Finite Difference Methods for Boundary Value Problems

October 2, 2013

Goals

- Learn steps to approximate BVPs using the Finite Difference Method
- Start with two-point BVP (1D)
- Investigate common FD approximations for $u'(x)$ and $u''(x)$ in 1D
- Use FD quotients to write a system of difference equations to solve two-point BVP
- Higher order accurate schemes
- Systems of first order BVPs
- Use what we learned from 1D and extend to Poisson's equation in 2D & 3D
- Learn how to handle different boundary conditions

Steps in the Finite Difference Approach to linear Dirichlet BVPs

- Overlay domain with grid
- Choose difference quotients to approximate derivatives in DE
- Write a difference equation at each node where there is an unknown
- Set up resulting system of equations as a matrix problem
- Solving resulting linear system efficiently
- Compute error when solution is known

Prototype Dirichlet BVP in 1D

$$-\frac{d}{dx}\left(p(x)\frac{du}{dx}\right)+q(x)u=f(x)\quad a<x<b\,, \tag{1}$$

$$u(a)=\alpha\qquad u(b)=\beta$$

When $p(x)=p$, a constant, we have

$$-pu''(x)+q(x)u=f(x)\quad a<x<b\,,$$

When $p=1$ and $q=0$ we have the Poisson equation

$$-u''(x)=f(x)\quad a<x<b$$

in one dimension. We will see that the minus sign is important.

Here $p(x)$, $q(x)$ are required to satisfy the bounds

$$0 < p_{\min} \leq p \leq p_{\max} \quad \text{and} \quad q_{\min} = 0 \leq q(x) \leq q_{\max}\,. \tag{2}$$

For existence and uniqueness we also require that f and q be continuous functions of x on the domain $[a, b]$ and that p has a continuous first derivative there.

Step 1: Overlay domain with a grid

Suppose that we subdivide our domain $[a, b]$ into $n + 1$ subintervals using the $(n + 2)$ uniformly spaced points x_i, $i = 0, 1, \ldots n + 1$ with

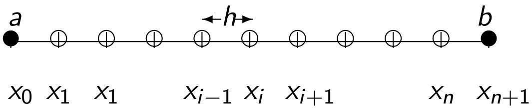
$$x_0 = a, \quad x_1 = x_0 + h, \ldots,$$

$$x_i = x_{i-1} + h, \ldots, \quad x_{n+1} = x_n + h = b$$

where

$$h = \frac{b - a}{n + 1}$$

- The points x_i are called the grid points or nodes.
- The nodes $x_1, x_2, \ldots, x_n$ are interior nodes (denoted by open circles in the diagram below)
- The two nodes x_0 and x_{n+1} are boundary nodes (denoted by solid circles in the diagram).



Step 2: Choose difference quotients to approximate derivatives in DE

For general $p(x)$ we have

$$-p(x)u''(x) - p'(x)u'(x) + q(x)u = f(x) \quad a < x < b\,.$$

So we need difference quotient approximations for both the first and second derivatives. So far we have approximations for the first derivative.

$$\textbf{Forward Difference:} \quad u'(x) = \frac{u(x+h) - u(x)}{h} + \mathcal{O}(h)$$

$$\textbf{Backward Difference:} \quad u'(x) = \frac{u(x) - u(x-h)}{h} + \mathcal{O}(h)$$

Difference quotient for $u''(x)$

A Taylor series expansion for $u(x+h)$ is

$$u(x+h) = u(x) + h\, u'(x) + \frac{h^2}{2!} u''(x) + \frac{h^3}{3!} u'''(x) + \mathcal{O}(h^4)\,. \qquad (3)$$

Now we want an approximation for $u''(x)$ but if we solve for it we get

$$\frac{h^2}{2!} u''(x) = u(x+h) - u(x) - hu'(x) - \frac{h^3}{3!} u'''(x) + \mathcal{O}(h^4)\,.$$

in (3) then we still have the $u'(x)$ term. However if we consider the Taylor series expansion for $u(x-h)$

$$u(x-h) = u(x) - h\, u'(x) + \frac{h^2}{2!} u''(x) - \frac{h^3}{3!} u'''(x) + \mathcal{O}(h^4) \qquad (4)$$

then we can eliminate the $u'(x)$ term by adding the two expansions; we have

$$u(x+h) = u(x) + h\,u'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \mathcal{O}(h^4)\,.$$

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

implies

$$u(x+h) + u(x-h) - 2u(x) = h^2 u''(x) + \mathcal{O}(h^4)$$

- Note that the terms involving h^3 cancel.
- This difference quotient is called a second centered difference quotient or a second order central difference approximation to $u''(x)$
- It is second order accurate.

Second centered difference:

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + \mathcal{O}(h^2) \qquad (5)$$

Another way to derive this approximation is to difference the forward and backward approximations to the first derivative, i.e.,

$$u''(x) \approx \frac{1}{h}\left[\text{Forward difference for } u'(x) - \text{Backward difference for } u'(x)\right]$$

which implies

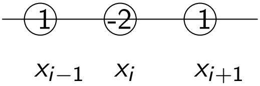
$$u''(x) \approx \frac{1}{h}\left[\frac{u(x+h)-u(x)}{h} - \frac{u(x)-u(x-h)}{h}\right]$$

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

hence the name second difference.

Finite Difference Stencil

Finite difference approximations are often described in a pictorial format by giving a diagram indicating the points used in the approximation. These are called finite difference stencils and this second centered difference is called a three point stencil for the second derivative in one dimension.



Finite difference quotient for $u'(x)$

- The forward or backward difference quotients for $u'(x)$ are first order
- The second centered difference for $u''(x)$ is second order
- So we need a second order approximation to $u'(x)$

If we subtract the expansions

$$u(x+h) = u(x) + h\,u'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \mathcal{O}(h^4)\,.$$

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

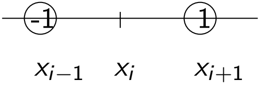
we get

$$u(x+h) - u(x-h) = 2hu'(x) + \mathcal{O}(h^3)$$

which gives the (first) centered difference

First centered difference: $$u'(x) = \frac{u(x+h) - u(x-h)}{2h} + \mathcal{O}(h^2)$$

It is described by the stencil



Step 3: Writing the Difference Equation

We have the ODE

$$-p(x)u''(x) - p'(x)u'(x) + q(x)u = f(x)$$

with the approximations

$$u''(x_i) \approx \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

$$u'(x_i) \approx \frac{u(x_{i+1}) - u(x_{i-1})}{2h}$$

$$\text{ODE:} \quad -p(x)u''(x) - p'(x)u'(x) + q(x)u = f(x)$$

Let $U_i \approx u(x_i)$ so that $U_0 = \alpha$, $U_1 = \beta$.
Using our difference quotients at each interior grid point x_i, $i = 1, \ldots, n$ we have

$$p(x_i)\left(\frac{-U_{i+1} + 2U_i - U_{i-1}}{h^2}\right) - p'(x_i)\left(\frac{U_{i+1} - U_{i-1}}{2h}\right) + q(x_i)U_i = f(x_i)\,.$$

At $i = 1$ we have

$$p(x_1)\left(\frac{-U_2 + 2U_1 - U_0}{h^2}\right) - p'(x_1)\left(\frac{U_2 - U_0}{2h}\right) + q(x_1)U_1 = f(x_1)\,,$$

$U_0 = \alpha$ is known so we take it to the right hand side of the equation

$$p(x_1)\left(\frac{-U_2 + 2U_1}{h^2}\right) - p'(x_1)\left(\frac{U_2}{2h}\right) + q(x_1)U_1 = f(x_1) + p(x_1)\frac{\alpha}{h^2} + p'(x_1)\frac{\alpha}{2h}\,,$$

Step 4: Write difference equations as linear system of equations

First consider the simple case when $p = 1$ and $q = 0$ then we have the equations

$$\begin{aligned} 2U_1 - U_2 &= h^2 f(x_1) + \alpha \\ -U_3 + 2U_2 - U_1 &= h^2 f(x_2) \\ -U_4 + 2U_3 - U_2 &= h^2 f(x_3) \\ &\vdots \\ -U_n + 2U_{n-1} - U_{n-2} &= h^2 f(x_{n-1}) \\ 2U_n - U_{n-1} &= h^2 f(x_n) + \beta \end{aligned}$$

The corresponding matrix problem is $A\vec{U} = \vec{F}$ where A is the matrix

$$\begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & & 0 \\ -1 & 2 & -1 & 0 & \cdots & & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ 0 & \cdots & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 2 \end{pmatrix} \tag{6}$$

with the vector of unknowns

$$\vec{U} = \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_{n-1} \\ U_n \end{pmatrix} \qquad \vec{F} = \begin{pmatrix} h^2 f(x_1) + \alpha \\ h^2 f(x_2) \\ \vdots \\ h^2 f(x_{n-1}) \\ h^2 f(x_n) + \beta \end{pmatrix}$$

The linear system is

- tridiagonal
- symmetric
- positive definite
- $\mathcal{O}(n)$ operations to solve
- Cholesky for tridiagonal system can be used $A = LL^T$ then forward solve $L\vec{Y} = \vec{F}$ and back solve $L^T\vec{U} = \vec{Y}$
- storage required is two vectors for matrix and one for $\vec{F}$
- Note that if we didn't have the minus sign in $-u''(x) = f(x)$ then the matrix would not be positive definite.

Example 1 - Homogeneous Dirichlet Boundary Conditions

We want to use finite differences to approximate the solution of the BVP

$$\begin{aligned} -u''(x) &= \pi^2 \sin(\pi x) \quad 0 < x < 1 \\ u(0) &= 0, \quad u(1) = 0 \end{aligned}$$

using $h = 1/4$. Our grid will contain five total grid points

$$x_0 = 0, \quad x_1 = 1/4, \quad x_2 = 1/2, \quad x_3 = 3/4, \quad x_4 = 1$$

and three interior points x_1, x_2, x_3. Thus we have three unknowns U_1, U_2, U_3. We will write the equation at each interior node to demonstrate that we get the tridiagonal system. We have

$$
\begin{aligned}
2U_1 - U_2 &= \frac{\pi^2}{16}\sin(\frac{\pi}{4}) \\
-U_1 + 2U_2 - U_3 &= \frac{\pi^2}{16}\sin(\frac{\pi}{2}) \\
-U_2 + 2U_3 &= \frac{\pi^2}{16}\sin(\frac{3\pi}{4})\,.
\end{aligned}
$$

Writing these three equations as a linear system gives

$$
\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix} = \frac{\pi^2}{16} \begin{pmatrix} \sin(\frac{\pi}{4}) \\ \sin(\frac{\pi}{2}) \\ \sin(\frac{3\pi}{4}) \end{pmatrix} = \begin{pmatrix} 0.436179 \\ 0.61685 \\ 0.436179 \end{pmatrix}.
$$

Solving this system gives $U_1 = 0.7446$, $U_2 = 1.0530$ and $U_3 = 0.7446$; the exact solution to this problem is $u = \sin(\pi x)$ so at the interior nodes we have the exact solution $(0.7071, 1, 0.7071)$.

Example 2 - Inhomogeneous Dirichlet BCs

Consider the BVP

$$\begin{aligned} -u''(x) &= \pi^2 \cos(\pi x) \quad 0 < x < 1 \\ u(0) &= 1, \quad u(1) = -1 \end{aligned}$$

whose exact solution is $u(x) = \cos(\pi x)$. Using the same grid $(h = 1/4)$ as in the previous example, we still have three unknowns so we write the equations at the three interior nodes

$$\begin{aligned} -U_0 + 2U_1 - U_2 &= \frac{\pi^2}{16} \cos(\frac{\pi}{4}) \\ -U_1 + 2U_2 - U_3 &= \frac{\pi^2}{16} \cos(\frac{\pi}{2})) \\ -U_2 + 2U_3 - U_4 &= \frac{\pi^2}{16} \cos(\frac{3\pi}{4})) \end{aligned}$$

Now $U_0 = 1$ and $U_4 = -1$ so we simply substitute these values into the equations and move the terms to the right hand side to get

$$
\begin{aligned}
2U_1 - U_2 &= \frac{\pi^2}{16}\cos(\frac{\pi}{4}) + 1 \\
-U_1 + 2U_2 - U_3 &= \frac{\pi^2}{16}\cos(\frac{\pi}{2})) \\
-U_2 + 2U_3 &= \frac{\pi^2}{16}\cos(\frac{3\pi}{4}) - 1
\end{aligned}
$$

Writing these three equations as a linear system gives

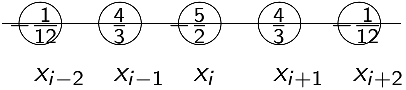
$$
\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}
\begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix}
=
\begin{pmatrix} 1.4362 \\ 0.0 \\ -1.4362 \end{pmatrix} .
$$

Solving this system gives $U_1 = 0.7181$, $U_2 = 0$ and $U_3 = -0.7181$; the exact solution at these interior nodes is $(0.7071, 0.0, -0.7071)$.

Higher order accurate scheme

To get a higher order scheme we need to include more points in the stencil

Five point stencil:



$$u''(x) = \frac{1}{h^2}\Big[-\frac{1}{12}u(x-2h)+\frac{4}{3}u(x-h)-\frac{5}{2}u(x)+\frac{4}{3}u(x+h) -\frac{1}{12}u(x+2h)\Big]+\mathcal{O}(h^4)$$

where we derive this by combining Taylor series expansions for $u(x-2h), u(x-h)$, $u(x+h)$, and $u(x+2h)$.

- If we have uniform points x_i, $i = 0, \ldots, n+1$, how many unknowns do we have for a Dirichlet 2-point BVP?
- What do you think the structure of the resulting matrix is?
- Do we handle the boundaries in the same way as the three-point stencil?

Summary of FD approximations

$u'(x)$	forward difference	$\frac{u(x+h)-u(x)}{h}$	$\mathcal{O}(h)$
$u'(x)$	backward difference	$\frac{u(x)-u(x-h)}{h}$	$\mathcal{O}(h)$
$u'(x)$	centered difference	$\frac{u(x+h)-u(x-h)}{2h}$	$\mathcal{O}(h^2)$
$u''(x)$	2^{nd} centered difference	$\frac{u(x+h)-2u(x)+u(x-h)}{h^2}$	$\mathcal{O}(h^2)$

$u''(x)$	five-point stencil (1D)	$\frac{1}{12h^2}\Big[-u(x-2h)+16u(x+h) -30u(x)+16u(x-h)-u(x+2h)\Big]$	$\mathcal{O}(h^4)$

Recall that for IVPs we made a LTE at each step and then the total or global error was the accumulated error over all the time steps.

Unlike IVPs, for BVPs the total error (assuming no roundoff and using a direct solver) is just due to the error in replacing the DE with a difference equation.

Calculating the numerical rate of convergence

We want to calculate the numerical rate of convergence for our simulations as we did for IVPs. However, in this case our solution is a vector rather than a single number. To calculate the numerical rate using the formula

$$r = \frac{\ln \frac{E_1}{E_2}}{\ln \frac{h_1}{h_2}}$$

we need a single number which represents the error so we use a vector norm. A commonly used norm is the standard Euclidean norm defined by

$$\|\vec{x}\|_2 = \Big[\sum_{i=1}^{n} x_i^2 \Big]^{1/2} \quad \text{or} \quad \|\vec{E}\|_2 = \Big[\frac{1}{n} \sum_{i=1}^{n} E_i^2 \Big]^{1/2}$$

for a vector in $\vec{x} \in R^n$. Other choices include the maximum norm $\| \cdot \|_\infty$ or the one-norm $\| \cdot \|_1$

Structure of code for Dirichlet 1D BVP

User specifies

- n, the number of interior grid points (alternately the grid spacing h);
- a and b, the right and left endpoints of interval;
- the boundary value at $x = a$ and at $x = b$,
- a routine for the forcing function $f(x)$
- a routine for the exact solution, if known.

Code could be structured as follows:

- compute $h = (b - a)/(n + 1)$;
- compute grid points $x(i)$, $i = 0, 1, 2, \ldots, n + 1$;
- set up the coefficient matrix and store efficiently; for example, for the three-point stencil the matrix can be stored as two vectors;
- set up the right hand side for all interior points;
- modify the first and last entries of the right hand side to account for inhomogeneous Dirichlet boundary data;
- solve the resulting linear system using an appropriate solver;
- output solution to file for plotting, if desired;
- compute the error vector and output a norm of the error (normalized) if the exact solution is known.

Example 3

$$-u''(x) = \pi^2 \sin(\pi x) \quad 0 < x < 1$$
$$u(0) = 0, \quad u(1) = 0$$

h	$\frac{\|E\|_2}{\|u\|_2}$	numerical rate
$\frac{1}{4}$	5.03588×10^{-2}	
$\frac{1}{8}$	1.27852×10^{-2}	1.978
$\frac{1}{16}$	3.20864×10^{-3}	1.994
$\frac{1}{32}$	8.02932×10^{-4}	1.999
$\frac{1}{64}$	2.00781×10^{-4}	2.000

Example 4

$$\begin{aligned} -u''(x) &= -2 \quad 0 < x < 1 \\ u(0) &= 0, \quad u(1) = 0 \end{aligned}$$

with exact solution $u(x) = x^2 - x$.

h	$\frac{\|E\|_2}{\|u\|_2}$	numerical rate
$\frac{1}{4}$	3.1402×10^{-16}	
$\frac{1}{8}$	3.1802×10^{-16}	

Why are we getting essentially zero for the error?

From the Taylor series derivation of the second centered difference

$$u(x+h)+u(x-h)-2u(x)=h^2u''(x)+2\frac{h^4}{4!}u''''(x)+\mathcal{O}(h^5)$$

and for our problem the exact solution is $u(x)=x^2-x$.

So $u'''(x)$ and all higher derivatives vanish and thus the approximation is exact.

Systems of BVPs in 1D

As an example consider

$$\begin{aligned} -u''(x) + v(x) &= f(x) \quad a < x < b \\ -v''(x) + u(x) &= g(x) \quad a < x < b \\ u(a) = 0 \quad u(b) &= 0 \\ v(a) = 0 \quad v(b) &= 0\,. \end{aligned}$$

Using 3 point stencil we have

$$\begin{aligned} -U_{i-1} + 2U_i - U_{i+1} + V_i &= f(x_i) \\ -V_{i-1} + 2V_i - V_{i+1} + U_i &= g(x_i) \end{aligned}$$

with the grid $x_0 = a, x_{n+1} = b,\ x_{i+1} = x_i + h,\ h = \dfrac{b-a}{n+1}$.

So at grid point (or node) x_i we have two unknowns U_i and V_i. This means we have a choice of how we want to number the unknowns. For example, we could number all of the U_i, $i = 1, \ldots, n$ and then the V_i or we could mix them up, e.g., $U_1, V_1, U_2, V_2, \ldots, U_n, V_n$. Now we will get the same solution either way but each leads to a different matrix problem and one may be easier to solve than the other.

First approach: Solution vector is $(U_1, U_2, \cdots, U_n, V_1, V_2, \cdots, V_n)^T$
We write all the equations for U_i in the first half of the matrix and all the equations for V_i in the second half.

$$\begin{aligned}
2U_1 - U_2 + V_1 &= f(x_1)\\
-U_1 + 2U_2 - U_3 + V_2 &= f(x_2)\\
&\vdots\\
-U_{n-1} + 2U_n + V_n &= f(x_n)\\
2V_1 - V_2 + U_1 &= g(x_1)\\
-V_1 + 2V_2 - V_3 + U_2 &= g(x_2)\\
&\vdots\\
-V_{n-1} + 2V_n + U_n &= g(x_n)\,.
\end{aligned}$$

Resulting $2n \times 2n$ matrix is

$$A = \begin{pmatrix} S & I \\ I & S \end{pmatrix}$$

where I is the $n \times n$ identity matrix and

$$S = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}.$$

What is the bandwidth of this matrix?

Second approach: Solution vector is

$$(U_1, V_1, U_2, V_2, \cdots, U_n, V_n)^T .$$

$$\begin{aligned}
2U_1 - U_2 + V_1 &= f(x_1) \\
2V_1 - V_2 + U_1 &= g(x_1) \\
-U_1 + 2U_2 - U_3 + V_2 &= f(x_2) \\
-V_1 + 2V_2 - V_3 + U_2 &= g(x_2) \\
&\vdots \\
-U_{n-1} + 2U_n + V_n &= f(x_n) \\
-V_{n-1} + 2V_n + U_n &= g(x_n) .
\end{aligned}$$

The coefficient matrix is

$$A = \begin{pmatrix} 2 & 1 & -1 & & & & & & \\ 1 & 2 & 0 & -1 & & & & & \\ -1 & 0 & 2 & 1 & -1 & & & & \\ & -1 & 1 & 2 & 0 & -1 & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & -1 & 0 & 2 & 1 & -1 & & \\ & & & -1 & 1 & 2 & 0 & -1 \\ & & & & -1 & 0 & 2 & 1 \\ & & & & & -1 & 1 & 2 \end{pmatrix}.$$

with a bandwidth of 5.

Moral: the way you number your unknowns can change the structure of your coefficient matrix.

Finite Differences for Poisson Equation in 2D

Let domain $\Omega = (0,1) \times (0,1)$, the unit square with boundary Γ.

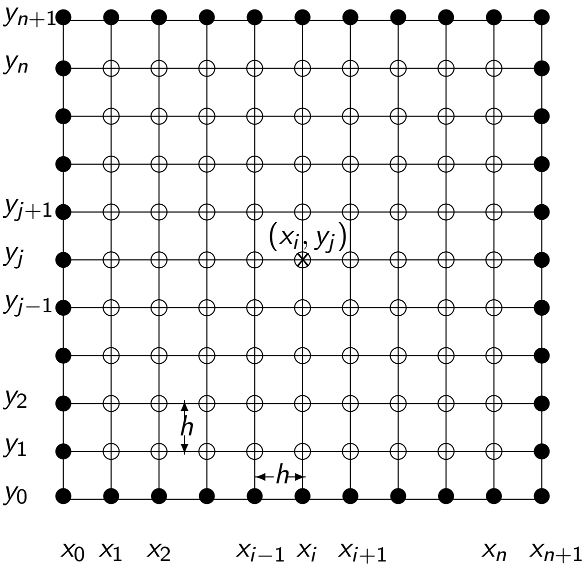
$$-\Delta u(x,y) = -(u_{xx} + u_{yy}) = f(x,y) \quad (x,y) \in \Omega, \quad u(x,y) = 0 \quad \text{on } \Gamma$$

Step 1: Overlay domain with grid

For simplicity set $\Delta x = \Delta y = h = 1/(n+1)$ and set

$$\begin{aligned} x_0 &= 0,\ x_1 = x_0 + h, \ldots,\ x_i = x_{i-1} + h, \ldots,\ x_{n+1} = x_n + h = 1 \\ y_0 &= 0,\ y_1 = y_0 + h, \ldots,\ y_j = y_{j-1} + h, \ldots,\ y_{n+1} = y_n + h = 1\,. \end{aligned}$$

for $i, j = 0, 1, \ldots, n, n+1$.


y_{n+1}
y_n
y_{j+1}
y_j
y_{j-1}
y_2
y_1
y_0
(x_i, y_j)
h
h
x_0 x_1 x_2 x_{i-1} x_i x_{i+1} x_n x_{n+1}

Step 2: Determine difference quotients to replace derivatives

$$U_{i,j} \approx u(x_i, y_j) \text{ for } i, j = 0, 1, 2, \ldots, n+1$$

To write our difference quotient for u_{xx} we simply use the second centered difference in x (holding y fixed)

$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2}$$

and then use the analogous difference quotient in the y direction

$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2}.$$

Step 3: Write difference equations at generic point (x_i, y_j)

$$\frac{-U_{i-1,j} + 2U_{i,j} - U_{i+1,j}}{h^2} + \frac{-U_{i,j-1} + 2U_{i,j} - U_{i,j+1}}{h^2} = f(x_i, y_j)\,.$$

Multiplying by h^2 and combining terms yields

$$-U_{i-1,j} + 4U_{i,j} - U_{i+1,j} - U_{i,j-1} - U_{i,j+1} = h^2 f(x_i, y_j) \qquad i, j = 1, 2, \ldots, n\,. \tag{7}$$

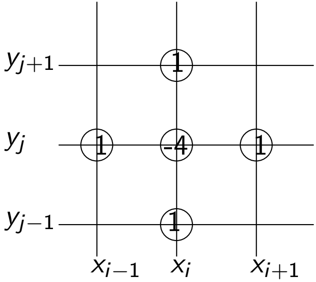
Clearly

$$U_{0,j} = U_{n+1,j} = 0, \quad j = 0, 1, \ldots, n+1$$

and

$$U_{i,0} = U_{i,n+1} = 0 \quad i = 0, 1, 2, \ldots, n+1$$

Five point stencil for Δu



Step 4: Set up coefficient matrix and right hand side

$$
\begin{aligned}
4U_{1,1} - U_{2,1} - U_{1,2} &= h^2 f(x_1, y_1) \\
-U_{1,1} + 4U_{2,1} - U_{3,1} - U_{2,2} &= h^2 f(x_2, y_1) \\
&\vdots \\
-U_{n-1,1} + 4U_{n,1} - U_{n,2} &= h^2 f(x_n, y_1) \\
\\
4U_{1,2} - U_{2,2} - U_{1,3} - U_{1,1} &= h^2 f(x_1, y_2) \\
-U_{1,2} + 4U_{2,2} - U_{3,2} - U_{2,3} - U_{2,1} &= h^2 f(x_2, y_2) \\
&\vdots \\
-U_{n-1,2} + 4U_{n,2} - U_{n,3} - U_{n,1} &= h^2 f(x_n, y_2),
\end{aligned}
$$

What is the dimension of the resulting matrix?

Ordering along each row, the unknown vector is

$$\left(U_{1,1}, U_{2,1}, \cdots, U_{n,1} \middle| U_{1,2}, U_{2,2}, \cdots, U_{n,2} \middle| \cdots \middle| U_{1,n}, U_{2,n}, \cdots, U_{n,n} \right)^T$$

$$A = \begin{pmatrix} S & -I & & & & \\ -I & S & -I & & & \\ & -I & S & -I & & \\ & & \ddots & \ddots & \ddots & \\ & & & -I & S & -I \\ & & & & -I & S \end{pmatrix}$$

which is spd block tridiagonal and where S is an $n \times n$ matrix defined by

$$S = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix}$$

Handling Boundary Conditions

Types of BCs: Dirichlet, Neumann and Mixed

Inhomogeneous Dirichlet BCs: $u(x, y) = g(x, y) \neq 0$ on Γ

- Approach 1
  - unknown at each interior node - n^2 unknowns
  - modify the right hand side for each equation that involves a boundary term
- Approach 2
  - unknown at every node (including boundaries) - $(n+2)^2$ unknowns
  - at each boundary node add an equation satisfying boundary condition; e.g., at (x_0, y_j) add equation $U_{0,j} = g(x_0, y_j)$. Doesn't change structure of matrix, just adds rows with a one on the diagonal.

Example 8

$$-\Delta u = f(x,y) = -2\cos \pi y + \pi^2 (1+x)^2 \cos \pi y \quad 0 < x, y < 1$$

$u(x,0) = (1+x)^2, u(x,1) = -(1+x)^2, u(0,y) = \cos \pi y, u(1,y) = 4\cos \pi y$

where $u(x,y) = (1+x)^2 \cos \pi y$

First approach - unknowns at interior nodes Set $h = 1/4$, at $(x_1, y_1) = (\frac{1}{4}, \frac{1}{4})$

$$-U_{0,1} + 4U_{1,1} - U_{2,1} - U_{1,0} - U_{1,2} = h^2 f(\frac{1}{4}, \frac{1}{4})$$

which gives

$$+4U_{1,1} - U_{2,1} - U_{1,2} = h^2 f(\frac{1}{4}, \frac{1}{4}) + \cos \frac{\pi}{4} + (1 + \frac{1}{4})^2$$

at $(x_2, y_1) = (\frac{1}{2}, \frac{1}{4})$

$$-U_{1,1} + 4U_{2,1} - U_{3,1} - U_{2,0} - U_{2,2} = h^2 f(\frac{1}{2}, \frac{1}{4})$$

which gives

$$-U_{1,1} + 4U_{2,1} - U_{3,1} - U_{2,2} = h^2 f(\frac{1}{2}, \frac{1}{4}) + (1 + \frac{1}{2})^2$$

at $(x_3, y_1) = (\frac{3}{4}, \frac{1}{4})$

$$-U_{2,1} + 4U_{3,1} - U_{4,1} - U_{3,0} - U_{3,2} = h^2 f(\frac{3}{4}, \frac{1}{4})$$

which gives

$$-U_{2,1} + 4U_{3,1} - U_{3,2} - U_{1,2} = h^2 f(\frac{3}{4}, \frac{1}{4}) + 4\cos\frac{\pi}{4} + (1 + \frac{3}{4})^2$$

Second approach - unknowns at every node

$$
\begin{aligned}
U_{0,0} &= (1+0)^2 \\
U_{1,0} &= (1+\frac{1}{4})^2 \\
U_{2,0} &= (1+\frac{1}{2})^2 \\
U_{3,0} &= (1+\frac{3}{4})^2 \\
U_{4,0} &= (1+1)^2 \\
U_{0,1} &= \cos\frac{\pi}{4} \\
-U_{0,1}+4U_{1,1}-U_{2,1}-U_{1,0}-U_{1,2} &= h^2 f(\frac{1}{4},\frac{1}{4}) \\
-U_{1,1}+4U_{2,1}-U_{3,1}-U_{2,0}-U_{2,2} &= h^2 f(\frac{1}{2},\frac{1}{4}) \\
-U_{2,1}+4U_{3,1}-U_{2,1}-U_{3,0}-U_{3,2} &= h^2 f(\frac{3}{4},\frac{1}{4}) \\
U_{4,1} &= 4\cos\frac{\pi}{4} \\
&\vdots
\end{aligned}
$$

Neumann Boundary Conditions

- Remember that when we impose a Neumann boundary condition the unknown itself is not given at the boundary so we have to solve for it there.
- This means that our unknowns are not just at the interior points but also at any point where a Neumann condition is specified.

Let $\Omega = (0,1) \times (0,1)$ and assume $\partial u / \partial \vec{n} = g(x,y)$ along the sides $x = 0$ and $x = 1$. Because the outer normal is $\pm \vec{i}$ this flux condition is just $\pm u_x = g$. This means that we have to replace u_x with a difference quotient and write this equation at the boundary node. We can use a one-sided difference such as

$$u_x(x_0, y_j) = \frac{U_{1,j} - U_{0,j}}{h} = g(x_0, y_j)$$

at the left boundary. The problem with this is that it is a first order accurate approximation whereas in the interior we are using a second order accurate approximation.

We have seen that the centered difference approximation

$$u_x(x_i, y_j) \approx \frac{u(x_{i+1}, y_j) - u(x_{i-1} y_j)}{2h}$$

is second order accurate. But if we write this at the point (x_0, y_j), then there is no grid point to its left because (x_0, y_j) lies on the boundary. To see how to implement this centered difference approximation for the Neumann boundary condition first consider the simplified case where $\partial u/\partial \vec{n} = 0$. The finite difference equation at the point (x_0, y_j) is

$$U_{-1,j} + 4U_{0,j} - U_{1,j} - U_{0,j+1} - U_{0,j-1} = h^2 f(x_0, y_j)$$

and the centered difference approximation to $-u_x = 0$ at (x_0, y_j) is

$$\frac{U_{1,j} - U_{-1,j}}{2h} = 0 \quad \Longrightarrow \quad U_{-1,j} = U_{1,j}\,.$$

We then substitute this into the difference equation at (x_0, y_j) to get

$$U_{1,j} + 4U_{0,j} - U_{1,j} - U_{0,j+1} - U_{0,j-1} = h^2 f(x_0, y_j)$$

or

$$4U_{0,j} - U_{0,j+1} - U_{0,j-1} = h^2 f(x_0, y_j)\,.$$

So we need to modify all the equations written at $x = 0$ or $x = 1$ where the Neumann boundary condition is imposed.

If the Neumann boundary condition is inhomogeneous we have

$$\frac{U_{1,j} - U_{-1,j}}{2h} = g(x_0, y_j) \quad \Longrightarrow \quad U_{-1,j} = U_{1,j} - 2hg(x_0, y_j)$$

and we substitute this into the difference equation for $U_{-1,j}$.

Of course if the domain is not a rectangle then the procedure is more complicated because the Neumann boundary condition $\partial u / \partial \vec{n}$ does not reduce to u_x or u_y.