Numerical Analysis - Part II

Anders C. Hansen

Lecture 2

Solving PDEs with finite difference methods

Approximation of ∇^2

Our goal is to solve the *Poisson equation*

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

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*

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

(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.)

Approximation of ∇^2

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

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

Approximation of ∇^2

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,

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

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.

Example of a grid on a square

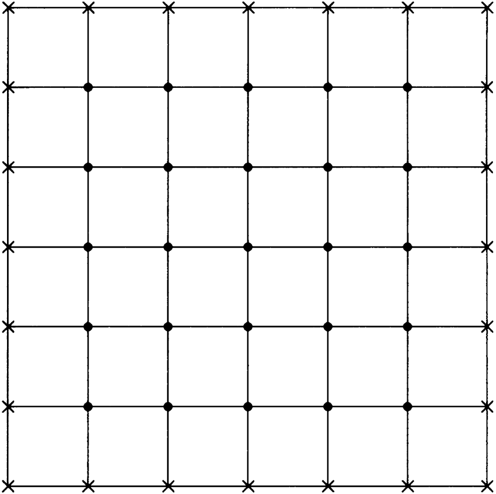


Figure : A square domain Ω with an equidistant grid.

Example of a grid on a more complicated domain

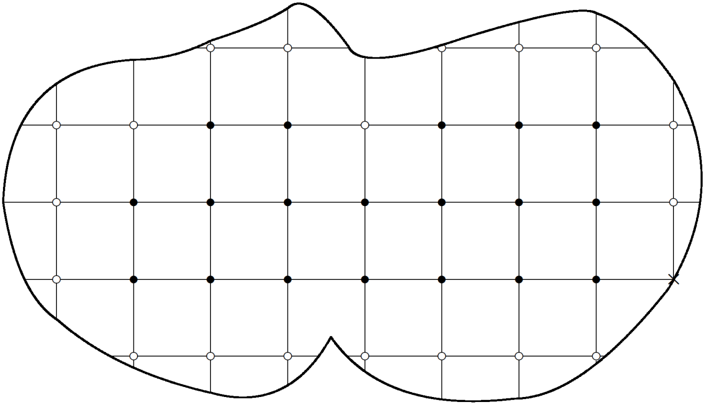


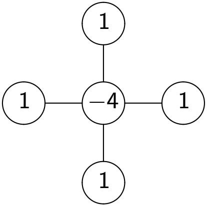
Figure : A more complicated domain Ω with an equidistant grid.

Computational stencil

We have the *five-point method*

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

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*



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

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.

Finite-difference discretization

Finite-difference discretization of $\nabla^2 u = f$ replaces the PDE by a large system of linear equations. In the sequel we pay special attention to the *five-point formula,* which results in the approximation

$$h^2\nabla^2 u(x,y) \approx u(x-h,y)+u(x+h,y)+u(x,y-h)+u(x,y+h)-4u(x,y)\,. \tag{5}$$

For the sake of simplicity, we restrict our attention to the important case of Ω being a *unit square*, where $h=\frac{1}{m+1}$ for some positive integer m. Thus, we estimate the m^2 unknown function values $u(ih,jh)_{i,j=1}^{m}$ (where $(ih,jh) \in \Omega$) by letting the right-hand side of (5) equal $h^2 f(ih,jh)$ at each value of i and j. This yields an $n \times n$ system of linear equations with $n = m^2$ unknowns $u_{i,j}$:

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = h^2 f(ih,jh)\,. \tag{6}$$

Obtaining the linear system of equations

(Note that when i or j is equal to 1 or m, then the values $u_{0,j}$, $u_{i,0}$ or $u_{i,m+1}$, $u_{m+1,j}$ are known boundary values and they should be moved to the right-hand side, thus leaving fewer unknowns on the left.) Having ordered grid points, we can write (6) as a linear system, say

$$A\mathbf{u} = \mathbf{b}\,.$$

Our present concern is to prove that, as $h \to 0$, the numerical solution (6) tends to the exact solution of the Poisson equation $\nabla^2 u = f$ (with appropriate Dirichlet boundary conditions).

Example of a grid on a square

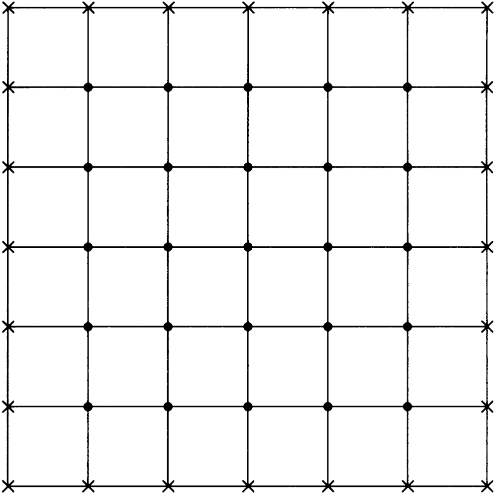


Figure : A square domain Ω with an equidistant grid.

Example 1 (Natural ordering)

The way the matrix A of this system looks depends of course on the way how the grid points (ih, jh) are being assembled in the one-dimensional array. In the *natural ordering*, when the grid points are arranged by columns, A is the following block tridiagonal matrix:

$$A = \begin{bmatrix} B & I & & & \\ I & B & I & & \\ & \ddots & \ddots & \ddots & \\ & & I & B & I \\ & & & I & B \end{bmatrix}, \qquad B = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 1 \\ & & & 1 & -4 \end{bmatrix}.$$

Before heading on let us prove the following simple but useful theorem whose importance will become apparent in the course of the lecture.

Theorem 2 (Gershgorin theorem)

All eigenvalues of an $n \times n$ matrix A are contained in the union of the Gershgorin discs in the complex plane:

$$\sigma(A) \subset \cup_{i=1}^{n} \Gamma_i \,, \qquad \Gamma_i := \{z \in \mathbb{C} : |z - a_{ii}| \leq r_i\}, \qquad r_i := \sum_{j \neq i} |a_{ij}| \,.$$

Proof of the Gershgorin theorem

Proof. Let λ be an eigenvalue of A. Choose a corresponding eigenvector $x = (x_j)$ so that one component x_i is equal to 1 and the others are of absolute value less than or equal to $x_i = 1$ and $|x_j| \leq 1$ $j \neq i$. There is always such an x, which can be obtained simply by dividing any eigenvector by its component with largest modulus. Since $Ax = \lambda x$, in particular

$$\sum_j a_{ij} x_j = \lambda x_i = \lambda.$$

So, splitting the sum and taking into account once again that $x_i = 1$, we get

$$\sum_{j \neq i} a_{ij} x_j + a_{ii} = \lambda.$$

Therefore, applying the triangle inequality,

$$|\lambda - a_{ii}| = \left| \sum_{j \neq i} a_{ij} x_j \right| \leq \sum_{j \neq i} |a_{ij}||x_j| \leq \sum_{j \neq i} |a_{ij}| = r_i.$$

The matrix A is symmetric and negative definite

Lemma 3

For any ordering of the grid points, the matrix A of the system (6) is symmetric and negative definite.

Proof I

Proof. Equation (6) implies that if $a_{ij} \neq 0$ for $i \neq j$, then the i-th and j-th points of the grid (ph, qh), are nearest neighbours. Hence $a_{ij} \neq 0$ implies $a_{ij} = a_{ji} = 1$, which proves the symmetry of A. Therefore A has real eigenvalues and eigenvectors.

It remains to prove that all the eigenvalues are negative. The arguments are parallel to the proof of Gershgorin theorem. Let $A\mathbf{x} = \lambda\mathbf{x}$, and let i be an integer such that $|x_i| = \max |x_j|$. With such an i we address the following identity (which is a reordering of the equation $(A\mathbf{x})_i = \lambda x_i$):

$$\underbrace{\left|(\lambda - a_{ii})\, x_i\right|}_{|\lambda+4|\,|x_i|} = \underbrace{\left|\, \textstyle\sum_{j\neq i}^{n} a_{ij} x_j\right|}_{\leq 4\,|x_i|} . \tag{7}$$

Here $a_{ii} = -4$ and $a_{ij} \in \{0, 1\}$ for $j \neq i$, with at most four nonzero elements on the right-hand side. It is seen that the case $\lambda > 0$ is impossible. Assuming $\lambda = 0$, we obtain $|x_j| = |x_i|$ whenever $a_{ij} = 1$, so we can alter the value of i in (7) to any of such j and repeat the same arguments. Thus, the modulus of every component of $\mathbf{x}$ would be $|x_i|$, but then the equations (7) that occur at the boundary of the grid and have fewer than four off-diagonal terms (see (6)) could not be true. Hence, $\lambda = 0$ is impossible too, hence $\lambda < 0$ which proves that A is negative definite. □

Proof II

Proof. Let U be any linear operator changing the grid ordering. Then U is clearly unitary ($\|Ux\|_2 = \|x\|_2$ for any x). Note that any matrix $\tilde{A}$ representing the the system of equations (6) can be written as $\tilde{A} = UAU^*$ for some unitary matrix U, where A is as in Example 1. Self-adjointness is preserved by unitary operators, and so is the spectrum. Thus, $\tilde{A}$ is self-adjoint (symmetric as it is real). Moreover, $\sigma(A)$ does not intersect the positive half plane by the Gershgorin theorem, so we only need to show that $0 \notin \sigma(A)$. If $Ax = 0$ then, by the definition of A, x must have elements of equal modulus, however, then the definition of B (that gives A) implies that $x = 0$. □

The eigenvalues of the matrix A

Proposition 4

The eigenvalues of the matrix A are

$$\lambda_{k,\ell} = -4\left(\sin^2\frac{k\pi h}{2}+\sin^2\frac{\ell\pi h}{2}\right), \qquad h = \frac{1}{m+1}\,, \qquad k,\ell = 1...m.$$

Proof. Let us show that, for every pair (k, ℓ), the vectors

$$v = (v_{i,j}), \quad v_{i,j} = \sin ix \sin jy, \quad \text{where} \quad x = k\pi h, \quad y = \ell\pi h,$$

are the eigenvectors of A. Indeed, for $i, j = 1...m$, we have

$$\begin{aligned} (Av)_{i,j} &= \sin(jy)\left[\sin(ix - x) - 2\sin(ix) + \sin(ix + x)\right] \\ &\quad + \sin(ix)\left[\sin(jy - y) - 2\sin(jy) + \sin(jy + y)\right] \\ &= \sin(jy)\sin(ix)\left[2\cos x - 2\right] + \sin(ix)\sin(jy)\left[2\cos y - 2\right] = \lambda v_{i,j}\,. \end{aligned}$$

Note that the terms $u_{i\pm1,j}, u_{i,j\pm1}$ do not appear in (6) for $i, j = 1$ or $i, j = m$, respectively, therefore (for such i, j) we should have dropped the corresponding components from above equation, but they are equal to zero because $\sin(i-1)x = 0$ for $i = 1$, while $\sin(i+1)x = 0$ for $i = m$, since $x = \frac{k\pi}{m+1}$. Thus, the eigenvalues are

$$\begin{aligned} \lambda_{k,\ell} = \left[2\cos x - 2\right] + \left[2\cos y - 2\right] &= -4\left(\sin^2\frac{x}{2} + \sin^2\frac{y}{2}\right) \\ &= -4\left(\sin^2\frac{k\pi h}{2} + \sin^2\frac{\ell\pi h}{2}\right). \end{aligned} \tag{8}$$

□

Remark 5

As a matter of independent mathematical interest, note that for $1 \le k, \ell \ll m$ we have $\sin x \approx x$, hence the eigenvalues for the discretized Laplacian ∇_h^2 are

$$\frac{\lambda_{k,\ell}}{h^2} \approx -\frac{4}{h^2}\left[\frac{k^2\pi^2h^2}{4} + \frac{\ell^2\pi^2h^2}{4}\right] = -(k^2+\ell^2)\pi^2 \,.$$

Now, recall (e.g. from the solution of the Poisson equation in a square by separation of variables in Maths Methods) that the *exact* eigenvalues of ∇^2 (in the unit square) are $-(k^2+\ell^2)\pi^2$, $k, \ell \in \mathbb{N}$, with the corresponding eigenfunctions $V_{k,\ell}(x,y) = \sin k\pi x \sin \ell\pi y$. So, the eigenvectors of the discretized ∇_h^2 are the values of $V_{k,\ell}(x,y)$ on the grid-points, and the eigenvalues of ∇_h^2 approximate those for continuous case.