2.1 Finite Difference Formulas via Taylor Series

1D Taylor Expansion

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2!}h^2 f''(x) + \dots + \frac{h^n}{n!} f^{(n)}(x) + \frac{h^{n+1}}{(n+1)!} f^{(n+1)}(c)$$

for some c between x and $x+h$

2D Taylor Expansion (e.g. Thomas Calc., p. 1041)

$$f(x+h, y+k) = f(x,y) + \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right) f \Big|_{(x,y)}$$

$$+ \frac{1}{2!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^2 f \Big|_{(x,y)}$$

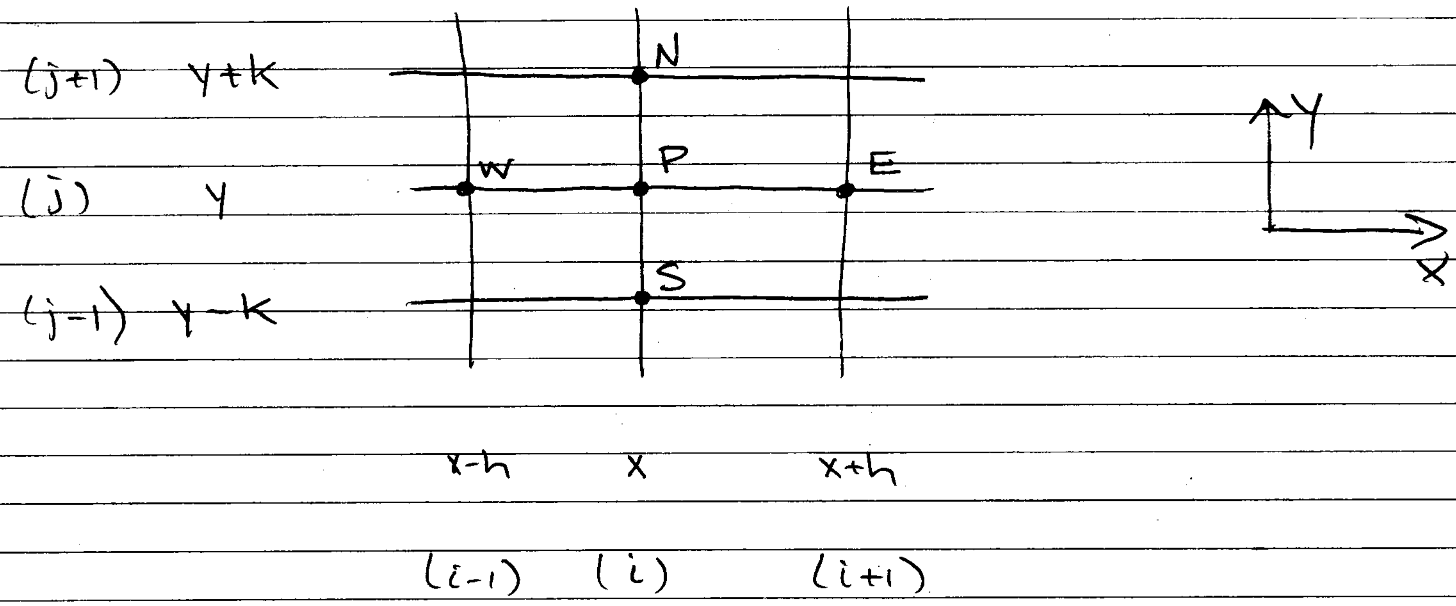
$$+ \frac{1}{3!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^3 f \Big|_{(x,y)} + \dots$$

$$+ \frac{1}{n!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^n f \Big|_{(x,y)} +$$

$$\frac{1}{(n+1)!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^{n+1} f \Big|_{(x+ch,\, y+ck)}$$

[last term evaluated on line segment between (x,y) and $(x+h, y+k)$]

Consider the rectangular grid in 2D...



Identify

$$\phi(x,y) = \phi_P = \phi_{i,j}$$

$$\phi(x+h,y) = \phi_E = \phi_{i+1,j}$$

$$\phi(x-h,y) = \phi_W = \phi_{i-1,j}$$

$$\phi(x,y+k) = \phi_N = \phi_{i,j+1}$$

$$\phi(x,y-k) = \phi_S = \phi_{i,j-1}$$

We shall identify derivative formulas for $\frac{\partial\phi}{\partial x}, \frac{\partial^2\phi}{\partial x^2}, \frac{\partial^2\phi}{\partial x\partial y}, \ldots$ at point P (i,j) in terms of function values at neighboring points $\phi_E, \phi_W, \phi_N, \phi_S$, and ϕ_P.

1D Cases (focus only on East/West direction – x-dependence only)

W P E

$$\boxed{\frac{d\phi}{dx}}$$

Note

$$\phi_E = \phi(x+h) = \phi(x) + h\phi'(x) + \frac{1}{2!}h^2\phi''(x) + \frac{1}{3!}h^3\phi'''(x) + \frac{1}{4!}h^4\phi^{(iv)}(x) + \ldots$$

and

$$\phi_W = \phi(x-h) = \phi(x) - h\phi'(x) + \frac{1}{2!}h^2\phi''(x) - \frac{1}{3!}h^3\phi'''(x) + \frac{1}{4!}h^4\phi^{(iv)}(x) + \ldots$$

subtracting those

$$\phi(x+h) - \phi(x-h) = 2h\phi'(x) + \frac{2}{3!}h^3\phi'''(x) + O(h^5)$$

Solving for $\phi'(x)$

$$\phi'(x) = \frac{\phi(x+h) - \phi(x-h)}{2h} - \underbrace{\frac{h^2}{3!}\phi'''(x) + \ldots}_{\text{error} \sim h^2\ [\text{second order}]}$$

The formula

$$\boxed{\left(\frac{d\phi}{dx}\right)_P = \frac{\phi_E - \phi_W}{2h}}$$

is called a second order accurate central difference formula for $\frac{d\phi}{dx}$ at $x = x_j$

Note:

$$\left(\frac{d\phi}{dx}\right)_P = \frac{\phi_E - \phi_P}{h} \qquad \underline{\text{Error}}\ \left(-\frac{1}{2} h \phi''(x)\right) \qquad \left[\text{see Exercise 2.1}\right]$$

and

$$\left(\frac{d\phi}{dx}\right)_P = \frac{\phi_P - \phi_W}{h} \qquad \left(+\frac{1}{2} h \phi''(x)\right)$$

are both first order accurate one-sided difference formulas for $\frac{d\phi}{dx}$

$$\boxed{\frac{d^2\phi}{dx^2}}$$

Add formulas for ϕ_E and ϕ_W

$$\phi_E + \phi_W = 2\phi_P + \frac{2}{2!} h^2 \phi''(x) + \frac{2}{4!} h^4 \phi^{iv}(x) + \ldots$$

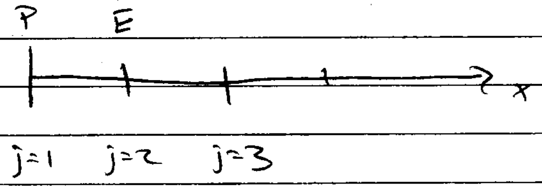
so
$$\phi''(x) = \left(\frac{d^2\phi}{dx^2}\right)_P = \frac{\phi_E - 2\phi_P + \phi_W}{h^2} + O(h^2)$$

so
$$\boxed{\left(\frac{d^2\phi}{dx^2}\right)_P = \frac{\phi_E - 2\phi_P + \phi_W}{h^2}}$$

is a second order accurate central difference formula for $\frac{d^2\phi}{dx^2}$ at $x = x_j$

$\boxed{\dfrac{d\phi}{dx} \text{ at boundaries}}$

<u>left boundary</u>



- to approximate $\frac{d\phi}{dx}$ at $x = x_1$ $(j=1)$ we could use the first order accurate

$$\left(\frac{d\phi}{dx}\right)_P = \frac{\phi_E - \phi_P}{h}$$

- to get a higher order accurate approximation we can use information at $j=3$

$$\begin{cases} \phi(x+h) = \phi(x) + h\phi'(x) + \frac{1}{2!}h^2\phi''(x) + \frac{1}{3!}h^3\phi'''(x) + \dots \\ \phi(x+2h) = \phi(x) + 2h\,\phi'(x) + \frac{1}{2!}4h^2\phi''(x) + \frac{8}{3!}h^3\phi'''(x) + \end{cases}$$

combine these so that the $h^2\phi''$ terms drop out...

$$4\phi(x+h) - \phi(x+2h) = 3\phi(x) + 2h\,\phi'(x) + O(h^3)$$

$$\phi'(x) = \frac{-3\phi(x) + 4\phi(x+h) - \phi(x+2h)}{2h} + O(h^2)$$

So

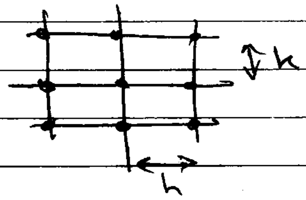
$$\boxed{\left(\frac{d\phi}{dx}\right)_{j=1} = \frac{-3\phi_1 + 4\phi_2 - \phi_3}{2h}}$$

2nd order accurate one-sided difference formula.

back to 2D

- $$\boxed{\frac{\partial^2 \phi}{\partial x \partial y}} = \frac{\partial}{\partial x}\left[\frac{\partial \phi}{\partial y}\right]$$ expand first in y and then x (or vice verse)

$$\frac{\partial}{\partial x}\left[\frac{\phi_{i,j+1} - \phi_{i,j-1}}{2k}\right] + O(k^2)$$



$$= \frac{\left(\frac{\phi_{i+1,j+1} - \phi_{i+1,j-1}}{2k}\right) - \left(\frac{\phi_{i-1,j+1} - \phi_{i-1,j-1}}{2k}\right)}{2h} + O(h^2, k^2)$$

$$\boxed{\begin{aligned} \frac{\partial^2 \phi}{\partial x \partial y} &= \frac{1}{4kh}\left[\phi_{i+1,j+1} - \phi_{i+1,j-1} - \phi_{i-1,j+1} + \phi_{i-1,j-1}\right] \\ &= \frac{1}{4kh}\left[\phi_{NE} - \phi_{SE} - \phi_{NW} + \phi_{SW}\right] \end{aligned}}$$

Error term: $-\frac{1}{hk}\left(\frac{hk^3}{3!}\frac{\partial^4 \phi}{\partial x^3 \partial y} + \frac{kh^3}{3!}\frac{\partial^4 \phi}{\partial x \partial y^3}\right)$

by combining terms from Taylor Expansion.

(see Exercise 2.4)

2.2 Parabolic Equations

Consider

$$\begin{cases} \dfrac{\partial \phi}{\partial t} = \dfrac{\partial^2 \phi}{\partial x^2} & \text{(1D Heat Eq.)} \\ \phi = 0 \quad \text{at } x = 0, 1 & \forall t \in [0, \infty \\ \phi = f(x) \quad \text{at } t = 0 & \forall x \in [0, 1] \end{cases}$$

exact sol.

$$\boxed{\phi = \sum_{n=1}^{\infty} a_n e^{-n^2\pi^2 t} \sin(n\pi x)}$$

satisfies PDE and b.c. $\phi = 0$ at $x = 0, 1$

require

$$f(x) = \sum_{n=1}^{\infty} a_n \sin(n\pi x)$$

$$\int_0^1 f(x) \sin m\pi x \, dx = \sum_{n=1}^{\infty} a_n \int_0^1 \sin m\pi x \sin n\pi x \, dx$$

$y = \pi x$

$$= \sum_{n=1}^{\infty} a_n \left[\frac{1}{\pi} \int_0^{\pi} \sin my \sin ny \, dy \right]$$

$$= \sum_{n=1}^{\infty} a_n \left[\frac{1}{\pi} \begin{cases} 0 & m \neq n \\ \frac{\pi}{2} & m = n \end{cases} \right]$$

$$= \frac{1}{2} a_m$$

so $$\boxed{a_n = \int_0^1 f(x) \sin n\pi x \, dx}$$

How can we solve this problem numerically?

- Discretize (in time and space!)

  Here we'll make use of our knowledge of methods for ODEs (IVPs + BVPs!).

Method of Lines

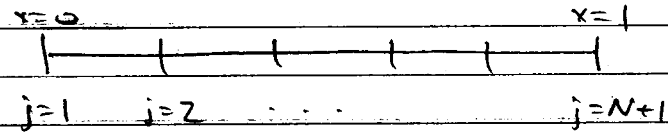
Consider the PDE

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} \qquad \begin{array}{l} \phi = 0 \text{ at } x = 0, 1 \\ \phi = f \text{ at } t = 0 \end{array}$$

The Method of Lines aims to convert this PDE into a system of ODEs in time (integrated along lines in time).

First, discretize the spatial derivative

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_{x=x_j} = \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}$$



Then

$$\left(\frac{\partial \phi}{\partial t}\right)_{x=x_j} = \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}$$

or

$$* \left\{ \begin{array}{ll} \dfrac{d}{dt}(\phi_j) = \dfrac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2} & j = 2, \ldots, N \\ \phi_1 = 0, \quad \phi_{N+1} = 0 & \end{array} \right.$$

depends on parameter h.

where we think of $\Phi_j = \Phi_j(t;h)$ and treat (*) as simply a system of ODEs (actually IVP given $\Phi_j = f(x_j)$ at $t=0$).

As we have seen, there are many tools available for us to solve IVPs — we shall make use of these here. Specifically, we'll examine both explicit (e.g. Euler, RK, ...) and implicit (Backward Euler, Crank-Nicolson, ...) schemes.

section 2.7

We shall address:

1. Error (section 2.3)
2. Consistency (section 2.4)
3. Convergence (section 2.5)
4. Stability (section 2.6)

next time...

For now we'll examine the mechanics of solving these problems...

Euler's Method

$$\frac{\phi_j^{i+1} - \phi_j^i}{k} = \frac{\phi_{j+1}^i - 2\phi_j^i + \phi_{j-1}^i}{h^2} \qquad \begin{array}{l} i = 1, 2, \dots \\ j = 2, \dots, N \end{array}$$

So
$$\boxed{\phi_j^{i+1} = \phi_j^i + \frac{k}{h^2}\left(\phi_{j+1}^i - 2\phi_j^i + \phi_{j-1}^i\right)}$$

(j index $\Rightarrow$ space i index $\Rightarrow$ time)

$$\left.\begin{array}{ll} \phi_1^i = 0 & \text{for all } i \\ \phi_{N+1}^i = 0 & \text{for all } i \end{array}\right\} \text{b.c.}$$

$$\left.\phi_j^1 = f(x_j) \quad \text{for all } j \right\} \text{i.c.}$$

Comments:

- This method is explicit — the solution at a new time value can be obtained directly from this formula for all points x_j at the old time
- There is a time step restriction on k for numerical stability (k must be sufficiently small).

  [MORE on this later...]

In matrix form this method is

$$\begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \\ \phi_N \end{bmatrix}^{i+1} = \underbrace{\begin{bmatrix} 1-2r & r & & 0 \\ r & 1-2r & r & \\ & r & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}}_{A = I + rT_{N-1}} \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \\ \phi_N \end{bmatrix}^{i}$$

where $r \equiv \dfrac{k}{h^2}$

so the solution can be updated by multiplication by matrix A.

$$T_{N-1} = \begin{bmatrix} -2 & 1 & & 0 \\ 1 & -2 & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}$$

Backward Euler

$$\frac{\phi_j^{i+1} - \phi_j^{i}}{k} = \frac{\phi_{j+1}^{i+1} - 2\phi_j^{i+1} + \phi_{j-1}^{i+1}}{h^2} \qquad \begin{array}{l} i = 1, 2, \ldots \\ j = 2, \ldots, N \end{array}$$

$$\boxed{\phi_j^{i+1} = \phi_j^{i} + \frac{k}{h^2}\left(\phi_{j+1}^{i+1} - 2\phi_j^{i+1} + \phi_{j-1}^{i+1} \right)}$$

+ b.c. and i.c.

In Matrix form

$$\underbrace{\begin{bmatrix} 1+2r & -r & & & 0 \\ -r & 1+2r & -r & & \\ & -r & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ 0 & & & \ddots & \ddots \end{bmatrix}}_{B = I - rT_{N-1}} \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \vdots \\ \phi_N \end{bmatrix}^{i+1} = \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \vdots \\ \phi_N \end{bmatrix}^{i}$$

here we need to solve a linear system to update the solution in time.

Comments:

- This method is implicit
- No stability time step restriction (Ascher + Petzold, p161)

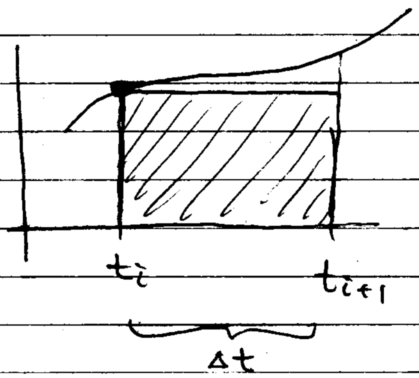
... back to ODE methods for $y' = f(t,y)$

rewrite this as

$$y_{i+1} = y_i + \int_{t_i}^{t_{i+1}} f(t,y)\,dt$$

and obtain approximation schemes by quadrature

Forward Euler



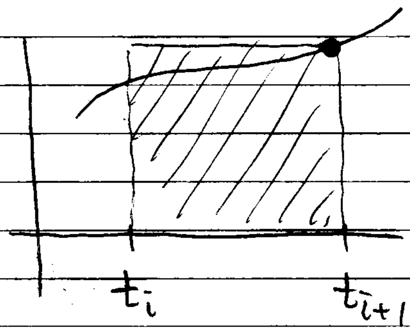
$$\int_{t_i}^{t_{i+1}} f(t,y)\,dt \approx \Delta t \cdot f(t_i, y_i)$$

so

$$\boxed{y_{i+1} = y_i + \Delta t\, f(t_i, y_i)}$$

first order accurate explicit

Backward Euler



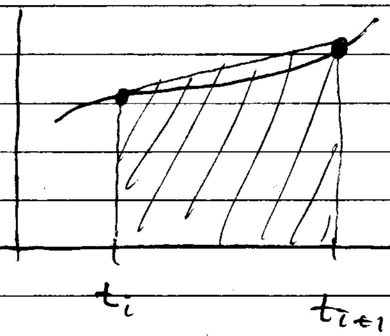
$$\int_{t_i}^{t_{i+1}} f(t,y)\,dt \approx \Delta t \cdot f(t_{i+1}, y_{i+1})$$

so

$$\boxed{y_{i+1} = y_i + \Delta t\, f(t_{i+1}, y_{i+1})}$$

first order accurate implicit

Trapezoid Rule



$$\int_{t_i}^{t_{i+1}} f(t,y)\,dt \approx \frac{\Delta t}{2}\left[f(t_i, y_i) + f(t_{i+1}, y_{i+1})\right]$$

so

$$\boxed{y_{i+1} = y_i + \frac{\Delta t}{2}\left[f(t_i, y_i) + f(t_{i+1}, y_{i+1})\right]}$$

second order accurate implicit

2.7 Crank-Nicolson

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} \qquad \begin{array}{l} \phi = 0 \text{ at } x = 0, 1 \\ \phi = f \text{ at } t = 0 \end{array}$$

$$\boxed{\frac{\phi_j^{i+1} - \phi_j^i}{k} = \frac{1}{2h^2}\left[\left(\phi_{j+1}^i - 2\phi_j^i + \phi_{j-1}^i\right) + \left(\phi_{j+1}^{i+1} - 2\phi_j^{i+1} + \phi_{j-1}^{i+1}\right)\right]}$$

+ b.c. and i.c. $\qquad r = \frac{k}{h^2}$

In matrix form

$$\underbrace{\begin{bmatrix} 2+2r & -r & & 0 \\ -r & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}}_{2I - rT_{N-1}} \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \phi_N \end{bmatrix}^{i+1} = \underbrace{\begin{bmatrix} 2-2r & r & & 0 \\ r & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}}_{2I + rT_{N-1}} \begin{bmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \phi_N \end{bmatrix}^{i}$$

where $\qquad T_{N-1} = \begin{bmatrix} -2 & 1 & & 0 \\ 1 & -2 & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}$