MA3227 Numerical Analysis II

Lecture 2: Finite Differences

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Finite Differences

Introduction

Consider Poisson's equation on $\Omega = (0, 1)$, i.e. the problem of finding $u : [0, 1] \to \mathbb{R}$ such that

$$-u''(x) = f(x) \text{ for } x \in (0, 1) \qquad \text{and} \qquad u(0) = u(1) = 0.$$

Any discretisation of this equation faces two fundamental challenges:

- A function $u : [0, 1] \to \mathbb{R}$ contains an infinite amount of information.
- Derivatives
$$u'(x) := \lim_{\delta \to 0} \frac{u(x + \delta) - u(x)}{\delta}$$
are not computable even if we could evaluate $u(x)$.

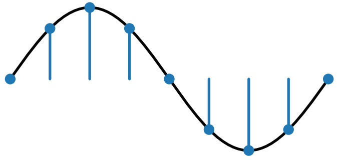
These problems can be tackled in different ways. In this module, we will focus on one particular way known as *finite difference discretisation*.

Finite Differences

Finite difference discretisation

Discretisation of functions:

Replace $u : [0,1] \to \mathbb{R}$ with vector of point values $u[i] := u\left(\frac{i}{n+1}\right)$.



Remarks:

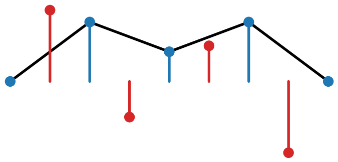
- We have $u[0] = u(0)$ and $u[n+1] = u(1)$.
  We typically exclude these i from the vector of point values since $u(0) = u(1) = 0$ according to the boundary conditions.
- We will frequently use the same symbol u to denote both a function $u(x)$ and the associated vector of point values $u[i] = u\left(\frac{i}{n+1}\right)$.

Finite Differences

Finite difference discretisation (continued)

Discretisation of derivatives:

Replace $u'(x)$ with $\tilde{u}'\left(\frac{i+1/2}{n+1}\right) := \dfrac{u\left(\frac{i+1}{n+1}\right) - u\left(\frac{i}{n+1}\right)}{1/(n+1)}$.



Iterating this idea for the second derivative $u''(x)$, we obtain

$$\begin{aligned}\tilde{u}''\left(\tfrac{i}{n+1}\right) &= \frac{\tilde{u}'\left(\frac{i+1/2}{n+1}\right) - \tilde{u}'\left(\frac{i-1/2}{n+1}\right)}{1/(n+1)} \\ &= (n+1)^2 \left(u\left(\tfrac{i+1}{n+1}\right) - 2\,u\left(\tfrac{i}{n+1}\right) + u\left(\tfrac{i-1}{n+1}\right)\right)\end{aligned}$$

Finite Differences

Finite difference discretisation (continued)

Copied from previous slide:

$$\tilde{u}''\left(\tfrac{i}{n+1}\right) = (n+1)^2 \left(u\left(\tfrac{i+1}{n+1}\right) - 2\,u\left(\tfrac{i}{n+1}\right) + u\left(\tfrac{i-1}{n+1}\right) \right).$$

This formula can be written as a matrix-vector product $\tilde{u}'' = \Delta_n u$,

$$\begin{pmatrix} \tilde{u}''\left(\tfrac{1}{n+1}\right) \\ \vdots \\ \tilde{u}''\left(\tfrac{n}{n+1}\right) \end{pmatrix} = (n+1)^2 \begin{pmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{pmatrix} \begin{pmatrix} u\left(\tfrac{1}{n+1}\right) \\ \vdots \\ u\left(\tfrac{n}{n+1}\right) \end{pmatrix}. \qquad (1)$$

Note that the first line of the above system of equations should be

$$\tilde{u}''\left(\tfrac{1}{n+1}\right) = (n+1)^2 \left(u\left(\tfrac{0}{n+1}\right) - 2\,u\left(\tfrac{1}{n+1}\right) + u\left(\tfrac{2}{n+1}\right) \right).$$

We can eliminate $u\left(\tfrac{0}{n+1}\right)$ in (1) since we know that $u\left(\tfrac{0}{n+1}\right) = u(0) = 0$. Same holds for $u\left(\tfrac{n+1}{n+1}\right)$.

Finite Differences

Finite difference discretisation (conclusion)

Finite difference discretisation of the Poisson equation consists in replacing Δu with $\Delta_n u_n$ where

$$\Delta_n := (n+1)^2 \begin{pmatrix} -2 & 1 & & & \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{pmatrix}, \qquad u_n \approx \begin{pmatrix} u\left(\frac{1}{n+1}\right) \\ \vdots \\ u\left(\frac{n}{n+1}\right) \end{pmatrix}.$$

This yields the linear system of equations

$$-\Delta_n u_n = f.$$

Writing code which computes this u_n is straightforward; see `solve_poisson()` in the code file for this lecture.

Finite Differences

Exercise

Derive the finite diff. discretisation of the operator $u \mapsto \frac{\partial}{\partial x}\big(D(x)\,\frac{\partial u}{\partial x}\big)$.
This operator describes diffusion in a medium where the diffusion coefficient $D(x)$ is spatially varying.

Discussion

Several steps in the above "derivation" of the finite differences equations are quite arbitrary.
Furthermore, we can check numerically that $u_n \neq u$ for any finite n.

Question: What makes finite differences a "good" scheme?

Answer: We can show that $u_n \to u$ for $n \to \infty$, and we can quantify the speed of convergence.

Finite Differences

We will use the following norm for our convergence analysis.

Weighted 2-norm

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

Remarks:

- $\|u\|_{2,n}$ is a trapezoidal-rule discretisation of $\sqrt{\int_0^1 u(x)^2 \, dx}$.
- $\|\mathbf{1}\|_{2,n} = \frac{\sqrt{n}}{\sqrt{n+1}} \to 1$ for $n \to \infty$ with $\mathbf{1}$ the vector of all ones.
- $\|A\|_{2,n} := \sup_{u \in \mathbb{R}^n} \frac{\|Au\|_{2,n}}{\|u\|_{2,n}} = \|A\|_2$ for all $A \in \mathbb{R}^{n \times n}$.

Finite Differences

Our convergence analysis is based on the following result.

Lemma

Let $u_n \in \mathbb{R}^n$ be the solution to $-\Delta_n u_n = f$. 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

- $\|\Delta_n^{-1}\|_{2,n}$: stability of discretised system.
  Measures how sensitive u_n is to perturbation in f.
- $\|\Delta_n u + f\|_{2,n}$: consistency of discretised system.
  Measures how well the exact solution u solves the discrete problem.

These two quantities can be analysed separately.

Finite Differences

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 need to determine smallest eigenvalue $\lambda_{\min}$.

Eigenvalues of continuous Laplacian

One can easily verify that the pairs

$$\lambda_k := -\pi^2 k^2, \qquad u_k(x) := \sin(\pi k x)$$

with $k \in \{1, 2, 3, \ldots\}$ satisfy

$$\Delta u_k(x) = \lambda_k \, u_k(x) \qquad \text{and} \qquad u_k(0) = u_k(1) = 0.$$

Hence, for the continuous Laplacian we have $|\lambda_{\min}| = \pi^2$.

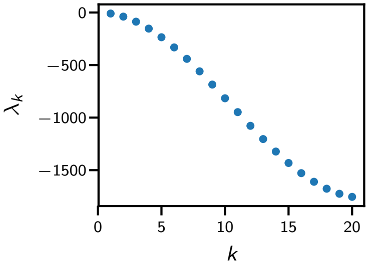
Finite Differences

Eigenvalues of discrete Laplacian

Through lengthy calculations, one can show that the eigenpairs of Δ_n are

$$\lambda_k = (n+1)^2 \left(2\cos\left(\pi \tfrac{k}{n+1}\right) - 2\right) \quad \text{and} \quad u_k[i] = \sin\left(\pi k \tfrac{i}{n+1}\right)$$

with $k \in \{1, \ldots n\}$.



We conclude

$$|\lambda_{\min}| = |\lambda_1| = (n+1)^2 \left(2\cos\left(\pi \tfrac{1}{n+1}\right) - 2\right) = \pi^2 + \mathcal{O}\left(n^{-2}\right)$$

and thus $\|\Delta_n^{-1}\|_{2,n} = \mathcal{O}(1)$, i.e. the discrete Laplacian is stable.

Finite Differences

Consistency of finite difference discretisation

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

$$\begin{aligned} u\big(\tfrac{i\pm 1}{n+1}\big) = u\big(\tfrac{i}{n+1}\big) &\pm \tfrac{1}{1!}\, u'\big(\tfrac{i}{n+1}\big)\tfrac{1}{n+1} \qquad + \tfrac{1}{2!}\, u''\big(\tfrac{i}{n+1}\big)\tfrac{1}{(n+1)^2} \\ &\pm \tfrac{1}{3!}\, u'''\big(\tfrac{i}{n+1}\big)\tfrac{1}{(n+1)^3} + \mathcal{O}\big(n^{-4}\big) \end{aligned}$$

yields

$$\begin{aligned} (\Delta_n u)_k &= (n+1)^2 \Big(u\big(\tfrac{i+1}{n+1}\big) - 2\, u\big(\tfrac{i}{n+1}\big) + u\big(\tfrac{i-1}{n+1}\big)\Big) \\ &= (n+1)^2 \Big(0 + 0 + \tfrac{2}{2!}\, u''\big(\tfrac{i}{n+1}\big)\, \tfrac{1}{(n+1)^2} + 0 + \mathcal{O}\big(n^{-4}\big)\Big) \\ &= u''\big(\tfrac{i}{n+1}\big) + \mathcal{O}\big(n^{-2}\big) \\ &= -f\big(\tfrac{i}{n+1}\big) + \mathcal{O}\big(n^{-2}\big). \end{aligned}$$

Hence, consistency error is $\|\Delta_n u + f\|_{2,n} = \mathcal{O}\big(n^{-2}\big)$.

Finite Differences

Convergence of finite difference discretisation

Combining the consistency and stability estimates yields

$$\|u - u_n\|_{n,2} \le \|\Delta_n^{-1}\|_{2,n} \, \|\Delta_n u + f\|_{2,n} = \mathcal{O}(1)\,\mathcal{O}\big(n^{-2}\big) = \mathcal{O}\big(n^{-2}\big).$$

See `convergence()`.

Applications of convergence estimate

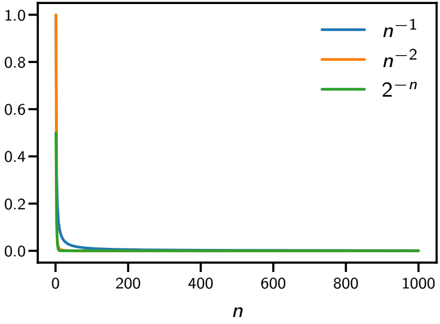
- Estimation of work required to reach sufficient accuracy.
- Compare different discretisation schemes.
- Code debugging.
  Example: replace $(n+1)^2$ with n^2 in definition of Δ_n and rerun `convergence()`.

Finite Differences

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 $\lesssim 10^{-2}$.

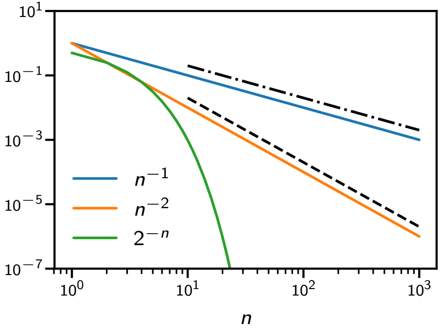


Finite Differences

Correct axes for convergence plots (continued)

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.

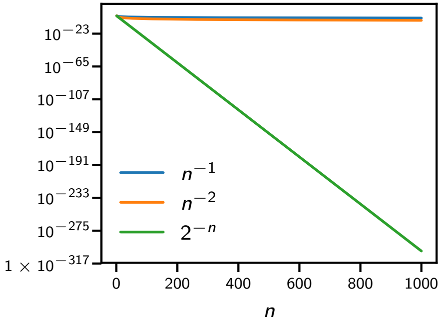


Finite Differences

Correct axes for convergence plots (continued)

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.



Finite Differences

Summary

- Finite-difference discretisation of $-\frac{\partial^2}{\partial x^2}$ leads to the linear system of equations

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

- Consistency and stability imply convergence:

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

  Stability $\|\Delta_n^{-1}\|_{2,n}$ can be estimated using eigenvalues.
  Consistency $\|\Delta_n u + f\|_{2,n}$ can be estimated using Taylor expansion.
- Finite difference discretisation: $\|u - u_n\|_{2,n} = \mathcal{O}\big(n^{-2}\big)$.