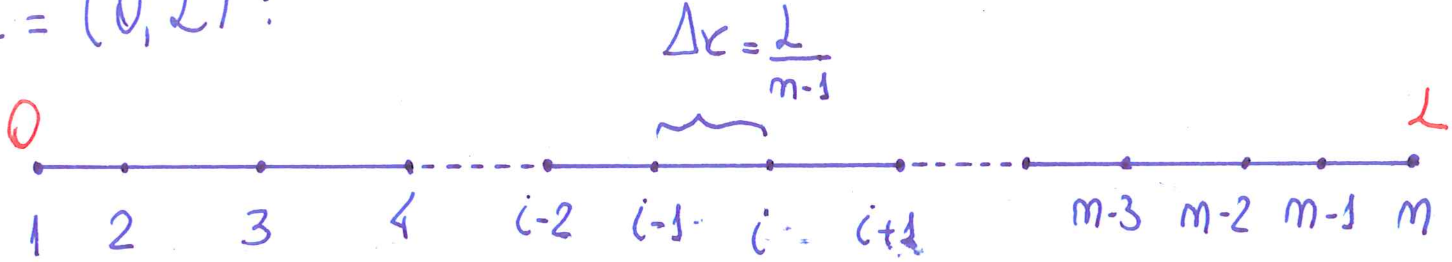
Finite Difference Methods (FDM)

↳ In FDM the derivatives of PDEs are approximated by linear combination of functions at the nodal points.

Initially, let's assume an 1D problem over a domain $\Omega = (0, L)$:



Now, in order to simplify our notation:

$$\begin{cases} \phi_i \simeq \phi(x_i), \quad i = 1, \dots, m \\ x_i = i \Delta x \end{cases} \Rightarrow \text{mesh size} : \Delta x = \frac{L}{n-1}$$

The derivative of $\phi(x)$ with respect ~~of~~ to $\underline{x}$ can be defined as

$$\frac{\partial \phi}{\partial x}(x_i) = \lim_{\Delta x \to 0} \frac{\phi(x_i + \Delta x) - \phi(x_i)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\phi(x_i) - \phi(x_i - \Delta x)}{\Delta x}$$

$$= \lim_{\Delta x \to 0} \frac{\phi(x_i + \Delta x) - \phi(x_i - \Delta x)}{2 \Delta x} \qquad (1)$$

All these above expressions are equivalent, i.e., the ~~expression~~ approximation converges to the derivative as $\Delta x \to 0$.

If Δx is sufficiently small (but finite) then,

$$\boxed{\begin{aligned} \frac{\partial \phi_i}{\partial x} &\approx \frac{\phi_{i+1} - \phi_i}{\Delta x} \quad \text{(forward diff)} \quad (2) \\ \frac{\partial \phi_i}{\partial x} &\approx \frac{\phi_i - \phi_{i-1}}{\Delta x} \quad \text{(backward diff)} \quad (3) \\ \frac{\partial \phi_i}{\partial x} &\approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} \quad \text{(central diff)} \quad (4) \end{aligned}}$$

We can analyse these approximations ~~by~~ through Taylor series expansion around the point x_i,

$$\phi(x) = \sum_{m=0}^{\infty} \frac{(x - x_i)^m}{m!} \left(\frac{\partial^m \phi}{\partial x^m} \right)_i ; \quad (5)$$

$$\phi_{i+1} = \phi_i + \Delta x \left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + \frac{(\Delta x)^3}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \dots$$
$$\dots + \frac{(\Delta x)^n}{n!}\left(\frac{\partial^n \phi}{\partial x^n}\right)_i + \underbrace{\frac{(\Delta x)^{n+1}}{(n+1)!}\left(\frac{\partial^{n+1} \phi}{\partial x^{n+1}}\right)_i (x^*)}_{(*)} \qquad (6)$$

The (*) term represents the error in the approximation if just the first n terms in the expansion is kept. Equation (6) is exact but x^* is unknown. For example, if we use Eqn. 6 with $n = 1$,

$$\frac{\phi_{i+1} - \phi_i}{\Delta x} = \left(\frac{\partial \phi}{\partial x}\right)_i + \underbrace{\frac{\Delta x}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i (x^*)}_{\text{truncation error } (\epsilon_T)} \qquad (7)$$

difference between the exact value and the numerical approximation

The order of a FD approximation is defined as (p)

constant

$$\lim_{\Delta x \to 0}\left(\frac{\epsilon_T}{\Delta x^p}\right) = \gamma \neq 0 \qquad (8)$$

This is equivalent to write:

$$\varepsilon_T = \mathcal{O}(\Delta x^p) \qquad (9)$$

In Eqn. 7, the forward difference is first-order accurate ($p=1$).

Now for backward difference, the Taylor series expansion (Eqn. 5) is:

$$\phi_{i-1} = \phi_i - \Delta x\left(\frac{\partial \phi}{\partial x}\right)_i + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i - \frac{(\Delta x)^3}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \dots \qquad (10)$$

Thus Eqns. (6) and (10) become:

forward diff

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\Delta x}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \dots \qquad (11)$$

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \dots \qquad (12)$$

backward diff

(11) + (12): central diff.

$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{(\Delta x)^2}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_i + \dots \qquad (13)$$

with:

$$\begin{cases} (11) & \mathcal{O}(\Delta x) \\ (12) & \mathcal{O}(\Delta x) \\ (13) & \mathcal{O}(\Delta x)^2 \end{cases}$$

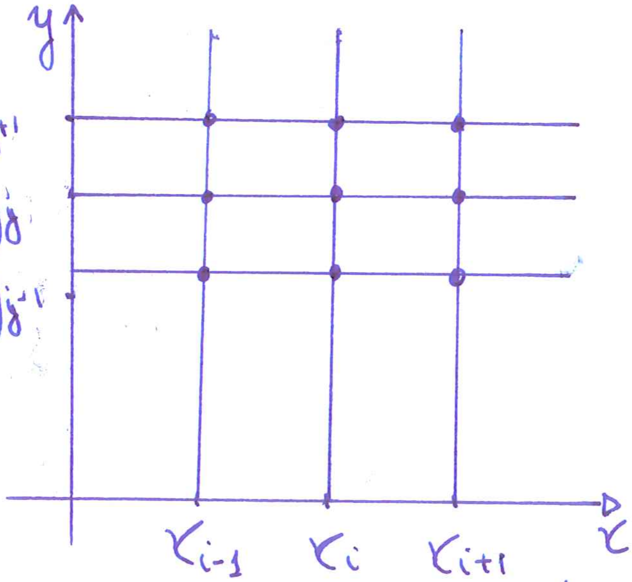
For higher-order derivatives we can generalise the previous procedure using Taylor series expansion.

Second-order derivatives can be obtained through

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i = \left[\frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial x}\right)\right]_i = \lim_{\Delta x \to 0} \frac{\left(\frac{\partial \phi}{\partial x}\right)_{i+1/2} - \left(\frac{\partial \phi}{\partial x}\right)_{i-1/2}}{\Delta x}$$

$$\approx \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2} \quad (14)$$

For 2D:



$$\frac{\partial^2 \phi}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial \phi}{\partial x}\right)$$

$$\left(\frac{\partial^2 \phi}{\partial x \partial y}\right)_{i,j} = \frac{\left(\frac{\partial \phi}{\partial y}\right)_{i+1,j} - \left(\frac{\partial \phi}{\partial y}\right)_{i-1,j}}{2\Delta x} + O(\Delta x)^2 \qquad (15)$$

$$\left(\frac{\partial \phi}{\partial y}\right)_{i+1,j} = \frac{\phi_{i+1,j+1} - \phi_{i+1,j-1}}{2\Delta y} + O(\Delta y)^2 \qquad (16)$$

$$\left(\frac{\partial \phi}{\partial y}\right)_{i-1,j} = \frac{\phi_{i-1,j+1} - \phi_{i-1,j-1}}{2\Delta y} + O(\Delta y)^2 \qquad (17)$$

Replacing (16) and (17) in (15)

$$\left(\frac{\partial^2 \phi}{\partial x \partial y}\right)_{i,j} = \frac{\phi_{i+1,j+1} - \phi_{i+1,j-1} - \phi_{i-1,j+1} + \phi_{i-1,j-1}}{4\Delta x \Delta y} + O\left[(\Delta x)^2, (\Delta y)^2\right] \qquad (18)$$

Examples

(a) 1D Poisson Elliptic PDE

$$\frac{\partial^2 \phi}{\partial x^2} = S(x) \quad \text{over } \Omega \in [0,1] \qquad (19.1)$$

If discretize the domain using $\underline{N}$ points (uniformly spaced, $\Delta x = 1/(N-1)$). $\rightarrow$ i.e., $x_i = \frac{i-1}{N-1}$

Here we can consider the solution of this PDE with two distinct boundary conditions:

(i) $\phi(0) = \alpha_1$ and $\phi(1) = \alpha_2$ (19.2)

(ii) $\phi(0) = \alpha_1$ and $\frac{\partial \phi}{\partial x}(1) = g$ (19.3)

For both cases, let's assume a central difference approximation in the interior nodes, i.e., $\hookrightarrow$ Eqn. 14

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2} + O(\Delta x)^2$$

Thus

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2} = S_i \qquad i = 2, \dots, N-1 \qquad (19.4)$$

For case (i) $\begin{cases} \phi_1 = \alpha_1 \\ \phi_N = \alpha_2 \end{cases}$ $\Rightarrow$ 2 eqns (Dirichlet BCs) + $N-2$ eqns (19.4)

N eqns & N unknowns

$\phi_{i-1} - 2\phi_i + \phi_{i+1}$

$$\begin{pmatrix} 1 & 0 & & \cdots & & & 0 \\ 1 & -2 & 1 & 0 & \cdots & & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & & \\ 0 & \cdots & 0 & 1 & -2 & 1 & 0 \\ 0 & \cdots & & 0 & 1 & -2 & 1 \\ 0 & & & \cdots & & 0 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_{N-2} \\ \phi_{N-1} \\ \phi_N \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ (\Delta x)^2 S_2 \\ (\Delta x)^2 S_3 \\ \vdots \\ (\Delta x)^2 S_{N-2} \\ (\Delta x)^2 S_{N-1} \\ \alpha_2 \end{pmatrix}$$

$\Downarrow$

$$\underline{\underline{A}}\, \underline{\phi} = \underline{S} \qquad (19.5)$$

$\underline{\underline{A}}$ is a non-singular matrix and admits a unique solution $\underline{\phi}$.

$\Rightarrow$ WELL-POSED ELLIPTIC EQN!

For case (ii) $\begin{cases} \phi_1 = \alpha_1 \\ \partial \phi_N / \partial x = g \end{cases}$ ← Dirichlet ← Neumann } BCs

The Neumann BC:

backward diff and $\mathcal{O}(\Delta x)$

$$\frac{\partial \phi_N}{\partial x} \approx \frac{\phi_N - \phi_{N-1}}{\Delta x} = g \qquad (19.6)$$

inconsistent with the second-order approx. used in $\partial^2\phi/\partial x^2$, thus

using a second-order centred difference approximation instead,

$$\frac{\partial \phi_N}{\partial x} \approx \frac{\phi_{N+1} - \phi_{N-1}}{\Delta x} = g \qquad (19.7)$$

Node $N+1$ is not readily available (outside the discretised domain), thus we should use the approximation at x_N,

$$\frac{\phi_{N+1} - 2\phi_N + \phi_{N-1}}{(\Delta x)^2} = s_N \qquad (19.8)$$

and replace ϕ_{N+1} from (19.7)

$$\frac{\phi_{N-1} + g\Delta x - 2\phi_N + \phi_{N-1}}{(\Delta x)^2} = s_N \qquad (19.9)$$

Now rearranging (19.9)

$$\phi_N - \phi_{N-1} = \underbrace{\frac{1}{2}\left[g\,\Delta x - S_N(\Delta x)^2\right]}_{h(x)} \qquad (19.10)$$

Thus the system of linear equations : (19.4) + (19.10) + BC1 ($\phi_1 = \alpha_1$)

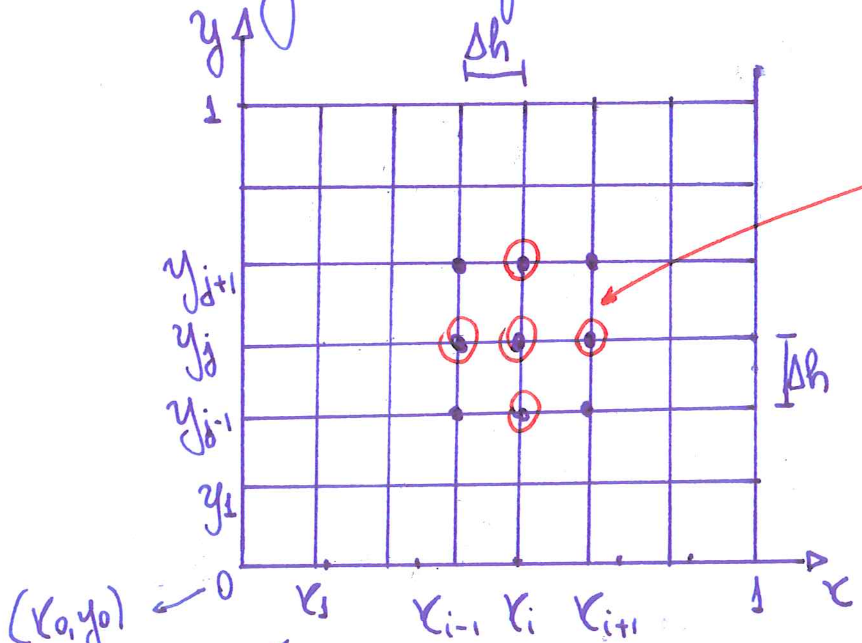
$$\begin{pmatrix} 1 & 0 & \cdots & & & & & 0 \\ 1 & -2 & 1 & 0 & \cdots & & & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & & 0 \\ & \ddots & & & & & & \\ 0 & & \cdots & 0 & 1 & -2 & 1 & 0 \\ 0 & & \cdots & & 0 & 1 & -2 & 1 \\ 0 & & \cdots & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_{N-2} \\ \phi_{N-1} \\ \phi_N \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ (\Delta x)^2 S_2 \\ (\Delta x)^2 S_3 \\ \vdots \\ (\Delta x)^2 S_{N-2} \\ (\Delta x)^2 S_{N-1} \\ h(x) \end{pmatrix}$$

(19.11)

(b) 2D Poisson PDE

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial x^2} + \dfrac{\partial^2 \phi}{\partial y^2} = S(x,y) & \text{over } \Omega = [0,1]\times[0,1] \\ \phi = 0 & \text{on } \Gamma = \partial\Omega \end{cases} \quad (20.1)$$

Assuming a uniform mesh $\Delta x = \Delta y = \Delta h$



$N = 1/\Delta h$

$i, j = 0, 1, \ldots, N$

The central-difference approximation (Eqns. 15-17 see) leads to: $(O(\Delta h)^2)$

$$\begin{cases} \dfrac{\phi_{i-1,j} + \phi_{i,j-1} - 4\phi_{i,j} + \phi_{i+1,j} + \phi_{i,j+1}}{(\Delta h)^2} = S_{i,j} & \forall i,j = 1,\ldots,N-1 \\ \phi_{i,0} = \phi_{i,N} = \phi_{0,j} = \phi_{N,j} = 0 & \forall i,j = 0,1,\ldots,N \end{cases} \quad (20.2)$$

In matricial form with,

$$\underset{\sim}{\phi} = \left(\phi_{1,1}\ \phi_{2,1} \dots \phi_{N-1,1}\ \phi_{1,2} \dots \phi_{N-1,2}\ \phi_{1,3} \dots \phi_{N-1,N-1}\right)^T$$

$$\underset{\sim}{S} = \left(S_{1,1}\ S_{2,1} \dots S_{N-1,1}\ S_{1,2} \dots S_{N-1,2}\ S_{1,3} \dots S_{N-1,N-1}\right)^T \times (\Delta h)^2$$

$$\underline{\underline{A}} = \begin{pmatrix} -4 & 1 & 0 & \dots & & & 0 \\ 1 & -4 & 1 & \dots & & & 0 \\ & & & \ddots & & & \\ & & & & 1 & -4 & 1 \\ 0 & \dots & & & & & \\ 0 & \dots & & & & 1 & -4 \end{pmatrix} \qquad (20.3)$$

$$\boxed{\underline{\underline{A}}\,\underset{\sim}{\phi} = \underset{\sim}{S}}$$