

Lecture 8: Solving the Heat, Laplace and Wave equations using finite difference methods

(Compiled 3 March 2014)

In this lecture we introduce the finite difference method that is widely used for approximating PDEs using the computer. We use the definition of the derivative and Taylor series to derive finite difference approximations to the first and second derivatives of a function. We then use these finite difference quotients to approximate the derivatives in the heat equation and to derive a finite difference approximation to the heat equation. Similarly, the technique is applied to the wave equation and Laplace's Equation. The technique is illustrated using an EXCEL spreadsheets.

Key Concepts: Finite Difference Approximations to derivatives, The Finite Difference Method, The Heat Equation, The Wave Equation, Laplace's Equation.

8 Finite Difference Methods

8.1 Approximating the Derivatives of a Function by Finite Differences

Recall that the derivative of a function was defined by taking the limit of a difference quotient:

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}. \quad (8.1)$$

Now to use the computer to solve differential equations we go in the opposite direction - we replace derivatives by appropriate difference quotients. If we assume that the function can be differentiated many times then Taylor's Theorem is a very useful device in determining the appropriate difference quotient to use. For example consider

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \frac{\Delta x^3}{3!} f^{(3)}(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) + \dots \quad (8.2)$$

Re-arranging terms in (2) and dividing by Δx we obtain

$$\frac{f(x + \Delta x) - f(x)}{\Delta x} = f'(x) + \frac{\Delta x}{2} f''(x) + \frac{\Delta x^2}{3!} f^{(3)}(x) + \dots$$

If we take the limit $\Delta x \rightarrow 0$ then we recover (1). But for our purposes it is more useful to retain the approximation

$$\begin{aligned} \frac{f(x + \Delta x) - f(x)}{\Delta x} &= f'(x) + \frac{\Delta x}{2} f''(\xi) \\ &= f'(x) + O(\Delta x). \end{aligned} \quad (8.3)$$

We retain the term $\frac{\Delta x}{2} f''(\xi)$ in (3) as a measure of the error involved when we approximate $f'(x)$ by the difference quotient $(f(x + \Delta x) - f(x))/\Delta x$. Notice that this error depends on how large f'' is in the interval $[x, x + \Delta x]$ (i.e. on the smoothness of f) and on the size of Δx . Since we like to focus on that part of the error we can control we say that the error term is of the order Δx - denoted by $O(\Delta x)$. Technically a term or function $E(\Delta x)$ is $O(\Delta x)$ if

$$\frac{E(\Delta x)}{\Delta x} \xrightarrow{\Delta x \rightarrow 0} \text{const.}$$

Now the difference quotient (3) is not the only one that can be used to approximate $f'(x)$. Indeed if we consider the expansion of $f(x - \Delta x)$:

$$f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) - \frac{\Delta x^3}{3!} f^{(3)}(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) + \dots \quad (8.4)$$

and we subtract (4) from (2) and divide by $(2\Delta x)$ we obtain:

$$\frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x} = f'(x) + \frac{\Delta x^2}{3!} f^{(3)}(\xi). \quad (8.5)$$

We notice that the error term associated with this form of difference approximation is $O(\Delta x^2)$, which converges more rapidly to zero as $\Delta x \rightarrow 0$.

In order to obtain an approximation to $f''(x)$ we add (2) to (4) which upon re-arrangement and dividing by Δx^2 leads to:

$$\frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} = f''(x) + \frac{1}{12} \Delta x^2 f^{(4)}(\xi). \quad (8.6)$$

Due to the symmetry of the difference approximations (5) and (6) about the expansion point x these are called central difference approximations. The difference approximation (3) is known as a forward difference approximation. We note that the central difference schemes (5) and (6) are second order accurate while the forward difference scheme (3) is only $O(\Delta x)$.

8.2 Solving the heat equations using Finite Difference

Consider the following initial-boundary value problem for the heat equation

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2} \quad 0 < x < 1, t > 0 \quad (8.7)$$

$$\text{BC: } u(0, t) = 0 \quad u(1, t) = 0 \quad (8.8)$$

$$\text{IC: } u(x, 0) = f(x). \quad (8.9)$$

The basic idea is to replace the derivatives in the heat equation by difference quotients. We consider the relationships between u at (x, t) and its neighbours a distance Δx apart and at a time Δt later.

Corresponding to the difference quotient approximations introduced in Section 1, we consider the following partial difference approximations.

Forward Difference in Time:

$$u(x, t + \Delta t) = u(x, t) + \Delta t \frac{\partial u}{\partial t}(x, t) + \frac{\Delta t^2}{2!} \frac{\partial^2 u}{\partial x^2}(x, t) + \dots$$

After re-arrangement and division by Δt :

$$\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \frac{\partial u}{\partial t}(x, t) + O(\Delta t). \quad (8.10)$$

Central Differences in Space:

$$\begin{aligned} u(x + \Delta x, t) &= u(x, t) + \Delta x \frac{\partial u}{\partial x}(x, t) + \frac{\Delta x^2}{2!} \frac{\partial^2 u}{\partial x^2}(x, t) + \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3}(x, t) + \frac{\Delta x^4}{4!} \frac{\partial^4 u}{\partial x^4}(x, t) + \dots \\ u(x - \Delta x, t) &= u(x, t) - \Delta x \frac{\partial u}{\partial x}(x, t) + \frac{\Delta x^2}{2!} \frac{\partial^2 u}{\partial x^2}(x, t) - \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3}(x, t) + \frac{\Delta x^4}{4!} \frac{\partial^4 u}{\partial x^4}(x, t) + \dots \end{aligned}$$

Adding and re-arranging:

$$\frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} = \frac{\partial^2 u}{\partial x^2}(x, t) + O(\Delta x^2). \quad (8.11)$$

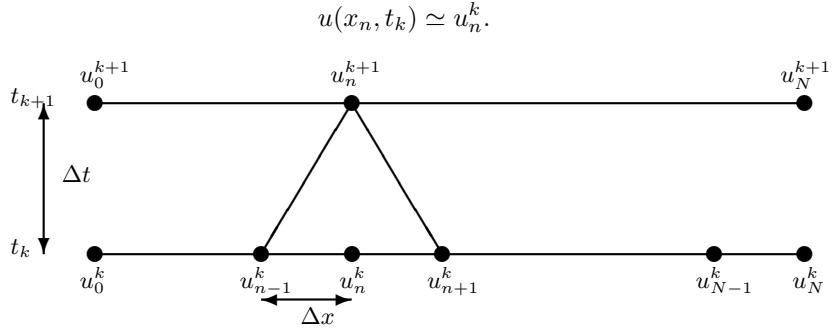
Substituting (2) and (3) into (1a) we obtain

$$\frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \alpha^2 \left(\frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2} \right) + O(\Delta t, \Delta x^2).$$

Re-arranging:

$$u(x, t + \Delta t) = u(x, t) + \alpha^2 \left(\frac{\Delta t}{\Delta x^2} \right) \{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)\}. \quad (8.12)$$

We subdivide the spatial interval $[0, 1]$ into $N + 1$ equally spaced sample points $x_n = n\Delta x$. The time interval $[0, T]$ is subdivided into $M + 1$ equal time levels $t_k = k\Delta t$. At each of these space-time sample points we introduce approximations:



$$u_n^{k+1} = u_n^k + \alpha^2 \left(\frac{\Delta t}{\Delta x^2} \right) (u_{n+1}^k - 2u_n^k + u_{n-1}^k)$$

↑ This is implemented in the spread sheets Heat0 and Heat.

Implementing Derivative Boundary Conditions:

Assume that the boundary conditions (1b) are changed to

$$\text{BC: } u(0, t) = 0, \quad \frac{\partial u}{\partial x}(1, t) = 0.$$

Consider a central difference approximation to $\frac{\partial u}{\partial x}(1, t)$, where $x_N = N\Delta x = 1$,

$$\frac{u(x_N + \Delta x, t) - u(x_N - \Delta x, t)}{\Delta x} = 0.$$

Re-arranging we obtain:

$$u(x_N + \Delta x, t) = u(x_N - \Delta x, t) \quad (*)$$

Since $x_N = 1$ we observe that $x_N + \Delta x$ is outside the domain we introduce an extra column u_{N+1} into which we copy the values u_{N-1} . In the column x_N we implement the same difference approximation for the Heat Equation, namely:

$$u_N^{k+1} = u_N^k + \alpha^2 \left(\frac{\Delta t}{\Delta x^2} \right) (u_{N+1}^k - 2u_N^k + u_{N-1}^k) \quad (**)$$

↑ This is implemented in the spread sheet Heat0f.

while $u_{N+1}^k = u_{N-1}^k$ (see (*)) since column u_{N-1}^k is copied to column u_{N+1}^k . Note that this BC could be implemented another way without introducing the additional column, by eliminating u_{N+1} from (*) and (**):

$$u_N^{k+1} = u_N^k + 2\alpha^2 \left(\frac{\Delta t}{\Delta x^2} \right) (u_{N-1}^k - u_N^k).$$

If this latter equation is implemented at x_N there is no need to introduce an extra column U_{N+1} or to implement the difference equation given in (**) as the the derivative boundary condition is taken care of automatically.

Stability of the Finite Difference Scheme for the heat equation

Consider the following finite difference approximation to the 1D heat equation:

$$u_n^{k+1} - u_n^k = \frac{\Delta t}{\Delta x^2} (u_{n+1}^k - 2u_n^k + u_{n-1}^k) \quad \text{where } u_n^k \simeq u(x_n, t_k)$$

Let $u_n^k = \phi_k e^{in\Delta x \theta}$ then

$$\begin{aligned} (\phi_{k+1} - \phi_k) e^{in\Delta x \theta} &= \frac{\Delta t}{\Delta x^2} (e^{i\Delta x \theta} - 2 + e^{-i\Delta x \theta}) \phi_k e^{in\Delta x \theta} \\ &= \frac{\Delta t}{\Delta x^2} [2 \cos(\theta \Delta x) - 2] \phi_k \end{aligned}$$

Therefore

$$\begin{aligned} \phi_{k+1} &= \phi_k - \frac{\Delta t}{\Delta x^2} 4 \sin^2 \left(\frac{\theta \Delta x}{2} \right) \phi_k \quad \cos(\theta \Delta x) - 1 = -2 \sin^2 \left(\frac{\theta \Delta x}{2} \right) \\ &= \left[1 - \frac{4\Delta t}{\Delta x^2} \sin^2 \left(\frac{\theta \Delta x}{2} \right) \right] \phi_k \end{aligned}$$

Now for stability we require that $|\phi_{k+1}| \leq |\phi_k|$ so that

$$\begin{aligned} \left| 1 - \frac{4\Delta t}{\Delta x^2} \sin^2 \left(\frac{\theta \Delta x}{2} \right) \right| &\leq 1 \\ \rightarrow -2 \leq -\frac{4\Delta t}{\Delta x^2} \sin^2 \left(\frac{\theta \Delta x}{2} \right) &\leq 0 \end{aligned}$$

The right inequality is satisfied automatically while the left inequality can be re-written in the form:

$$\frac{4\Delta t}{\Delta x^2} \sin^2 \left(\frac{\theta \Delta x}{2} \right) \leq 2$$

Since $\sin(\) \leq 1$ this condition is satisfied for all θ provided

$$\Delta t \leq \frac{\Delta x^2}{2} \tag{8.13}$$

Exercises on finite Differences applied to the Heat Equation

Exercise 1 Numerical Instability:

(a) Change the Δt in cell D1 from 0.001 to 0.05 and you will observe what is known as a numerical instability. Now change Δt to 0.00625, which is known as the stability boundary predicted by (8.13) and observe what happens. Now let $\Delta t = 0.006$ and observe the abrupt change in the solution - it is much closer to what we would expect.

(b) Derive the stability condition for the finite difference approximation of the 1D heat equation when $\alpha^2 \neq 1$.

$$\text{i.e. } u_n^{k+1} - u_n^k = \frac{\alpha^2 \Delta t}{\Delta x^2} (u_{n+1}^k - 2u_n^k + u_{n-1}^k)$$

Exercise 2 Truncation Error: The instability noted in 1 above is not the only source of error in the numerical approximation. Although numerical instability is evident for a parameter choice that is unstable, the other type of error is present in almost every type of numerical approximation scheme. This class of error results from discarding the $O(\Delta x^2)$ and $O(\Delta t)$ terms in (2) and (3) when we replace derivatives in (1a) by difference quotients. This error is known as the truncation error. To determine the truncation error change the spread sheet to implement the initial condition

$$f(x) = \begin{cases} 2x & 0 < x < 1/2 \\ 2(1-x) & 1/2 \leq x < 1 \end{cases}.$$

Now code up the Fourier Series (in another spread sheet) that is derived in Lecture 10, Exercise 10.1 and compare the numerical solution to the 'exact' Fourier Series solution with 50 terms. The difference between the two is mainly due to the truncation error since the round-off error is about 10^{-12} and does not grow if stable parameters are used.

Exercise 3 Derivative Boundary Conditions: Implement a derivative boundary condition the left endpoint $x = 0$. Check the numerical solution against the problem solved in Lecture 11.

8.3 Finite Difference scheme for the 1D Wave Equation

Consider the following initial boundary value problem for the Wave Equation:

$$u_{tt} = c^2 u_{xx} \quad 0 < x < L \quad (8.14)$$

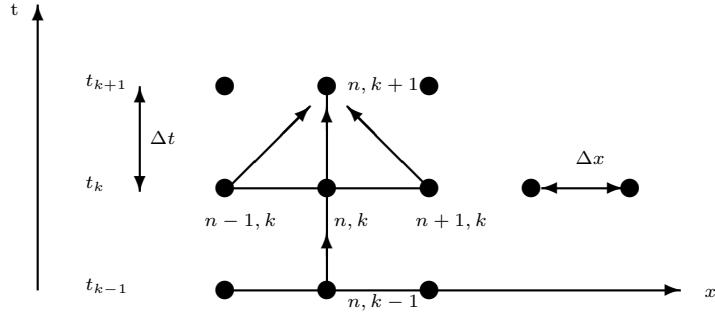
$$\text{BC: } u(0, t) = 0 \quad u(L, t) = 0 \quad (8.15)$$

$$\text{IC: } u(x, 0) = f(x) \quad (8.16)$$

$$\frac{\partial u}{\partial t}(x, 0) = g(x) \quad (8.17)$$

We introduce a finite difference mesh $x_n = n\Delta t$, $t_k = k\Delta t$ and let the corresponding nodal values be denoted by

$$u_n^k \simeq u(x_n, t_k).$$



Now approximating derivatives by central differences both in space and time we obtain

$$\frac{u_n^{k+1} - 2u_n^k + u_n^{k-1}}{\Delta t^2} = c^2 \left(\frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{\Delta x^2} \right) + O(\Delta x^2, \Delta t^2). \quad (8.18)$$

$$\begin{aligned} \text{Therefore } u_n^{k+1} &= 2u_n^k - u_n^{k-1} + \left(\frac{c\Delta t}{\Delta x} \right)^2 (u_{n+1}^k - 2u_n^k + u_{n-1}^k) \\ &= \underbrace{r^2 u_{n+1}^k + 2(1 - r^2) u_n^k + r^2 u_{n-1}^k}_{\text{time level } k} - \underbrace{u_n^{k-1}}_{\text{time level } k-1} \end{aligned} \quad (8.19)$$

Here $r = (c\Delta t / \Delta x)$ is known as the Courant Number. We observe that the Discrete Equation (8.19) involves three distinct levels in which known data is transferred from steps $k-1$ and k to step $k+1$.

Initial Conditions - Starting the Solution

The 3-level scheme poses some challenges when imposing the initial conditions. If we imagine a row of false mesh points at time $t = -\Delta t = t_{-1}$, then the initial velocity condition (8.17) can be approximated using central differences as:

$$\frac{u_n^1 - u_n^{-1}}{2\Delta t} = g(x_n)$$

therefore

$$u_n^{-1} = u_n^2 - 2\Delta t g(x_n) \quad (8.20)$$

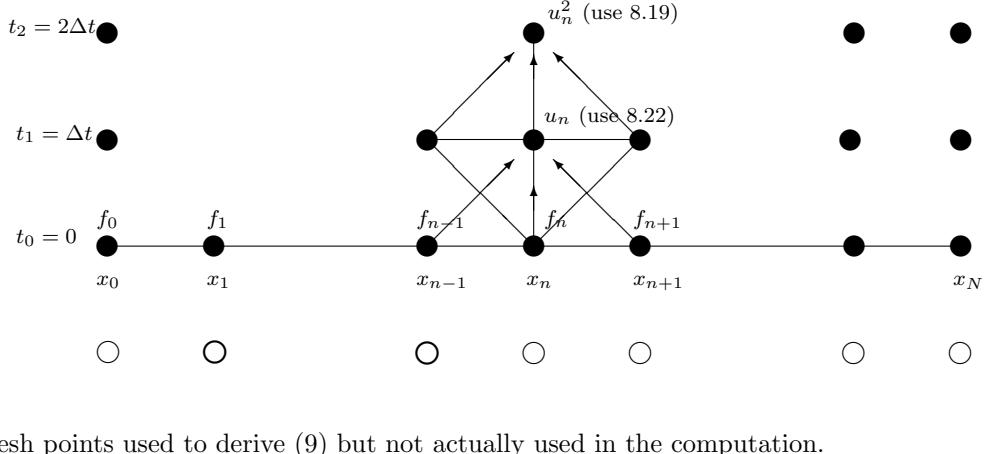
Now we assume that the Discrete Wave Equation (8.19) also holds at $t = 0$ so that

$$u_n^1 = r^2 u_{n+1}^0 + 2(1 - r^2) u_n^0 + r^2 u_{n-1}^0 - u_n^{-1} \quad (8.21)$$

Now substituting (8.20) into (8.21) and re-arranging we obtain:

$$u_n^1 = \frac{1}{2}(r^2 u_{n+1}^0 + 2(1 - r^2)u_n^0 + r^2 u_{n-1}^0) + \Delta t g(x_n) \quad (8.22)$$

Since $u_n^0 = f(x_n)$ and $g(x_n)$ are known, we are now in a position to specify the first two rows of nodes. This is sufficient to start the recursion (6) for all subsequent steps.



Stability of the Finite Difference Scheme for the wave equation Consider the following finite difference approximation to the 1D wave equation:

$$u_n^{k+1} = r^2 u_{n+1}^k + 2(1 - r^2)u_n^k + r^2 u_{n-1}^k - u_n^{k-1}. \quad (8.23)$$

and as in the case of the heat equation, substitute $u_n^k = \phi_k e^{in\Delta x \theta}$ into (10)

$$e^{in\Delta x \theta} \phi_{k+1} = (r^2 e^{i\Delta x \theta} + 2(1 - r^2) + r^2 e^{-i\Delta x \theta}) e^{in\Delta x \theta} \phi_k - e^{in\Delta x \theta} \phi_{k-1}$$

Cancelling terms and using the double angle formulae

$$\phi_{k+1} = 2(1 + r^2(\cos \Delta x \theta - 1)) \phi_k - \phi_{k-1} \quad (8.24)$$

$$= 2 \left(1 - 2r^2 \sin^2 \frac{\Delta x \theta}{2} \right) \phi_k - \phi_{k-1} \quad (8.25)$$

If we now assume that ϕ_k has the following exponential form $\phi_k = G^k$ then (8.25) reduces to the following quadratic equation:

$$G^2 - 2\gamma G + 1 = 0 \quad (8.26)$$

where $\gamma = (1 - 2r^2 \sin^2 \frac{\Delta x \theta}{2})$. The solutions of this quadratic equation are given by

$$G_{1,2} = \gamma \pm \sqrt{\gamma^2 - 1} \quad (8.27)$$

Now since G_1 and G_2 are the roots of this quadratic we may conclude that

$$(G - G_1)(G - G_2) = G^2 - (G_1 + G_2)G + G_1 G_2 = 0 \quad (8.28)$$

Comparing the last terms in these two quadratic equations (8.26) and (8.28) we conclude that

$$G_1 G_2 = 1. \quad (8.29)$$

However, for stability of solutions for the form $\phi_k = G^k$, we require that $|G_1| \leq 1$ and $|G_2| \leq 1$. Given the constraint (8.29), the only possibility, if the solutions are to be stable, is that $|G_1| = |G_2| = 1$. Thus G must fall on the unit disk, which implies that

$$|\gamma| \leq 1$$

Thus

$$\left| 1 - 2r^2 \sin^2 \frac{\Delta x \theta}{2} \right| \leq 1$$

or

$$-1 \leq 1 - 2r^2 \sin^2 \frac{\Delta x \theta}{2} \leq 1$$

so that

$$-2 \leq -2r^2 \sin^2 \frac{\Delta x \theta}{2} \leq 0 \quad (8.30)$$

The second inequality in (17) is satisfied automatically, while the first leads to the condition

$$r^2 \sin^2 \frac{\Delta x \theta}{2} \leq 1$$

Since the maximum value that $\sin^2 \frac{\Delta x \theta}{2}$ can achieve is 1, we conclude that the condition for stability is

$$r = (c \Delta t / \Delta x) \leq 1$$

or

$$\Delta t \leq \frac{\Delta x}{c} \quad (8.31)$$

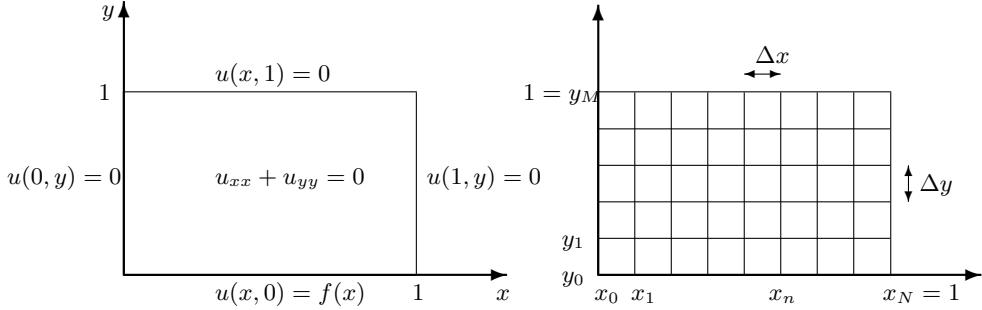
The condition (18), which imposes an upper bound on the time step that can be used, is known as the Courant-Friedrichs-Lowy or CFL condition.

8.4 Solving Laplace's Equation using finite differences

Consider the boundary value problem

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad 0 < x, y < 1 \quad (8.32)$$

$$\text{BC: } u(0, y) = 0; \quad u(1, y) = 0; \quad u(x, 0) = f(x); \quad u(x, 1) = 0. \quad (8.33)$$



As before we replace the second derivatives in (1a) by central difference quotients that are second order accurate:

$$\frac{u(x + \Delta x, y) - 2u(x, y) + u(x - \Delta x, y)}{\Delta x^2} = \frac{\partial^2 u}{\partial x^2}(x, y) + O(\Delta x^2) \quad (8.34)$$

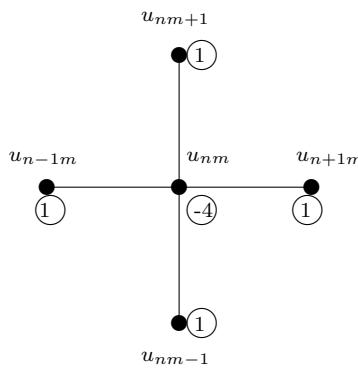
$$\frac{u(x, y + \Delta y) - 2u(x, y) + u(x, y - \Delta y)}{\Delta y^2} = \frac{\partial^2 u}{\partial y^2}(x, y) + O(\Delta y^2). \quad (8.35)$$

We partition the interval $0 \leq x \leq 1$ into $(N + 1)$ equally spaced nodes $x_n = n\Delta x$ and the interval $0 \leq y \leq 1$ into $(M + 1)$ equally spaced nodes $y_m = m\Delta y$. Replacing the derivatives in (1a) by the difference quotients in (3) and (4) and representing the mesh values at (x_n, y_m) by $u_{nm} \simeq u(x_n, y_m)$ we obtain:

$$\frac{u_{n+1m} - 2u_{nm} + u_{n-1m}}{\Delta x^2} + \frac{u_{nm+1} - 2u_{nm} + u_{nm-1}}{\Delta y^2} = (u_{xx} + u_{yy})_{(x_n, y_m)} + O(\Delta x^2, \Delta y^2).$$

If we choose $\Delta x = \Delta y$ then we obtain

$$u_{n+1m} + u_{n-1m} + u_{nm+1} + u_{nm-1} - 4u_{nm} = 0 \quad 1 \leq n, m \leq (N - 1), (M - 1). \quad (8.36)$$



This is known as the finite difference 'Stencil' that relates u_{nm} to its 4 nearest neighbours.

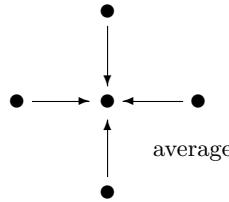
This is a system of $(N - 1) \times (M - 1)$ unknowns for the values of u_{nm} interior to the domain - recall the boundary values are already specified!

8.4.1 Solving the System of Equations by Jacobi Iteration

This is a procedure to solve the system of Equation (3) by looping through each of the mesh points and updating u_{nm} according to (3) assuming that the nearest neighbours already have values close to the exact solution. This procedure is repeated until the changes that are made in each iteration falls below a certain tolerance.

To implement this iterative procedure we observe that the discrete Laplace Equation (5) can be re-written in the form:

$$u_{nm}^{k+1} = \frac{u_{n+1m}^k + u_{n-1m}^k + u_{nm+1}^k + u_{nm-1}^k}{4} \quad (8.37)$$



Thus u_{nm} is the average value of its nearest neighbours. Note that a new superscript index k has been introduced to represent the nodal values at the k th iteration. Thus iteration can be viewed as taking successive neighbour averages until there is no change, at which point the value of u_{mn} equals the average of the values at its mesh neighbours. This mean value property is a discrete form of a fundamental property of any solution to Laplace's Equation.

To implement the iterative procedure (6) on a spread sheet, go to the *Tools Menu* at the top of the screen and click on the *Options Tab*. Then select the *Calculation Tab*. Check the *Iteration* box. If you set the number of iterations to 5 say, then if you start with zero values throughout the interior of the domain (as you should if you cut and paste as demonstrated in class), you will see the values percolate 5 cells into the domain from the non zero boundary condition $f(x) = \sin(\pi x)$. You can choose a surface plot to visualize the solution. Now hold down the *F9* key and watch the solution move to equilibrium. This iterative process essentially uses diffusion on a pseudo time scale to take the solution to equilibrium.

Exercises for Laplace's Equation:

Exercise 4 Implement a 0 derivative BC along the lines $x = 0$ and $x = 1$. Plot a cross section of the results along $y = 1/2$. To ensure that $\frac{\partial u}{\partial x}(0, y) = 0 = \frac{\partial u}{\partial x}(1, y)$.

Exercise 5 Implement an inhomogeneous term for Poisson's Equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad 0 < x, y < 1.$$

Introduce finite difference quotients, assume $\Delta x = \Delta y$ to arrive at the iterative formula:

$$u_{nm}^{k+1} = \frac{(u_{n+1m}^k + u_{n-1m}^k + u_{nm+1}^k + u_{nm-1}^k - \Delta x^2 f(x_n, y_m))}{4}. \quad (*)$$

It may be useful to calculate the values of f_{nm} on a separate sheet in which the same cell values as those for u_{nm} are maintained. Then the values of f_{nm} can be referenced in the calculation of u_{nm} according to (*).