Numerical Analysis - Part II

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Lecture 1

Solving PDEs with finite difference methods

Approximation of ∇^2

Our goal is to solve the *Poisson equation*

$$\nabla^2 u = f \qquad (x, y) \in \Omega, \qquad (1)$$

where $\nabla^2 = \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is the Laplace operator and Ω is an open connected domain of $\mathbb{R}^2$ with a Jordan boundary, specified together with the *Dirichlet boundary condition*

$$u(x, y) = \phi(x, y) \qquad (x, y) \in \partial\Omega. \qquad (2)$$

(You may assume that $f \in C(\Omega)$, $\phi \in C^2(\partial\Omega)$, but this can be relaxed by an approach outside the scope of this course.)

We cannot solve

$$\nabla^2 u = f \qquad (x, y) \in \Omega, \tag{3}$$

directly, meaning that we typically do not have a closed form solution u, nor can we solve (3) directly on a computer.
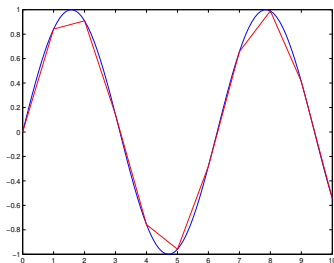
However, we do know how to solve a linear system of equations

$$Ax = y, \qquad A \in \mathbb{R}^{N \times N}, \quad x, y \in \mathbb{R}^N.$$
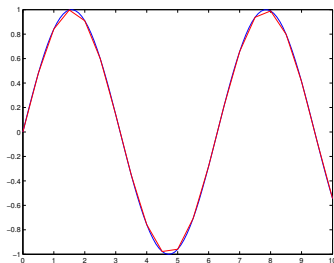
Discretising functions

Consider a function $f : [0, 10] \to \mathbb{R}$. We can "approximate" f with a vector $x = \{f(0), f(h), \ldots, f(10)\}$, where $h > 0$ is called the step size.

Approximating with step size $h = 1$

Approximating with step size $h = 0.5$

Figure : Left: The sin function approximated on a grid of 11 points.
Right: The sin function approximated on a grid of 21 points.

If we can "approximate" a function u with a vector x, what should be the approximation of the operator ∇^2?

Crazy Idea: Use finite differences! After all, the derivative is the limit of differences of the function with some scaling. Indeed,

$$u'(a) = \lim_{h \to 0} \frac{u(a+h) - u(a)}{h}.$$

Approximation of ∇^2

To this end we impose on Ω a square grid with uniform spacing of $h > 0$ and replace

$$\nabla^2 u = f \qquad (x, y) \in \Omega,$$

by a *finite-difference* formula. For simplicity, we require for the time being that $\partial\Omega$ 'fits' into the grid: if a grid point lies inside Ω then all its neighbours are in $\mathrm{cl}\,\Omega$. We will discuss briefly in the sequel grids that fail this condition.

Approximation of ∇^2

Since $\nabla^2 = \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, we need to consider a finite-difference approximation of second derivatives.

Proposition 1

Let $g \in C^4[a, b]$ and $x \in (a + h, b - h)$. Then

$$\Delta_h^2 g(x) := g(x-h) - 2g(x) + g(x+h) = h^2 g''(x) + \frac{1}{12} h^4 g^{(4)} + \mathcal{O}(h^6). \tag{4}$$

Proof. Expanding into Taylor series,

$$
\begin{aligned}
g(x + h) - g(x) &= & hg'(x) + \tfrac{1}{2!} h^2 g''(x) + \tfrac{1}{3!} h^3 g'''(x) + \cdots \\
g(x - h) - g(x) &= & -hg'(x) + \tfrac{1}{2!} h^2 g''(x) - \tfrac{1}{3!} h^3 g'''(x) + \cdots
\end{aligned}
$$

and adding two expressions, we see that the terms with odd derivatives vanish, and the LHS of (4) is equal to $\sum_{k=1}^{m} \frac{2}{(2k)!} h^{2k} g^{(2k)}(x) + \mathcal{O}(h^{2m+2})$, where we took $m = 2$. $\qquad\square$

Remark 2
In approximation of the second derivative g'' by the second central difference $\Delta_h^* g(x) = g(x - h) - 2g(x) + g(x + h)$, it is sometimes useful to know the terms of higher order:

$$\frac{1}{h^2}[g(x-h)-2g(x)+g(x+h)] = g''(x)+\frac{1}{12}h^2 g^{(\mathrm{iv})}+\frac{1}{360}h^4 g^{(\mathrm{vi})}+\mathcal{O}(h^6).$$

Corollary 3

The approximation

$(\Delta_{h,x}^2 + \Delta_{h,y}^2)\, u(x, y)$
$= u(x - h, y) + u(x + h, y) + u(x, y - h) + u(x, y + h) - 4u(x, y)$
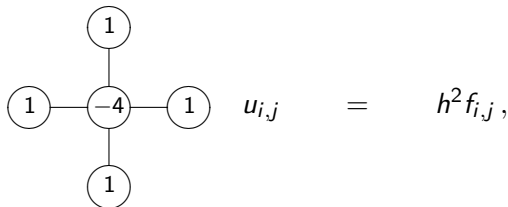$\approx h^2 \nabla^2 u(x, y)$

(5)

produces a local error of $\mathcal{O}(h^4)$.

Approximation of ∇^2

The aforementioned analysis justifies the *five-point method*

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = h^2 f_{i,j}, \qquad (ih, jh) \in \Omega, \ (6)$$

where $f_{i,j} = f(ih, jh)$ are given, and $u_{i,j} \approx u(ih, jh)$ is an approximation to the exact solution. It is usually denoted by the following *computational stencil*

$$u_{i,j} \quad = \quad h^2 f_{i,j},$$

Whenever $(ih, jh) \in \partial\Omega$, we substitute appropriate Dirichlet boundary values. Note that the outcome of our procedure is a set of linear algebraic equations whose solution approximates the solution of the Poisson equation (1) at the grid points.
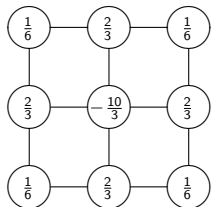
Approximation of ∇^2

It is easy (but laborious) to produce higher-order methods. You may verify, for example, that the stencil

$$u_{i,j} = h^2 f_{i,j}$$

produces a local error of $\mathcal{O}(h^6)$. (This scheme is just a linear combination of two five-point methods with steps h and $2h$, respectively.) Needless to say, the implementation of this method is more complicated, since we might be 'missing' points near the boundary. Moreover, the set of algebraic equations that needs to be solved is less sparse than for the 5-point method, hence its solution is more expensive.

Approximation of ∇^2

It is considerably easier to implement the *nine-point method*

$$u_{i,j} \qquad = \qquad h^2 f_{i,j}$$

but, as such, it again produces error of $\mathcal{O}(h^4)$. However, this can be remedied by a clever trick of adding the term $\frac{1}{12}h^4\nabla^2 f$ to the right-hand side, with the 5-point approximation to $h^2\nabla^2 f$, which increases the order to $\mathcal{O}(h^6)$ (see Exercise 1).
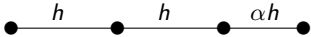
Approximation of ∇^2

Since the boundary often fails to fit exactly into a square grid, we sometimes need to approximate ∇^2 using non-equispaced points. Clearly, it is enough to be able to approximate a second directional derivative w.r.t. each variable and subsequently 'synthetize' an approximation to ∇^2.

For example, suppose that grid points are given with the spacing

$\bullet \xrightarrow{h} \bullet \xrightarrow{\alpha h} \bullet$, where $0 < \alpha \leq 1$. It is easy to verify by a Taylor expansion that

$$
\frac{2}{\alpha + 1}g(x - h) - \frac{2}{\alpha}g(x) + \frac{2}{\alpha(\alpha + 1)}g(x + \alpha h)
$$
$$
= g''(x)h^2 + \frac{1}{3}(\alpha - 1)g'''(x)h^3 + \mathcal{O}(h^4),
$$

with error of $\mathcal{O}(h^3)$ (note that $\alpha = 1$ gives, as expected, $\mathcal{O}(h^4)$).

Approximation of ∇^2

Better approximation can be obtained by taking two equispaced points on the 'interior' side, i.e. ●——h——●——h——●——αh——● as follows:

$$\frac{\alpha - 1}{\alpha + 2}g(x - 2h) - \frac{2(\alpha - 2)}{\alpha + 1}g(x - h) + \frac{\alpha - 3}{\alpha}g(x)$$
$$+ \frac{6}{\alpha(\alpha + 1)(\alpha + 2)}g(x + \alpha h) = h^2 g''(x) + \mathcal{O}(h^4).$$