MA5233 Computational Mathematics

Lecture 5: Poisson Equation

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Poisson Equation

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

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

Poisson Equation

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:

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

Poisson Equation

Derivation of the Poisson equation

- Combining conservation of mass with divergence theorem yields

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

  Hences

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

- 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.

Poisson Equation

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

Poisson Equation

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.

Poisson Equation

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

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

Poisson Equation

Example: heat flow through wall

- Consider wall of thickness L with diffusion constant D.
- 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,

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

Poisson Equation

Discretising the Poisson equation

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

Functions:

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

Derivatives:

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

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

Second derivative simplifies to

$$(\Delta_n u)_k = (n+1)^2 \left(f_{k+1} - 2f_k + f_{k-1} \right).$$

Poisson Equation

Discretising the Poisson equation

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

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

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

Remarks

- Replacing
$$\frac{\partial u}{\partial x} \quad \longrightarrow \quad \frac{u(x + \frac{\Delta x}{2}) - u(x - \frac{\Delta x}{2})}{\Delta x}$$
is know as *finite difference discretisation*.
- How do we know that this is a good scheme?

Poisson Equation

Assessing the quality of a discretisation

Recall: A good factorisation algorithm was one which was

- accurate (relative errors are $\mathcal{O}\big(\varepsilon_{\text{mach}}\big)$), 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: $e_n = \mathcal{O}\big(2^{-n}\big)$
- Bad algorithm: $e_n = \mathcal{O}\big(\log_2(n)^{-1}\big)$

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

Poisson Equation

Notation 1

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

Notation 2

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

- 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 $f(0) = f(1) = 0$.

Poisson Equation

Theorem

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

$$-\Delta u = f \qquad \text{and} \qquad -\Delta_n u_n = f.$$

Then,

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

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

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!

Poisson Equation

Consistency of finite difference discretisation

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

$$\begin{aligned} u\left(\tfrac{k\pm1}{n+1}\right) = u\left(\tfrac{k}{n+1}\right) &\pm \tfrac{1}{1!}\, u'\left(\tfrac{k}{n+1}\right)\tfrac{1}{n+1} \qquad + \tfrac{1}{2!}\, u''\left(\tfrac{k}{n+1}\right)\tfrac{1}{(n+1)^2} \\ &\pm \tfrac{1}{3!}\, u'''\left(\tfrac{k}{n+1}\right)\tfrac{1}{(n+1)^3} + \tfrac{1}{4!}\, u''''\left(\tfrac{k}{n+1}\right)\tfrac{1}{(n+1)^4} + o\left(n^{-4}\right) \end{aligned}$$

yields

$$\begin{aligned} (\Delta_n u)_k &= (n+1)^2 \left(u\left(\tfrac{k+1}{n+1}\right) - 2\, u\left(\tfrac{k}{n+1}\right) + u\left(\tfrac{k-1}{n+1}\right)\right) \\ &= u''\left(\tfrac{k}{n+1}\right) + \tfrac{1}{4!}\, u''''\left(\tfrac{k}{n+1}\right)\tfrac{1}{(n+1)^2} + o\left(n^{-4}\right) \\ &= -f\left(\tfrac{k}{n+1}\right) + \tfrac{1}{4!}\, u''''\left(\tfrac{k}{n+1}\right)\tfrac{1}{(n+1)^2} + o\left(n^{-4}\right). \end{aligned}$$

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

Poisson Equation

Stability of finite difference discretisation

- Δ_n is a symmetric matrix.
- For such matrices, it holds $\|\Delta_n^{-1}\|_{2,n} = \|\Delta_n^{-1}\|_2 = |\lambda_{\min}|^{-1}$, where $\lambda_{\min}$ 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 $\|\Delta_n^{-1}\|_{2,n} \geq C$ for some C independent of n.

Poisson Equation

Eigenfunctions of continuous Laplacian Δ

Observations:

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

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

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

Hence, eigenpairs of Δ are given by

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

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

Poisson Equation

Eigenfunctions of discrete Laplacian Δ_n

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

To verify this, it is convenient to split

$$(u_\ell)_k = \frac{1}{2\iota}\Big(\exp\big(\pi\iota\tfrac{\ell k}{n+1}\big) - \exp\big(-\pi\iota\tfrac{\ell k}{n+1}\big)\Big) =: \frac{1}{2\iota}\Big((e_\ell)_k - (e_{-\ell})_k\Big)$$

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

$$\begin{aligned}
(\Delta_n\, e_\ell)_k &= (n+1)^2 \Big((e_\ell)_{k+1} - 2\,(e_\ell)_k + (e_\ell)_{k-1}\Big) \\
&= (n+1)^2 \Big(\exp\big(\pi\iota\tfrac{\ell\,(k+1)}{n+1}\big) - 2\,\exp\big(\pi\iota\tfrac{\ell k}{n+1}\big) + \exp\big(\pi\iota\tfrac{\ell\,(k-1)}{n+1}\big)\Big) \\
&= (n+1)^2 \Big(\exp\big(\pi\iota\tfrac{\ell}{n+1}\big) + \exp\big(\pi\iota\tfrac{\ell}{n+1}\big) - 2\Big)\,\exp\big(\pi\iota\tfrac{\ell k}{n+1}\big) \\
&= \underbrace{(n+1)^2 \Big(2\cos\big(\pi\tfrac{\ell}{n+1}\big) - 2\Big)}_{\lambda_\ell}(e_\ell)_k.
\end{aligned}$$

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

Poisson Equation

Eigenfunctions of discrete Laplacian Δ_n

For $k = 1$, we have

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

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,

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

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

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

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

Poisson Equation

Convergence of finite difference discretisation

Combining the consistency and stability estimates yields

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

Applications of convergence estimate

- Estimation of work required to reach sufficient accuracy.
- Code debugging!

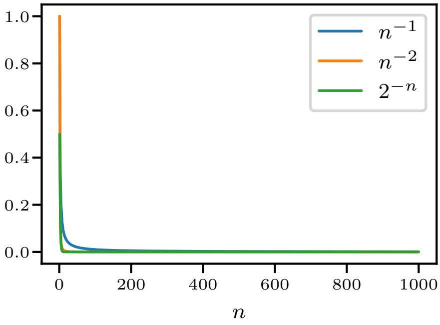
  Try replacing the $(n+1)^2$ scaling of Δ_n with n^2 and see what happens to the convergence rate.

Poisson Equation

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 $\lesssim 10^{-2}$.

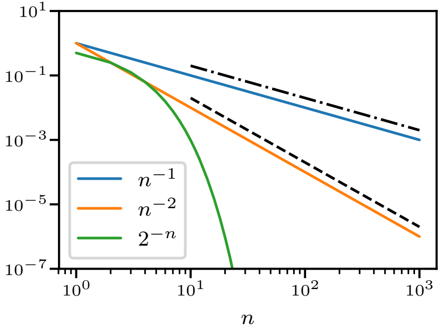


Poisson Equation

Correct axes for convergence plots

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

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

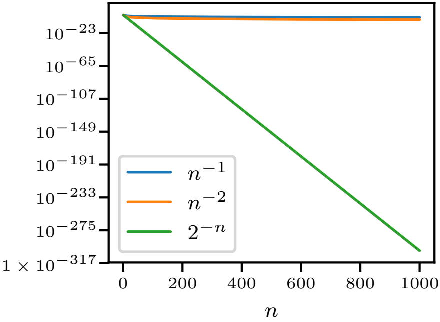


Poisson Equation

Correct axes for convergence plots

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

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



Poisson Equation

References and further reading

- Consistency and stability theorem:
  `http://www-users.math.umn.edu/~arnold/papers/stability.pdf`