

MAST90026 Computational Differential Equations: Week 5

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Classification of 2nd order partial differential equations

A linear second order partial differential equation can be written as

$$Au_{xx} + Bu_{xy} + Cu_{yy} = F(x, y, u, u_x, u_y)$$

where A, B and C may be functions of x and y . Based on the local value of the coefficients the equations are classified as follows:

$$B^2 - 4AC > 0 \quad \text{Hyperbolic}$$

$$B^2 - 4AC = 0 \quad \text{Parabolic}$$

$$B^2 - 4AC < 0 \quad \text{Elliptic}$$

Example

$$-\nabla^2 u = f,$$

The Poisson equation, elliptic,

$$\nabla^2 u = u_t,$$

The diffusion equation, parabolic,

$$\nabla^2 u = u_{tt},$$

The wave equation, hyperbolic.

Elliptic equation

Consider (a subclass of) the elliptic PDEs:

$$-\nabla \cdot (D(x, y) \nabla u) = f(x, y),$$

where $D > 0$ to satisfy ellipticity.

Possible boundary conditions:

- Dirichlet BC: $u = g_D(x, y)$ on $\partial\Omega$.
- Neumann BC: $q \cdot \vec{n} = g_N(x, y)$ on $\partial\Omega$
- Robin BC: $\alpha u + \beta q \cdot \vec{n} = g_R$ on $\partial\Omega$

where $q = -D(x, y) \nabla u$.

Discretisation of domain

Questions:

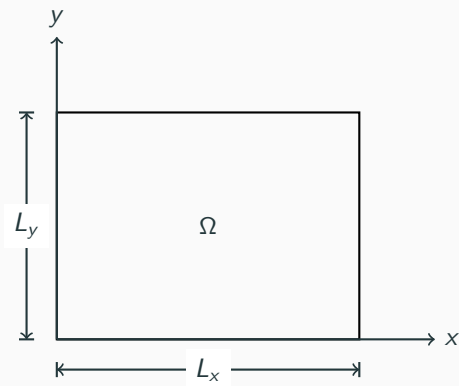
- How to handle the curved boundaries?
- How to define the mesh in 2D?

To avoid the problem, considering a rectangle aligned with the axes. In addition, we consider Poisson equation by assuming $D = 1$.

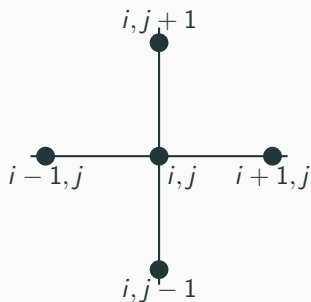
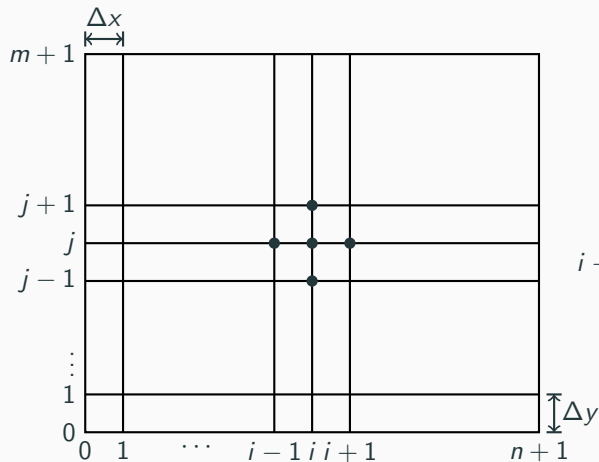
Poisson equation in 2D

$$\begin{aligned} -\nabla^2 u(x, y) &= f(x, y), & \text{in } \Omega, \\ u &= g_D, & \text{on } \partial\Omega. \end{aligned}$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$



Discretization of domain



$$\Delta x = \frac{L_x}{n+1}, \quad \Delta y = \frac{L_y}{m+1}, \quad x_i = i\Delta x, \quad y_j = j\Delta y$$

Approximation of differential operator

Use central finite difference on each direction:

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_{i,j} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}$$

$$\left. \frac{\partial^2 v}{\partial y^2} \right|_{i,j} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2}$$

Five point stencil:

$$-\nabla^2 u_{ij} \approx -\frac{1}{\Delta x^2} (u_{i-1,j} - 2u_{ij} + u_{i+1,j}) - \frac{1}{\Delta y^2} (u_{i,j-1} - 2u_{ij} + u_{i,j+1})$$

In particular, $\Delta x = \Delta y = h$:

$$-\nabla^2 u_{ij} \approx -\frac{1}{h^2} (u_{i-1,j} + u_{i,j-1} - 4u_{ij} + u_{i+1,j} + u_{i,j+1})$$

Equations

$-u_{xx} - u_{yy} = f$ suggests:

$$-\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} - \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f_{i,j}$$

$$u_{0,j} = g_D(x_0, y_j), u_{n+1,j} = g_D(x_{n+1}, y_j) \quad 1 \leq j \leq m$$

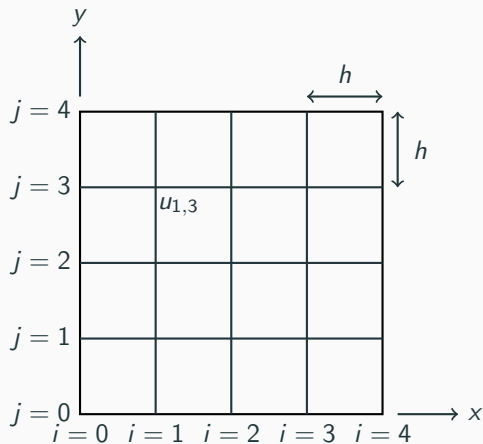
$$u_{i,0} = g_D(x_i, y_0), u_{i,m+1} = g_D(x_i, y_{m+1}) \quad 1 \leq i \leq n$$

$$\Rightarrow A\vec{u} = \vec{f}$$

Example of Poisson equation in 2D

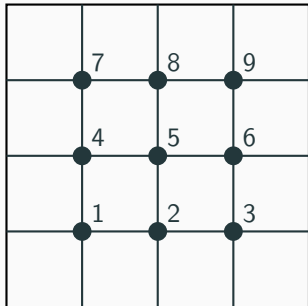
$$m = n = 3$$

$$\Delta x = \Delta y = h$$

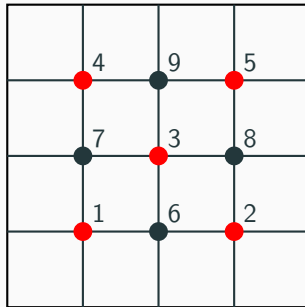


Numbering scheme

Natural rowwise ordering



Red-black ordering



Equation at internal points – natural rowwise ordering

$$\text{Eqn.1:} \quad -\frac{1}{h^2} (-4u_1 + u_2 + u_4) = f_{1,1} + \frac{u_{0,1} + u_{1,0}}{h^2}$$

$$\text{Eqn.2:} \quad -\frac{1}{h^2} (u_1 - 4u_2 + u_3 + u_5) = f_{2,1} + \frac{u_{2,0}}{h^2}$$

$$\text{Eqn.3:} \quad -\frac{1}{h^2} (u_2 - 4u_3 + u_6) = f_{3,1} + \frac{u_{3,0} + u_{4,1}}{h^2}$$

$$\text{Eqn.4:} \quad -\frac{1}{h^2} (u_1 - 4u_4 + u_5 + u_7) = f_{1,2} + \frac{u_{0,2}}{h^2}$$

$$\text{Eqn.5:} \quad -\frac{1}{h^2} (u_2 + u_4 - 4u_5 + u_6 + u_8) = f_{2,2}$$

$$\text{Eqn.6:} \quad -\frac{1}{h^2} (u_3 + u_5 - 4u_6 + u_9) = f_{3,2} + \frac{u_{4,2}}{h^2}$$

$$\text{Eqn.7:} \quad -\frac{1}{h^2} (u_4 - 4u_7 + u_8) = f_{13} + \frac{u_{0,3} + u_{1,4}}{h^2}$$

$$\text{Eqn.8:} \quad -\frac{1}{h^2} (u_5 + u_7 - 4u_8 + u_9) = f_{2,3} + \frac{u_{2,4}}{h^2}$$

$$\text{Eqn.9:} \quad -\frac{1}{h^2} (u_6 + u_8 - 4u_9) = f_{33} + \frac{u_{3,4} + u_{4,3}}{h^2}.$$

Example: matrix and vector – natural rowwise ordering

$$A = \frac{1}{h^2} \left[\begin{array}{ccc|cc|cc} 4 & -1 & & -1 & & & \\ & -1 & 4 & & -1 & & \\ & & -1 & 4 & & -1 & \\ \hline -1 & & & 4 & -1 & & -1 \\ & -1 & & -1 & 4 & -1 & \\ & & -1 & & -1 & 4 & -1 \\ \hline & & & -1 & & 4 & -1 \\ & & & & -1 & & -1 \\ & & & & & -1 & 4 \end{array} \right]$$

Assume $g_D = 0$, we have

$$f = (f_{1,1}, f_{2,1}, f_{3,1}, f_{1,2}, f_{2,2}, f_{3,2}, f_{1,3}, f_{2,3}, f_{3,3})^T$$

General finite difference method

$$-\frac{1}{\Delta y^2}u_{i,j-1}-\frac{1}{\Delta x^2}u_{i-1,j}+2\left(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}\right)u_{i,j}-\frac{1}{\Delta x^2}u_{i+1,j}-\frac{1}{\Delta y^2}u_{i,j+1}=f_{i,j}.$$

Let $\vec{u}_j = (u_{1,j}, u_{2,j}, \dots, u_{n,j})^T$ for $1 \leq j \leq m$.

Rewrite as

$$D\vec{u}_{j-1} + C\vec{u}_j + D\vec{u}_{j+1} = \vec{f}_j;$$

where

$$C = \begin{bmatrix} 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & -\frac{1}{\Delta x^2} & & & \\ -\frac{1}{\Delta x^2} & 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & -\frac{1}{\Delta x^2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{\Delta x^2} & 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & -\frac{1}{\Delta x^2} \\ & & & -\frac{1}{\Delta x^2} & 2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) \end{bmatrix}$$

General finite difference method (Continue)

$$D = \begin{bmatrix} -\frac{1}{\Delta y^2} & & & & \\ & -\frac{1}{\Delta y^2} & & & \\ & & \ddots & & \\ & & & -\frac{1}{\Delta y^2} & \\ & & & & -\frac{1}{\Delta y^2} \end{bmatrix}, \vec{f}_j = \begin{pmatrix} f_{1,j} + \frac{1}{\Delta x^2} g_D(x_0, y_j) \\ f_{2,j} \\ \vdots \\ f_{n-1,j} \\ f_{n,j} + \frac{1}{\Delta x^2} g_D(x_{n+1}, y_j) \end{pmatrix}$$

$$C, D : (n \times n)$$

Linear system

$$A\vec{u} = \begin{bmatrix} C & D & & & \\ D & C & D & & \\ & \ddots & \ddots & \ddots & \\ & & D & C & D \\ & & & D & C \end{bmatrix} \begin{pmatrix} \vec{u}_1 \\ \vec{u}_2 \\ \vdots \\ \vec{u}_{m-1} \\ \vec{u}_m \end{pmatrix} = \begin{pmatrix} \vec{f}_1 - D\vec{u}_0 \\ \vec{f}_2 \\ \vdots \\ \vec{f}_{m-1} \\ \vec{f}_m - D\vec{u}_{m+1} \end{pmatrix}.$$

A: **Block** $(m \times m)$ tridiagonal matrix.

Implementation of 2D FDM

Kronecker product: If S is a $m \times n$ matrix and T is a $p \times q$ matrix, then the Kronecker product of S and T is $mp \times nq$ given by

$$S \otimes T = \begin{pmatrix} s_{11}T & \cdots & s_{1n}T \\ \vdots & & \\ s_{m1}T & \cdots & s_{mn}T \end{pmatrix}.$$

Implementation of 2D FDM (Continue)

Using Kronecker product, we can see that

$$A = \begin{bmatrix} C & & & & \\ & C & & & \\ & & \ddots & \ddots & \ddots \\ & & & C & \\ & & & & C \end{bmatrix} + \begin{bmatrix} O & D & & & \\ D & O & D & & \\ & \ddots & \ddots & \ddots & \\ & & D & O & D \\ & & & D & O \end{bmatrix} = I_m \otimes C + E \otimes D;$$

where I_m is the $m \times m$ identities matrix and

$$E = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{bmatrix}.$$

In Matlab, you can use the function `kron(S, T)` to compute $S \otimes T$.

Truncation error

$$\begin{aligned} & - \frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j))}{\Delta x^2} \\ & - \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1}))}{\Delta y^2} = f(x_i, y_j) \\ & \underbrace{- \frac{\Delta x^2}{12} \frac{\partial^4 u}{\partial x^4}(x_i + \theta_i^x \Delta x, y_j) - \frac{\Delta y^2}{12} \frac{\partial^4 u}{\partial y^4}(x_i, y_j + \theta_j^y \Delta y)}_{\tau_{i,j}} \end{aligned}$$

For $u \in \mathcal{C}^4$, $\tau_{i,j} \sim \mathcal{O}(\Delta x^2, \Delta y^2)$ for all i, j

Convergence

Original scheme

$$A\vec{u} = \vec{f}.$$

Consistency

$$A\hat{u} = \vec{f} + \vec{\tau}.$$

Error equation

$$\mathbf{E} = -A^{-1}\vec{\tau}.$$

Taking norms

$$\begin{aligned}\|\mathbf{E}\| &= \| -A^{-1}\vec{\tau} \| \\ &\leq \|A^{-1}\| \|\vec{\tau}\| \\ &\leq \|A^{-1}\| Ch^2.\end{aligned}$$

Recap of FD Methods

Easy for simple geometry e.g. rectangles.

Convergence theory can be tricky.

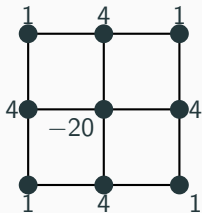
Produces large sparse matrices, even in 2D.

Curved Regions also make finite difference methods messy, but possible. See for example 'Immersed Interface Method' Ref: Li & Leveque 1994.

Nonlinear elliptic PDEs can be tackled by quasi-linearisation or by Newton's method and its variants

For easy problems ($-\nabla^2 u = f$) on a square there are special 'fast Poisson solvers' that don't generalize to the variable coefficient case, or other coordinate systems.

9-point stencil



Finite difference scheme:

$$\nabla_9^2 u_{ij} = \frac{1}{6h^2} [4u_{i-1,j} + 4u_{i+1,j} + 4u_{i,j-1} + 4u_{i,j+1} + u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 20u_{i,j}].$$

Truncation error of 9-point stencil

Compute:

$$\nabla_9^2 u(x_i, y_j) = \nabla^2 u + \underbrace{\frac{1}{12} h^2 (u_{xxxx} + 2u_{xxyy} + u_{yyyy})}_{\tau_{ij}} + O(h^4),$$

Reformulate:

$$\begin{aligned}\tau_{ij} &= \frac{1}{12} h^2 \nabla^2 (\nabla^2 u) + O(h^4) \\ &= -\frac{1}{12} h^2 \nabla^2 f + O(h^4).\end{aligned}$$

Observation: if we know f analytically, we can evaluate the first term of τ_{ij} .

Example: $f = 0$ then error is $O(h^4)$, $\nabla_9^2 u = 0 \rightarrow A_9 \vec{u} = \vec{b}$, $\tau = O(h^4)$.

4th Order method for Poisson equation

For Poisson equation:

$$-\nabla_9^2 u = f + \frac{1}{12} h^2 \nabla^2 f + O(h^4),$$

Consider different problem:

$$-\nabla_9^2 u = f + \frac{1}{12} h^2 \nabla^2 f = \tilde{f},$$

then

$$-\nabla^2 u + \frac{1}{12} h^2 \nabla^2 \tilde{f} + O(h^4) = \tilde{f},$$

therefore

$$-\nabla^2 u + \frac{1}{12} h^2 \nabla^2 f + O(h^4) = f + \frac{1}{12} h^2 \nabla^2 f,$$

so

$$-\nabla^2 u + O(h^4) = f,$$

i.e. we've solved $-\nabla^2 u = f$ to $O(h^4)$.

Unknown right hand side

If we don't know f analytically, but just at grid points. Just form

$$\begin{aligned}\tilde{f}_{i,j} &= f_{i,j} + \frac{1}{12} h^2 \nabla_5^2 f_{i,j} \\ &= f_{i,j} + \frac{1}{12} h^2 (\nabla^2 f + O(h^2)) \\ &= f_{i,j} + \frac{1}{12} h^2 \nabla^2 f_{i,j} + O(h^4),\end{aligned}$$

Method of deferred corrections

Solve $A_5 \vec{u} = \vec{f}$ which gives \vec{u} with an error $O(h^2)$. We know

$$\tau_{ij} = \frac{1}{12} h^2 (u_{xxxx} + u_{yyyy}) + O(h^4).$$

Then, since $A_5 \hat{u} - \vec{f} = \tau$ and $A_5 \vec{u} - \vec{f} = \vec{0}$,

$$A_5(\vec{u} - \hat{u}) = -\vec{\tau} \Rightarrow A_5 E = -\tau.$$

We now attempt to use \vec{u} to estimate τ . For example we can use central differences to get u_{xxxx} and u_{yyyy} to $O(h^2)$. Then we obtain

$$\hat{\tau} = \vec{\tau} + O(h^4),$$

and solve

$$A_5 E = -\hat{\tau},$$

then update

$$\tilde{\vec{u}} = \hat{\vec{u}} - E,$$

which has improved our estimate to $O(h^4)$.

End of week 5!