot(J^{-1}\cdot\nabla\tilde{\varphi}_s)\det J\,\mathrm{d}X$$

Numerical integration

Numerical integration over reference cell triangles and tetrahedra:

$$\int_{\tilde{\Omega}^r} g\,\mathrm{d}X = \sum_{j=0}^{n-1} w_j g(\bar{\boldsymbol{X}}_j)$$

Module `numint.py` contains different rules:

```
>>> import numint
>>> x, w = numint.quadrature_for_triangles(num_points=3)
>>> x
[(0.16666666666666666, 0.16666666666666666),
 (0.66666666666666666, 0.16666666666666666),
 (0.16666666666666666, 0.66666666666666666)]
>>> w
[0.16666666666666666, 0.16666666666666666, 0.16666666666666666]
```

- Triangle: rules with $n = 1, 3, 4, 7$ integrate exactly polynomials of degree $1, 2, 3, 4$, resp.
- Tetrahedron: rules with $n = 1, 4, 5, 11$ integrate exactly polynomials of degree $1, 2, 3, 4$, resp.