Numerical Methods for Differential Equations

Chapter 4: From Finite Differences to Finite Elements

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1. Integration by parts

Logarithmic norm of matrix

$$\mu_2[A] = \max_{x \neq 0} \frac{x^{\mathrm{T}} A x}{x^{\mathrm{T}} x} \quad \Rightarrow \quad x^{\mathrm{T}} A x \leq \mu_2[A] \cdot x^{\mathrm{T}} x$$

For $\mathrm{d}^2/\mathrm{d}x^2$, introduce the *inner product*

$$\langle u, v \rangle = \int_0^1 \bar{u}(x) v(x) \, \mathrm{d}x \quad \Rightarrow \quad \|u\|_2^2 = \langle u, u \rangle$$

The logarithmic norm of $\mathrm{d}^2/\mathrm{d}x^2$

Can we find a constant $\mu_2[\mathrm{d}^2/\mathrm{d}x^2]$ such that

$$\langle u, u'' \rangle \leq \mu_2[\mathrm{d}^2/\mathrm{d}x^2] \cdot \|u\|_2^2$$

for all functions $u \in C_0^2[0, 1]$?

Yes, and $\mu_2[\mathrm{d}^2/\mathrm{d}x^2] = -\pi^2$

Integration by parts

$$\int_0^1 uv' \, \mathrm{d}x = [uv]_0^1 - \int_0^1 u'v \, \mathrm{d}x$$

Because $u(0) = u(1) = 0$, this can be written

$$\langle u, v' \rangle = -\langle u', v \rangle$$

Apply to $\mathrm{d}^2/\mathrm{d}x^2 \quad \Rightarrow$

$$\langle u, u'' \rangle = -\langle u', u' \rangle = -\|u'\|_2^2$$

Sobolev's lemma

Lemma *For all functions u with $u(0) = u(1) = 0$ it holds that*

$$\|u'\|_2 \geq \pi \|u\|_2$$

Proof Fourier analysis (Parseval's theorem)

$$u = \sqrt{2} \sum_{k=1}^{\infty} c_k \sin k\pi x \quad \Rightarrow \quad u' = \pi \sqrt{2} \sum_{k=1}^{\infty} k\, c_k \cos k\pi x$$

implies $\|u'\|_2 \geq \pi \|u\|_2$

Note Equality for $u(x) = \sin \pi x$

Logarithmic norm of $\mathrm{d}^2/\mathrm{d}x^2$ on $[0,1]$

We now have

$$\langle u, u'' \rangle = -\langle u', u' \rangle = -\|u'\|_2^2 \leq -\pi^2 \|u\|_2^2$$

Theorem *The logarithmic norm of* $\mathrm{d}^2/\mathrm{d}x^2$ *on* $C_0^2[0,1]$ *is*

$$\mu_2[\mathrm{d}^2/\mathrm{d}x^2] = -\pi^2$$

Corollary *The 2pBVP* $u'' = f(x)$ *with* $u(0) = u(1) = 0$ *has a unique solution with* $\|u\|_2 \leq \|f\|_2/\pi^2$

2. Linear operators and adjoint operators

Definition Given an operator A,

$$\langle v, Au \rangle = \langle A^* v, u \rangle$$

defines the adjoint operator A^*

Example For vectors and matrices, A^{T} is the adjoint of A, as

$$\langle v, Au \rangle = v^{\mathrm{T}} A u = (A^{\mathrm{T}} v)^{\mathrm{T}} u = \langle A^* v, u \rangle$$

A matrix is "self-adjoint" (symmetric) if $A = A^{\mathrm{T}}$

Example 1 $\mathrm{d}^2/\mathrm{d}x^2$ is *self-adjoint* on $C_0^2[0,1]$

Proof Integrate twice by parts $\langle v, u'' \rangle = -\langle v', u' \rangle = \langle v'', u \rangle$

Example 2 $\mathcal{L} = \dfrac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\dfrac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)$ is self-adjoint on $C_0^2[0,1]$

$$\begin{aligned}
\langle v, \mathcal{L}u \rangle = \langle v, (pu')' + qu \rangle &= \langle v, (pu')' \rangle + \langle v, qu \rangle \\
&= -\langle v', pu' \rangle + \langle qv, u \rangle \\
&= -\langle pv', u' \rangle + \langle qv, u \rangle \\
&= \langle (pv')', u \rangle + \langle qv, u \rangle \\
&= \langle (pv')' + qv, u \rangle = \langle \mathcal{L}v, u \rangle = \langle \mathcal{L}^* v, u \rangle
\end{aligned}$$

Example 3 $\mathcal{L} = \mathrm{d}/\mathrm{d}x$ is *anti-selfadjoint* on $C_0^2[0,1]$

Proof Integrate by parts, $\langle v, u' \rangle = -\langle v', u \rangle$, so $\mathcal{L}^* = -\mathcal{L}$

Some are neither self-adjoint nor anti-selfadjoint

Example 4 $\mathcal{L} = \dfrac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\dfrac{\mathrm{d}}{\mathrm{d}x}\right) + \dfrac{\mathrm{d}}{\mathrm{d}x} + q(x)$

The latter tend to be "trouble-makers"

Eigenvalues of self-adjoint operators are real

Let $Au = \lambda u$, then $\lambda = \bar{\lambda}$ because

$$\begin{aligned}\lambda\|u\|_2^2 &= \langle u, \lambda u\rangle = \langle u, Au\rangle = \langle A^* u, u\rangle \\ &= \langle Au, u\rangle = \langle \lambda u, u\rangle = \bar{\lambda}\|u\|_2^2\end{aligned}$$

(Anti-selfadjoint operators have imaginary eigenvalues)

Eigenvectors are orthogonal – let $Au = \lambda u$ and $Av = \mu v$, then

$$\begin{aligned}\lambda\langle v, u\rangle &= \langle v, Au\rangle = \langle A^* v, u\rangle \\ &= \langle Av, u\rangle = \mu\langle v, u\rangle\end{aligned}$$

So $\lambda \neq \mu$ implies orthogonality, $\langle v, u\rangle = 0$

3. Elliptic operators

Definition *An operator is elliptic if for all* $u \neq 0$

$$\langle u, Au \rangle > 0$$

Example $-\mathrm{d}^2/\mathrm{d}x^2$ on $C_0^2[0,1]$

Proof Integrate by parts

$$-\langle u, u'' \rangle = \langle u', u' \rangle \geq \pi^2 \langle u, u \rangle$$

by Sobolev's lemma

Elliptic operators...

More generally,

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)$$

is elliptic if $p(x) > 0$ and $q(x) \geq 0$

Example Poisson equation

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y)$$

$-\Delta$ is an elliptic operator

Positive definite operators

Definition *An operator is positive definite if it is self-adjoint and elliptic*

Example $-\mathrm{d}^2/\mathrm{d}x^2$ as $\mu_2[\mathrm{d}^2/\mathrm{d}x^2] = -\pi^2$ on $C_0^2[0,1]$

Negative Laplacian $-\Delta$ (leads to FEM theory)

Procedure

Analyze the differential operator, discretize to preserve symmetry and ellipticity, using high order (if possible) and adaptive grids

4. From Finite Differences to Finite Elements

Start with linear differential equation

$$\mathcal{A}u = f \qquad + \quad \text{boundary conditions}$$

Finite Difference Method (FDM) *The main idea*

- *Replace functions* u and f *by vectors*
- *Replace differential operator* $\mathcal{A}$ *by matrix*
- *Obtain a linear system of equations*

Example 1D Poisson equation $\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}\, u = f(x) \;\rightarrow\; T_{\Delta x} u = f$

Finite Elements and the Galerkin method

Galerkin Method (FEM) *The main idea*

- *Approximate function* u *by polynomials* v
- *Keep differential operator* $\mathcal{A}$ *as is*
- *Insert* v *into original equation*
- *Choose* v *to minimize the residual* $\|\mathcal{A}v - f\|_{L^2}$

Choose v as a piecewise polynomial satisfying boundary conditions, and find the best approximation using integration by parts

This is in principle a least squares approximation

Best approximation = least squares

Let $\{\varphi_j\}$ be a polynomial basis, and make the *ansatz*

$$v(x) = \sum_{j=1}^{N} c_j \varphi_j(x)$$

Minimizing $\|\mathcal{A}v - f\|_2$ is equivalent to requiring that *the residual is orthogonal to each and every φ_i*

$$\langle \varphi_i, \mathcal{A}v - f \rangle = 0 \qquad \forall i$$

This is *least-squares approximation*

Best approximation...

As $\mathcal{A}$ is linear,

$$\mathcal{A}v = \mathcal{A}\sum_{j=1}^{N} c_j\varphi_j = \sum_{j=1}^{N} c_j\mathcal{A}\varphi_j$$

Then

$$\langle \varphi_i, \mathcal{A}v - f\rangle = 0 \quad \Leftrightarrow \quad \sum_{j=1}^{N}\langle \varphi_i, \mathcal{A}\varphi_j\rangle c_j = \langle \varphi_i, f\rangle$$

Linear system of equations $Ac = b$ with $\sum a_{ij}c_j = b_i$, and where

$$a_{ij} = \langle \varphi_i, \mathcal{A}\varphi_j\rangle \qquad\qquad b_i = \langle \varphi_i, f\rangle$$

The system is assembled from the basis $\{\varphi_i\}$ and the operator $\mathcal{A}$

5. Weak formulation

If $-u'' = f$ then *for all* v satisfying $v(0) = v(1) = 0$

$$\langle v, -u'' \rangle = \langle v, f \rangle$$

Integrate by parts and use Dirichlet boundary data to get

Weak formulation $\quad \langle v', u' \rangle = \langle v, f \rangle \quad \forall v$

Note

- u only needs to be *once* continuously differentiable, *not twice*
- Integration by parts corresponds to a "Choleski factorization" of the positive definite operator

Weak formulation and energy norm

Definition *The energy norm is defined by* $a(v, u) = \langle v', u' \rangle$ *and the weak formulation can be written:*

Find a function u *such that for all test functions* v *it holds*

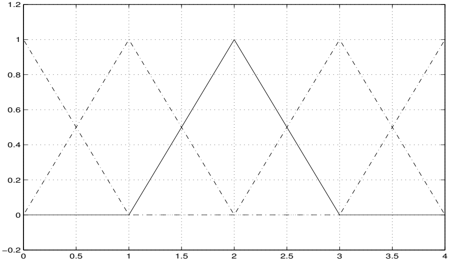
$$a(v, u) = \langle v, f \rangle$$

What functions? Choose a polynomial space $\mathcal{V}$ with basis $\{\varphi_j\}$, satisfying the boundary conditions, and require $v \in \mathcal{V}$ and $u \in \mathcal{V}$, all defined on suitable grid $\{x_i\}$

The Finite Element Method (FEM)

Given grid $\{x_i\}$, choose *piecewise linear basis polynomials*

$\varphi_j(x_i) = 1$ if $i = j$, otherwise 0



Piecewise linear interpolant $v \approx u$ can be written

$$v(x) = \sum_{j=1}^{N} c_j \varphi_j(x)$$

Note $v(x_i) = c_i \approx u(x_i)$

Best approximation $a(v,u) = \langle v, f\rangle$, with $u, v \in \mathcal{V}$, leads to

$$a(\varphi_i, \sum_{j=1}^{N} c_j\varphi_j) = \langle \varphi_i, f\rangle$$

which is equivalent to the *finite element equation $Kc = b$*

$$\sum_{j=1}^{N} \langle \varphi_i', \varphi_j'\rangle c_j = \langle \varphi_i, f\rangle \qquad \forall \varphi_i \in \mathcal{V}$$

The *stiffness matrix K* with elements $\{\langle \varphi_i', \varphi_j'\rangle\}_{i,j=1}^{N}$ can be computed as soon as the basis $\{\varphi_j\}$ has been constructed

The right-hand side vector b depends on the data f

Assume an equidistant grid with spacing Δx and note that

$$
\begin{aligned}
\varphi_i'(x) &= 1/\Delta x && x \in [x_{i-1}, x_i] \\
\varphi_i'(x) &= -1/\Delta x && x \in [x_i, x_{i+1}] \\
\varphi_i'(x) &= 0 && \text{elsewhere}
\end{aligned}
$$

Then

$$\langle \varphi_i', \varphi_i' \rangle = \int_{x_{i-1}}^{x_{i+1}} \frac{1}{\Delta x^2} \, \mathrm{d}x = \frac{2}{\Delta x}$$

$$\langle \varphi_i', \varphi_{i-1}' \rangle = \langle \varphi_i', \varphi_{i+1}' \rangle = \int_{x_i}^{x_{i+1}} \frac{-1}{\Delta x^2} \, \mathrm{d}x = \frac{-1}{\Delta x}$$

$$\langle \varphi_i', \varphi_j' \rangle = 0 \qquad \text{otherwise}$$

Stiffness matrix

For equidistant grid with spacing Δx the *stiffness matrix* is

$$K_{\Delta x} = \frac{1}{\Delta x} \operatorname{tridiag}(-1 \qquad 2 \quad -1)$$

Note

- The stiffness matrix is $K_{\Delta x} = -\Delta x \cdot T_{\Delta x}$
- It is *positive definite*, therefore nonsingular
- Smallest eigenvalue $\lambda_1[K_{\Delta x}] \approx \pi^2 \Delta x$

Mass matrix

Compute RHS integrals using numerical integration

$$\langle \varphi_i, f \rangle \approx \langle \varphi_i, \sum_{j=0}^{N} f_j \varphi_j \rangle = \sum_{k=-1}^{1} f_{i+k} \langle \varphi_i, \varphi_{i+k} \rangle$$

Need to compute $\langle \varphi_i, \varphi_{i+k} \rangle = \int_{x_{i-1}}^{x_{i+1}} \varphi_i(x) \varphi_{i+k}(x) \, \mathrm{d}x$

The integrals are $\langle \varphi_i, \varphi_i \rangle = 2\Delta x/3$ and $\langle \varphi_i, \varphi_{i+1} \rangle = \Delta x/6$

For equidistant grid with spacing Δx the *mass matrix* is

$$M_{\Delta x} = \frac{\Delta x}{6} \, \mathrm{tridiag}(1 \quad 4 \quad 1)$$

Assembling the system of equations

Finite element equation for $-u'' = f$ is a tridiagonal system

$$K_{\Delta x}\, c = M_{\Delta x} f$$

with *stiffness matrix*

$$K_{\Delta x} = \frac{1}{\Delta x}\,\mathrm{tridiag}(-1 \quad 2 \quad -1)$$

and *mass matrix*

$$M_{\Delta x} = \frac{\Delta x}{6}\,\mathrm{tridiag}(1 \quad 4 \quad 1)$$

Advantages of the Finite Element Method

- Produces "continuous solution" not only on grid points
- Boundary conditions built into test functions
- In PDEs, easy to work with complex geometries
- Can easily use nonuniform grids
- Can also use basis of higher degree splines
- Rich theoretical foundation

Note Weak formulation allows using piecewise linear approximations, in spite of $v'' = 0$ for such "solutions"