MA3227 Numerical Analysis II

Midterm Assignment

Deadline: 8 March 2021, 12 noon
Total marks: 15

1 Poisson's equation with variable diffusion coefficient

In this assignment, we will develop a finite difference discretisation for the one-dimensional Poisson equation with variable diffusion coefficient and homogeneous Dirichlet boundary conditions, i.e. the following partial differential equation.

Problem statement
Given $D, f : [0,1] \to \mathbb{R}$, find $u : [0,1] \to \mathbb{R}$ such that $u(0) = u(1) = 0$ and

$$-\tfrac{\partial}{\partial x}\Big(D(x)\,\tfrac{\partial u}{\partial x}(x)\Big) = f(x) \qquad \text{for all } x \in (0,1). \tag{1}$$

This equation can be used e.g. to model the temperature distribution $u(x)$ on your CPU:

- The zero boundary conditions represent the fact that the surface of your CPU is kept at a constant temperature by the cooling system.
- The source term $f(x)$ represents the heat generated by the various CPU components.
- The diffusion coefficient $D(x)$ represents the spatially varying thermal conductivity.

Let us begin by developing some intuition for this equation.

Task 1 [1 mark] `example()` plots the solution $u(x)$ of (1) for

$$D(x) = \begin{cases} 1.0 & \text{if } x \geq 0.5 \\ 0.1 & \text{if } x < 0.5 \end{cases} \qquad \text{and} \qquad f(x) = 1.0.$$

Explain why $u(x)$ assumes its maximum value for $x \in [0, 0.5]$ rather than $x \in [0.5, 1]$. Your answer should refer only to physical intuition and not involve any computations.

Next, let us derive a finite-difference discretisation.

Task 2 [1 mark] Show that the usual finite difference approximation

$$\tfrac{\partial u}{\partial x}\big(\tfrac{i}{n+1}\big) \approx (n+1)\,\Big(u\big(\tfrac{i+1/2}{n+1}\big) - u\big(\tfrac{i-1/2}{n+1}\big)\Big)$$

gives rise to the approximation

$$\tfrac{\partial}{\partial x}\Big(D(x)\,\tfrac{\partial u}{\partial x}(x)\Big)\big(\tfrac{i}{n+1}\big) \approx \dots$$
$$(n+1)^2\,\Big(D\big(\tfrac{i-1/2}{n+1}\big)\,u\big(\tfrac{i-1}{n+1}\big) - \Big(D\big(\tfrac{i-1/2}{n+1}\big) + D\big(\tfrac{i+1/2}{n+1}\big)\Big)\,u\big(\tfrac{i}{n+1}\big) + D\big(\tfrac{i+1/2}{n+1}\big)\,u\big(\tfrac{i+1}{n+1}\big)\Big).$$

Task 2 suggests that we replace the continuous PDE (1) with the linear system of equations

$$-\Delta_n u_n = f$$

where $u_n, f \in \mathbb{R}^n$ denote the usual (approximate) vectors of point values

$$u_n[i] \approx u\big(\tfrac{i}{n+1}\big), \qquad f[i] = f\big(\tfrac{i}{n+1}\big), \qquad i = 1, \ldots, n,$$

and $\Delta_n \in \mathbb{R}^{n \times n}$ denotes the discrete Laplacian now given by

$$(\Delta_n u)[i] = (n+1)^2 \left(D\big(\tfrac{i-1/2}{n+1}\big)\, u[i-1] - \left(D\big(\tfrac{i-1/2}{n+1}\big) + D\big(\tfrac{i+1/2}{n+1}\big) \right) u[i] + D\big(\tfrac{i+1/2}{n+1}\big)\, u[i+1] \right).$$

Let us next assess the convergence of this discretisation using the stability and consistency lemma presented in class.

Task 3 [3 marks] Show that if $D(x) \geq \varepsilon > 0$ for all $x \in [0,1]$, then

$$\|\Delta_n^{-1}\|_{2,n} \;\leq\; \varepsilon^{-1} \qquad \text{for all } n \in \mathbb{N}.$$

Hint. Use the energy method. Fourier analysis does not work here because of the variable diffusion coefficient $D(x)$.

Task 4 [3 marks] Show that if $u(x)$ is four times continuously differentiable, then

$$\|f + \Delta_n u\|_{2,n} \;=\; O\big(n^{-2}\big) \qquad \text{for } n \to \infty.$$

Hint. The proof is analogous to what we did in class, but it is more tedious because of the extra $D(x)$ factors. Plan ahead how you want to proceed and try to stay as organised as possible.

Tasks 3 and 4 together with the stability and consistency lemma show that our finite difference scheme is second-order convergent, i.e.

$$\|u_n - u\|_{2,n} = O\big(n^{-2}\big) \qquad \text{for } n \to \infty.$$

In addition, our finding in Task 3 indicates that

$$\|u_n\|_{2,n} \;\leq\; \|\Delta_n^{-1}\|_{2,n}\, \|f\|_{2,n} \;=\; O(\varepsilon^{-1})\; \|f\|_{2,n},$$

i.e. $\|u_n\|_{2,n}$ may grow beyond bounds for vanishing $\varepsilon > 0$ and fixed $\|f\|_{2,n}$. This mathematical has an intuitive interpretation.

Task 5 [1 mark] Motivate why $u(x)$ may grow beyond bounds for vanishing $D(x)$ and fixed $f(x)$ by referring to the physical meaning of (1).

Hint. Recall your findings from Task 1. You may also want to run `example()` repeatedly for increasingly smaller values of $D([0, 0.5])$ to see the corresponding changes in $u(x)$.

Warning. The following assumes familiarity with some topics of Lecture 5 which I did not cover before recess week. You may wish to wait until Monday 1 March (first Monday after recess week) before proceeding.

Finally, let us consider the problem of solving the linear system of equations $-\Delta_n u_n = f$. Since we are tackling a one-dimensional PDE, this could be done in optimal $O(n)$ runtime using the LU factorisation, but we shall ignore this possibility for the purpose of this exercise and consider the conjugate gradients method instead.

We have seen in class that the conjugate gradients method applied to $-\Delta_n u_n = f$ with $D(x) = 1$ requires $O(n)$ iterations, and `n_iterations()` demonstrates that the same is also true for a nontrivial $D(x)$. We therefore conclude conjugate gradients needs preconditioning to be effective.

A simple but usually effective preconditioner for Poisson-like differential equations is given by

$$P = V \Lambda V^T$$

where

$$V[i,k] = \sqrt{\tfrac{2}{n+1}}\, \sin\!\big(\pi k \, \tfrac{i}{n+1}\big), \qquad \Lambda[k,\ell] = \begin{cases} 2\,(n+1)^2 \left(1 - \cos\!\big(\pi \tfrac{k}{n+1}\big)\right) & \text{if } k = \ell, \\ 0 & \text{otherwise} \end{cases}$$

denotes the eigendecomposition of $-\Delta_n$ for $D(x) = 1$ (cf. Lecture 3). This so-called *Fourier preconditioner* allows us to evaluate

$$P^{-1}\, v = V \Lambda^{-1}\, V^T v$$

quickly because the matrix-vector products $V^T v$ and $V v$ can be evaluated in $O\big(n\,\log(n)\big)$ runtime using an algorithm known as the Fast Fourier Transform (FFT), and $\Lambda^{-1}\, v$ can trivially be evaluated in $O(n)$ runtime.

Task 6 [6 marks] `fourier_preconditioning()` plots the convergence histories of conjugate gradients with no preconditioning and Fourier preconditioning applied to $-\Delta_n u_n = f$ with a diffusion coefficient $D(x)$ given by

$$D(x) = 1 + (1 - \varepsilon)\, x\, (1 - x).$$

Relate the following observations to what we have seen in Lecture 5.

1. Unpreconditioned conjugate gradients converges to the exact solution after 50 iterations for $\varepsilon = 1$ but fails to do so for $\varepsilon < 1$.
2. Fourier-preconditioned conjugate gradients converges in a single iteration for $\varepsilon = 1$ but converges increasingly more slowly for $\varepsilon \to 0$.
