MA5233 Computational Mathematics

Lecture 5: Poisson Equation

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Poisson equation

- Linear systems often arise as discretisations of partial differential equations (PDEs).
- ► These linear systems have a special structure which allows for much faster algorithms.
- Poisson equation is the most famous of all PDEs.

Outline

- ► Introduction to the Poisson equation
- ► Solving the Poisson equation using finite differences
- Convergence of the finite difference discretisation

Poisson equation

Given $\Omega \subset \mathbb{R}^n$ and $f: \Omega \to \mathbb{R}$, find $u: \Omega \to \mathbb{R}$ such that

$$\begin{cases} -\Delta u(x) = f(x) & \forall x \in \Omega, \\ u(x) = 0 & \forall x \in \partial \Omega. \end{cases}$$

 $\Delta:=\frac{\partial^2}{\partial x_1^2}+\ldots+\frac{\partial^2}{\partial x_n^2}$ is called the Laplacian operator.

Physical interpretation

	f	и
diffusion	particle source / sink	concentration
heat	heat source / sink	temperature
electrostatics	charge distribution	potential

Derivation of the Poisson equation

Fick's law of diffusion: net flux is given by

$$\vec{J} = -D \nabla u = -D \begin{pmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_n} \end{pmatrix}.$$

Conservation of mass:

$$\frac{\partial}{\partial t} \int_{\Omega'} u \, dx = - \int_{\partial \Omega'} \vec{n} \cdot \vec{J} \, dx + \int_{\Omega'} f \, dx.$$

Divergence / Gauss's theorem:

$$\int_{\partial\Omega'} \vec{n} \cdot \vec{J} dx = \int_{\Omega'} \nabla \cdot \vec{J} dx = \int_{\Omega'} \left(\frac{\partial J_1}{\partial x_1} + \ldots + \frac{\partial J_n}{\partial x_n} \right) dx$$

Derivation of the Poisson equation

Combining conservation of mass with divergence theorem yields

$$\int_{\Omega'} \left(\frac{\partial u}{\partial t} + \nabla \cdot \vec{J} - f \right) dx = 0 \qquad \forall \Omega' \subset \Omega.$$

Hence

$$\frac{\partial u}{\partial t} + \nabla \cdot \vec{J} - f = 0.$$

▶ Inserting steady-state condition $\frac{\partial u}{\partial t} = 0$ and Fick's law yields

$$-\nabla\cdot(D\,\nabla u)=f.$$

In electrostatics, D represents the electrical permittivity of a given material.

Terminology

Equations:

- ▶ Poisson equation: $-\Delta u = f$ (elliptic)
- ▶ Laplace equation: $-\Delta u = 0$ (elliptic)
- ▶ Heat equation: $\frac{\partial u}{\partial t} = \Delta u + f$ (parabolic)

Boundary conditions:

- ▶ homogeneous Dirichlet: u(x) = 0
- ▶ inhomogeneous Dirichlet: u(x) = g(x)
- ▶ Neumann: $\vec{n} \cdot \nabla u = g(x)$

Physical interpretation of boundary conditions

Homogeneous Dirichlet, u(x) = 0:

- ▶ Diffusion: particles reaching $\partial\Omega$ get trapped.
- Heat: constant temperature on boundary.
- ► Electrostatics: constant potential on boundary.

Neumann, $\vec{n} \cdot \nabla u(x) = g(x)$:

- Diffusion & heat: prescribed flux across boundary.
- ► Electrostatics: prescribed charges on boundary.

Handling inhomogeneous Dirichlet boundary conditions

$$\begin{cases} -\Delta u = f & \text{on } \Omega \\ u = g & \text{on } \partial \Omega \end{cases}$$

is equivalent to $u = u_0 + g$ where

$$\begin{cases} -\Delta u_0 = f + \Delta g & \text{on } \Omega \\ u_0 = 0 & \text{on } \partial \Omega \end{cases}$$

Example: heat flow through wall

- ► Consider wall of thickness *L* with diffusion constant *D*.
- \blacktriangleright Assume there is a temperature difference ΔT across the wall.
- Let u(x) denote the temperature as function of distance x to the left end of the wall.

Temperature distribution u(x) satisfies the 1D Poisson equation

$$\begin{cases} -\frac{\partial}{\partial x} D \frac{\partial}{\partial x} u = 0 & \text{on } \Omega = [0, L], \\ u(0) = 0, & u(L) = \Delta T. \end{cases}$$

Solution u(x) and heat flux J are given by, respectively,

$$u(x) = \frac{\Delta T}{L} x$$
 and $J = -\frac{D \Delta T}{L}$.

Discretising the Poisson equation

Assuming $\Omega = [0, 1]$, u(0) = u(1) = 0 and D = 1 for now.

Functions:

- ▶ Introduce mesh $\Omega_n := \{x_k := \frac{k}{n+1} \mid k = 0, \dots, n+1\}.$
- ▶ Replace function f(x) with vector of point values $f_k := f(x_k)$.

Derivatives:

$$(\nabla_n u)_{k+\frac{1}{2}} := rac{f_{k+1} - f_k}{1/(n+1)} pprox \nabla u(x_{k+\frac{1}{2}})$$

$$(\Delta_n u)_k := rac{(\nabla_n u)_{k+\frac{1}{2}} - (\nabla_n u)_{k-\frac{1}{2}}}{1/(n+1)} pprox \Delta u(x_k)$$

Second derivative simplifies to

$$(\Delta_n u)_k = (n+1)^2 (u_{k+1} - 2u_k + u_{k-1}).$$

Discretising the Poisson equation

Replacing Δ with Δ_n in $-\Delta u = f$ yields

$$(n+1)^{2}\begin{pmatrix}2&-1&&\\-1&\ddots&\ddots&\\&\ddots&\ddots&-1\\&&-1&2\end{pmatrix}\begin{pmatrix}u\left(\frac{1}{n+1}\right)\\\vdots\\u\left(\frac{n}{n+1}\right)\end{pmatrix}=\begin{pmatrix}f\left(\frac{1}{n+1}\right)\\\vdots\\f\left(\frac{n}{n+1}\right)\end{pmatrix}.$$

Note that boundary points $u(\frac{0}{n+1})$ and $u(\frac{n+1}{n+1})$ do not appear in linear system since we already know these values.

See 5_poission_equation.jl for how to do this in Julia.

Remarks

► Replacing

$$\frac{\partial u}{\partial x} \longrightarrow \frac{u(x + \frac{\Delta x}{2}) - u(x - \frac{\Delta x}{2})}{\Delta x}$$

is know as finite difference discretisation.

▶ How do we know that this is a good scheme?

Assessing the quality of a discretisation

Recall: A good factorisation algorithm was one which was

- lacktriangle accurate (relative errors are $\mathcal{O}(\varepsilon_{\mathsf{mach}})$), and
- fast (as little floating-point operations as possible).

This assessment no longer works for discretisations: Increasing mesh size n increases FLOP count but reduces error.

New performance metric: error e_n as a function of mesh size n.

- ▶ Good algorithm: $e_n = \mathcal{O}(2^{-n})$
- ▶ Bad algorithm: $e_n = \mathcal{O}(\log_2(n)^{-1})$

Hence, we want a theorem of the form $||u - u_n|| = \mathcal{O}(g(n))$.

Notation 1

We use the same symbol f to denote both a function $f:[0,1]\to\mathbb{R}$ and vector of point-values $f=\left(f(\frac{1}{n+1})\ldots f(\frac{n}{n+1})\right)^T$. Context will clarify the intended meaning.

Notation 2

$$||f||_{2,n} := \frac{1}{\sqrt{n+1}} \sqrt{\sum_{k=1}^{n} f(\frac{k}{n+1})^2} = \frac{||f||_2}{\sqrt{n+1}}.$$

- ► For now: extra factor $\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$ is needed to ensure that the magnitude of $||f||_{2,n}$ is independent of n.
- We will see later that $||f||_{2,n}$ corresponds to a trapezoidal rule discretisation of $\sqrt{\int_0^1 f(x)^2 dx}$, assuming f(0) = f(1) = 0.

Theorem

Assume function u and point-values u_n satisfy, respectively,

$$-\Delta u = f$$
 and $-\Delta_n u_n = f$.

Then,

$$||u-u_n||_{2,n} \leq ||\Delta_n^{-1}||_{2,n} ||\Delta_n u + f||_{2,n}.$$

Proof.
$$u - u_n = \Delta_n^{-1} (\Delta_n u - \Delta_n u_n) = \Delta_n^{-1} (\Delta_n u + f).$$

Remarks

- ▶ $\|\Delta_n^{-1}\|_{2,n}$: conditioning of discretised system. Confusingly, this is commonly referred to as *stability*.
- ▶ $\|\Delta_n u + f\|_{2,n}$: consistency of discretised system. Measures how well exact solution u solves the discrete problem.

Statement to remember

Consistency and stability imply convergence!

Consistency of finite difference discretisation

Assume $u \in C^4([0,1])$. Inserting the Taylor expansion

$$\begin{split} u\big(\frac{k\pm 1}{n+1}\big) &= u\big(\frac{k}{n+1}\big) \pm \frac{1}{1!} \; u'\big(\frac{k}{n+1}\big) \frac{1}{n+1} &+ \frac{1}{2!} \; u''\big(\frac{k}{n+1}\big) \frac{1}{(n+1)^2} \\ &\pm \frac{1}{3!} \; u'''\big(\frac{k}{n+1}\big) \frac{1}{(n+1)^3} + \frac{1}{4!} \; u''''\big(\frac{k}{n+1}\big) \frac{1}{(n+1)^4} + o\big(n^{-4}\big) \end{split}$$

yields

$$(\Delta_{n}u)_{k} = (n+1)^{2} \left(u(\frac{k+1}{n+1}) - 2u(\frac{k}{n+1}) + u(\frac{k-1}{n+1}) \right)$$

$$= u''(\frac{k}{n+1}) + \frac{2}{4!} u''''(\frac{k}{n+1}) \frac{1}{(n+1)^{2}} + o(n^{-2})$$

$$= -f(\frac{k}{n+1}) + \frac{2}{4!} u''''(\frac{k}{n+1}) \frac{1}{(n+1)^{2}} + o(n^{-2}).$$

Hence, consistency error is $\|\Delta_n u + f\|_{2,n} \le \frac{2}{4!} \|u''''\|_{[0,1]} \frac{1}{(n+1)^2} + o(n^{-2}).$

Stability of finite difference discretisation

- $ightharpoonup \Delta_n$ is a symmetric matrix.
- For such matrices, it holds $\|\Delta_n^{-1}\|_{2,n} = \|\Delta_n^{-1}\|_2 = |\lambda_{\min}|^{-1}$, where λ_{\min} is the eigenvalue of Δ_n of smallest magnitude.
- ▶ Hence, we are looking for u such that $\Delta_n u = \lambda u$.

Outline for the following slides:

- ► Consider continuous case $\Delta u(x) = \lambda u(x)$ for inspiration.
- ► Guess discrete eigenvectors based on continuous eigenfunctions.
- ▶ Verify $\|\Delta_n^{-1}\|_{2,n} \ge C$ for some C independent of n.

Eigenfunctions of continuous Laplacian Δ

Observations:

 $ightharpoonup rac{\partial^2 u}{\partial x^2}(x) = \lambda \, u(x)$ is satisfied by

$$\lambda = -\pi^2 \ell^2$$
 and
$$\begin{cases} u(x) = \sin(\pi \ell x), \\ u(x) = \cos(\pi \ell x). \end{cases}$$

▶ Only $u(x) = \sin(\pi \ell x)$ with $\ell \in \{1, 2, ...\}$ satisfies u(0) = u(1) = 0.

Hence, eigenpairs of Δ are given by

$$\lambda_{\ell} := -\pi^2 \ell^2$$
 and $u_{\ell}(x) := \sin(\pi \ell x)$.

We observe $\lambda_{\min} = -\pi^2 \neq 0$.

Eigenfunctions of discrete Laplacian Δ_n

Educated guess: eigenvectors of Δ_n are given by $(u_\ell)_k := \sin(\pi \frac{\ell k}{n+1})$.

To verify this, it is convenient to split

$$(u_{\ell})_{k} = \frac{1}{2\iota} \left(\exp\left(\pi\iota \frac{\ell k}{n+1}\right) - \exp\left(-\pi\iota \frac{\ell k}{n+1}\right) \right) =: \frac{1}{2\iota} \left((e_{\ell})_{k} - (e_{-\ell})_{k} \right)$$

We compute, for $k \in \{2, \ldots, n-1\}$,

$$\begin{split} (\Delta_n \, e_\ell)_k &= (n+1)^2 \left((e_\ell)_{k+1} - 2 \, (e_\ell)_k + (e_\ell)_{k-1} \right) \\ &= (n+1)^2 \left(\exp \left(\pi \iota \frac{\ell \, (k+1)}{n+1} \right) - 2 \, \exp \left(\pi \iota \frac{\ell \, k}{n+1} \right) + \exp \left(\pi \iota \frac{\ell \, (k-1)}{n+1} \right) \right) \\ &= (n+1)^2 \left(\exp \left(\pi \iota \frac{\ell}{n+1} \right) + \exp \left(-\pi \iota \frac{\ell}{n+1} \right) - 2 \right) \, \exp \left(\pi \iota \frac{\ell \, k}{n+1} \right) \\ &= \underbrace{(n+1)^2 \left(2 \cos \left(\pi \frac{\ell}{n+1} \right) - 2 \right) (e_\ell)_k}. \end{split}$$

By linearity, it holds $(\Delta_n u_\ell)_k = \lambda_\ell (u_\ell)_k$ for $k \in \{2, \dots, n-1\}$.

Eigenfunctions of discrete Laplacian Δ_n

For k = 1, we have

$$(\Delta_n e_\ell)_1 = \lambda_\ell (e_\ell)_k - \exp \left(\pi \iota \frac{\ell \, 0}{n+1}\right) = \lambda_\ell (e_\ell)_k - 1.$$

Hence $(\Delta_n u_\ell)_1 = \lambda_\ell (u_\ell)_1$, and similarly one can show $(\Delta_n u_\ell)_n = \lambda_\ell (u_\ell)_n$

Conclusion: eigenvalues and eigenvectors of Δ_n are given by, respectively,

$$\lambda_\ell = (n+1)^2 \left(2\cos\left(\pi\frac{\ell}{n+1}\right) - 2\right) \quad \text{and} \quad (u_\ell)_k = \sin\left(\pi\frac{\ell k}{n+1}\right)$$

for $\ell \in \{1, \dots n\}$.

Minimal eigenvalue is obtained for $\ell = 1$:

$$\lambda_{\min} = (n+1)^2 \left(2\cos\left(\frac{\pi}{n+1}\right) - 2 \right) = -\pi^2 + \mathcal{O}(n^{-2}).$$

Convergence of finite difference discretisation

Combining the consistency and stability estimates yields

$$||u - u_n||_{n,2} \le \underbrace{\pi^2}_{||\Delta_n||_{2,n}} \underbrace{\frac{2}{4!} ||u''''||_{[0,1]} \frac{1}{(n+1)^2}}_{||\Delta_n u + f||_{2,n}} + o(n^{-2}).$$

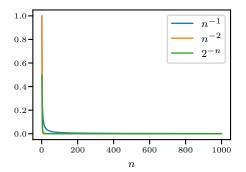
Applications of convergence estimate

- Estimation of work required to reach sufficient accuracy.
- Code debugging! Try replacing the $(n+1)^2$ scaling of Δ_n with n^2 and see what happens to the convergence rate.

Correct axes for convergence plots

Bad choice: linear scale for both x and y axis.

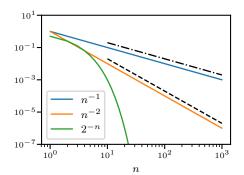
- ▶ Different decay behaviours all look the same.
- ▶ You cannot see errors $\lesssim 10^{-2}$.



Correct axes for convergence plots

Good choice for algebraic decay: logarithmic scale for both x and y axis.

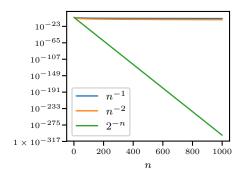
- $ightharpoonup n^{\alpha}$ decay leads to straight line.
- Add reference lines (black lines below) so order of decay α can be easily inferred.



Correct axes for convergence plots

Good choice for exponential decay: linear scale for x axis, logarithmic scale for y axis.

- $ightharpoonup a^{-n}$ decay leads to straight line.
- ▶ If there is an estimate for *a* from theory, add reference line for comparison.



References and further reading

► Consistency and stability theorem:

http://www-users.math.umn.edu/~arnold/papers/stability.pdf