Finite differences in 2D and 3D problems. Heat equation. Laplace equation.

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Heat equation

The most general form of the heat equation in 3D is as follows:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) + Q, \qquad (1)$$

where
$T(x, y, z, t)$ - temperature
ρ - density
c_p - heat capacity
k_x, k_y, and k_z - thermal conductivities in x, y, and z direction
$Q(x, y, z, t)$ - heat production function (volumetric heat flux)

In general, quantities ρ, c_p, k_x, k_y, and k_z could be functions of both x, y, z and t (or T)

Heat equation

However, within if the expected spatial/temporal temperature variations are not too huge, ρ, c_p, k_x, k_y, and k_z can be considered constant. Also, for most materials the thermal conductivity is isotropic, i.e. $k_x = k_y = k_z$. Finally, if no heat is supplied to the system other than through heat exchange with the environment then $Q = 0$. With that the heat equation gets simplified to the following form:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T, \tag{2}$$

where constant α is called thermal diffusivity.

Heat equation

When boundary conditions are constant (i.e. do not change with time) temperature distribution T do not change with time ($\frac{\partial T}{\partial t} = 0$) after initial equilibration. Hence we deal with a stationary problem

$$\nabla^2 T = 0, \tag{3}$$

The above equation is called the Laplace equation.

Finite difference discretization in 2D

For simplicity, let us consider the 2D case. To approximate the Laplacian operator, we can use finite-differences. For example, The simplest three-point approximations for second derivatives give:

$$f''_{xx}(x,y) = \frac{f(x-h,y) - 2f(x,y) + f(x+h,y)}{h^2},$$

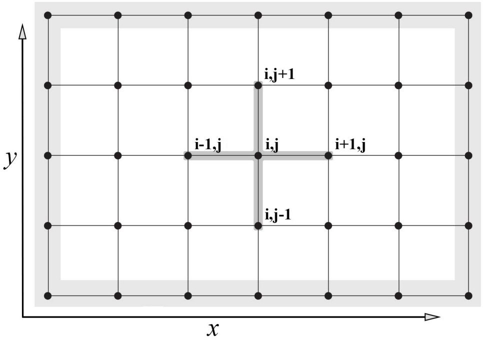
$$f''_{yy}(x,y) = \frac{f(x,y-h) - 2f(x,y) + f(x,y+)}{h^2},$$

and

$$\nabla^2 f(x,y) = \frac{f(x-h,y) + f(x,y-h) - 4f(x,y) + f(x+h,y) + f(x,y+h)}{h^2}. \tag{4}$$

Laplace operator in 2D

When we look at the 2D grid representing function $f(x, y)$, we can see a 5-point stencil



$$\nabla^2 f_{i,j} = \frac{f_{i-1,j} + f_{i,j-1} - 4f_{i,j} + f_{i+1,j} + f_{i,j+1}}{h^2}. \tag{5}$$

Solution in 2D

Expression (5) gives us $N = N_x \times N_y$ (N is the toal number of grid points) homogenious linear equations. When we incorporate boundary conditions, it yields a system of $N - N_b$ inhomogenious equations with a sparce matrix, where N_b is the number of points where the boundary conditions are given. We can solve these equations directly (e.g. with the help of LAPACK) and obtain the solution of the Laplace equation.

Iterative scheme in 2D

Alternatively, we could employ an iterative approach to solving the Laplace equation on a grid. If $\nabla^2 f = 0$ then each point on the grid must satisfy the condition

$$f_{i-1,j} + f_{i,j-1} - 4f_{i,j} + f_{i+1,j} + f_{i,j+1} = 0, \tag{6}$$

or

$$f_{i,j} = \frac{1}{4}\left(f_{i-1,j} + f_{i,j-1} + f_{i+1,j} + f_{i,j+1}\right). \tag{7}$$

This suggests that if we do iterations in the form (p is the iteration number)

$$f_{i,j}^{(p+1)} = \frac{1}{4}\left(f_{i-1,j}^{(p)} + f_{i,j-1}^{(p)} + f_{i+1,j}^{(p)} + f_{i,j+1}^{(p)}\right), \tag{8}$$

which in this particular case amounts to representing f as an average of its closest 4 neighbours, then after some time we will converge/approach to the exact solution.

Iterative scheme in 3D

In 3D case this becomes

$$f_{i,j,k}^{(p+1)} = \frac{1}{6}\left(f_{i-1,j,k}^{(p)} + f_{i,j-1,k}^{(p)} + f_{i,j,k-1}^{(p)} + f_{i+1,j,k}^{(p)} + f_{i,j+1,k}^{(p)} f_{i,j,k+1}^{(p)}\right). \tag{9}$$

It is important that we do not change grid points that represent boundary conditions (e.g. the exterior points if the boundary conditions are defined on the exterior surface of the numerical grid)