Formulas for finite differences

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1 Basics

Taylor series

$$u(x+h) = u(x) + \frac{h}{1!}\frac{\partial u}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{h^3}{3!}\frac{\partial^3 u}{\partial x^3} + \dots$$

2 One dimension

Forward difference

$$u(x+h) = u(x) + \frac{h}{1!}\frac{\partial u}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 u}{\partial x^2} + + \frac{h^3}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^4\big)$$

We divide by h:

$$\frac{u(x+h)}{h} = \frac{u(x)}{h} + \frac{\partial u}{\partial x} + \frac{h}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big)$$

Rearange:

$$\frac{\partial u}{\partial x} = \frac{u(x+h) - u(x)}{h} - \frac{h}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big) \tag{1}$$

Finally:

$$\frac{\partial u}{\partial x} = \frac{u(x+h) - u(x)}{h} + \mathcal{O}(h)$$

Backward difference

$$u(x-h) = u(x) - \frac{h}{1!}\frac{\partial u}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{h^3}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^4\big)$$

We divide by h:

$$\frac{u(x-h)}{h} = \frac{u(x)}{h} - \frac{\partial u}{\partial x} + \frac{h}{2!}\frac{\partial^2 u}{\partial x^2} + - \frac{h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big)$$

Rearange:

$$\frac{\partial u}{\partial x} = \frac{u(x) - u(x-h)}{h} + \frac{h}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big) \tag{2}$$

Finally:

$$\frac{\partial u}{\partial x} = \frac{u(x) - u(x-h)}{h} + \mathcal{O}(h)$$

Central difference Take a sum of forward and backward, Equation 1 and Equation 5:

$$2\frac{\partial u}{\partial x} = \frac{u(x+h) - u(x-h)}{h} - \frac{2h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big) \tag{3}$$

Divide by two:

$$\frac{\partial u}{\partial x} = \frac{u(x+h) - u(x-h)}{2h} - \frac{1h^2}{3!}\frac{\partial^3 u}{\partial x^3} + \mathcal{O}\big(h^3\big) \tag{4}$$

Finally:

$$\frac{\partial u}{\partial x} = \frac{u(x+h) - u(x-h)}{2h} + \mathcal{O}\big(h^2\big) \tag{5}$$

Central difference of second derivative It is not exactly central difference of a central difference. That would have a wide stencil. Bad. Instead try writing at halfs.

$$u''(x) = \frac{u'(x+h/2) - u'(x-h/2)}{h}$$

$$u'(x \pm h) = \frac{u(x \pm h/2 + h/2) - u(x \pm h/2 - h/2)}{h}$$

Pluging in...

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

3 Solving systems of equations

Gauss seidel formula From Wikipedia. We have

$$A = \underbrace{\begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}}_{L_*} + \underbrace{\begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}}_{U}.$$

We do:

$$A\mathbf{x} = \mathbf{b} \tag{6}$$
$$(L_* + U)\mathbf{x} = \mathbf{b} \tag{7}$$
$$L_*\mathbf{x} + U\mathbf{x} = \mathbf{b} \tag{8}$$
$$L_*\mathbf{x} = \mathbf{b} - U\mathbf{x} \tag{9}$$

The Gauss–Seidel method now solves the left hand side of this expression for $\mathbf{x}$, using previous value for $\mathbf{x}$ on the right hand side. Analytically, this may be written as:

$$\mathbf{x}^{(k+1)} = L_*^{-1}\left(\mathbf{b} - U\mathbf{x}^{(k)}\right).$$

However, by taking advantage of the triangular form of L_*, the elements of $\mathbf{x}^{(k+1)}$ can be computed sequentially for each row i using forward substitution:

$$x_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k)}\right), \quad i = 1, 2, \dots, n$$

4 COSI/U4

4.1 Instationary diffusion

Forward Euler scheme It is an explicit scheme in time (from Taylor expansion):

$$u(t^{n+1}, x) = u(t^n, x) + \Delta t f(t^n, x, u(t^n, x))$$

Implicit Euler

$$u(t^{n+1}, x) = u(t^n, x) + \Delta t f\left(t^{n+1}, x, u(t^{n+1}, x)\right)$$

Heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} = \frac{\lambda}{\rho c_p}\frac{\partial^2 T}{\partial x^2}$$

Discretised form

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}$$

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2}\left[T_{i+1}^n - 2T_i^n + T_{i-1}^n\right]$$

$$T_i^{n+1} = \left(1 - \frac{2\alpha\Delta t}{(\Delta x)^2}\right)T_i^n + \frac{\alpha\Delta t}{(\Delta x)^2}\left[T_{i+1}^n + T_{i-1}^n\right]$$

4.2 Von Neumann stability analysis

The von Neumann method is based on the decomposition of the errors into Fourier series. To illustrate the procedure, consider the one-dimensional heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

defined on the spatial interval L, which can be discretized in this case, using the FTCS discretization scheme as

$$u_j^{n+1} = u_j^n + r\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right), \quad r = \frac{\alpha\,\Delta t}{(\Delta x)^2}$$

and the solution u_j^n of the discrete equation approximates the analytical solution $u(x,t)$ of the PDE on the grid.

Define the round-off error ϵ_j^n as

$$\epsilon_j^n = N_j^n - u_j^n$$

where u_j^n is the solution of the discretized equation that would be computed in the absence of round-off error, and N_j^n is the numerical solution. The error satisfies the solution since the exact solution does that as well.

$$\epsilon_j^{n+1} = \epsilon_j^n + r\left(\epsilon_{j+1}^n - 2\epsilon_j^n + \epsilon_{j-1}^n\right)$$

Both solution and error have the same behaviour with respect to time. We assume periodic conditions. Equation is linear, so we can say:

$$\epsilon(x,t) = \sum_{m=-M}^{M} e_m = \sum_{m=-M}^{M} E_m(t) e^{ik_m x}$$

The wavenumber is defined as

$$k_m = \frac{\pi m}{L}, \quad m = -M, \ldots, -1, 0, 1, \cdots M, \quad M = \frac{L}{\Delta X}$$

The amplitude E_m is the function of time. We can only consider one of the error frequencies:

$$\epsilon_j^n = E_m(t) e^{ik_m x} \tag{10}$$

$$\epsilon_j^{n+1} = E_m(t+\Delta t) e^{ik_m x} \tag{11}$$

$$\epsilon_{j+1}^n = E_m(t) e^{ik_m (x+\Delta x)} \tag{12}$$

$$\epsilon_{j-1}^n = E_m(t) e^{ik_m (x-\Delta x)}, \tag{13}$$

Inserting into the equations (I divided by $E_m(t)$ for the sake of space):

$$\frac{E_m(t+\Delta t) e^{ik_m x}}{E_m(t)} = e^{ik_m x} + r\left(e^{ik_m(x+\Delta x)} - 2e^{ik_m x} + e^{ik_m(x-\Delta x)}\right)$$

Now dividing by the $e^{ik_m x}$

$$\frac{E_m(t+\Delta t)}{E_m(t)} = 1 + r\left(e^{ik_m \Delta x} - 2 + e^{-ik_m \Delta x}\right)$$

If we set $\phi = k_m \Delta x$, note that $e^{i\phi} = i\sin(\phi) + \cos(\phi)$ and remember that sin is antysymmetric and cos is symmetric

$$\frac{E_m(t+\Delta t)}{E_m(t)} = 1 + r\left(i\sin(\phi) + \cos\phi - 2 - i\sin\phi + \cos\phi\right)$$

$$G = \frac{E_m(t+\Delta t)}{E_m(t)} = 1 - 2r\left(\cos\phi - 1\right) = 1 + 4r\sin^2\frac{\phi}{2}$$

We have also used the property of $2\sin^2(\phi/2) = 1 - \cos\phi$. The condition for stability is $|G| \neq 1$.

$$\left|1 - 4r\sin^2(\theta/2)\right| \leq 1$$

The $\sin^2$ is always positive.

$$4r\sin^2(\theta/2) \leq 2$$