Math 315: Numerical Analysis
Emory University
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Numerical Differentiation

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1 Introduction

Partial differential Equations (PDEs) are cool. One could easily spend your entire academic career really understanding one single PDE.
The first difference is that we discretize the continuous problem and do computations at those discrete points

2 Difference Quotient as Motivation

In calculus I, we learn the limit definiton of the derivative

Definition 2.1 (Limit Definition of a derivative)**.** Let f be a differentiable function, then we can write the derivitive of f at x by the limit of the difference quotient:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

This means that if we use a small h, we can approximate the derivative of a function with the difference quotient.

Remark. What is a good h that we should use? If we choose h too large, then the finite difference approximation will not be accurate, but if we pick h too small, we might end up with numerical error considerations.

2.1 First Order Approximation

2.1.1 Deriving the Rule

Theorem 2.1 (Taylor's Theorem)**.**

$$\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{f''(\xi)}{2}h^2, \quad \xi \in (x, x+h) \\
&= f(x) + hf'(x) + \mathcal{O}\big(h^2\big) \\
hf'(x) &= f(x+h) - f(x) + \mathcal{O}\big(h^2\big) \\
f'(x) &\approx \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)
\end{aligned}$$

Definition 2.2 (Forward Difference Approximation).

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h) \tag{1}$$

Definition 2.3 (Backward Difference Approximation).

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h) \tag{2}$$

Definition 2.4 (Centered Difference Approximation).

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}\big(h^2\big) \tag{3}$$

2.1.2 In Matrix Form

Using the uniform discretization, we can see

$$A_{\mathrm{F}} f(x) = \frac{1}{h} \begin{pmatrix} -1 & 1 & & & & & 0 \\ & -1 & 1 & & & & \\ & & \ddots & \ddots & & & \\ & & & -1 & 1 & & \\ & & & & \ddots & \ddots & \\ 0 & & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_i) \\ f(x_{i+1}) \\ \vdots \\ f(x_n) \end{pmatrix}$$

$$A_{\mathrm{B}} f(x) = \frac{1}{h} \begin{pmatrix} 1 & -1 & & & & & 0 \\ & 1 & -1 & & & & \\ & & \ddots & \ddots & & & \\ & & & 1 & -1 & & \\ & & & & \ddots & \ddots & \\ 0 & & & & & 1 & -1 \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_i) \\ f(x_{i+1}) \\ \vdots \\ f(x_n) \end{pmatrix}$$

$$A_{\mathrm{C}} f(x) = \frac{1}{h} \begin{pmatrix} -1 & 1 & & & & & & 0 \\ -1 & 0 & 1 & & & & & \\ & \ddots & \ddots & \ddots & & & & \\ & & -1 & 0 & 1 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & -1 & 0 & 1 & \\ & & & & & -1 & 0 & 1 \\ 0 & & & & & & -1 & 1 \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{i-1}) \\ f(x_i) \\ f(x_{i+1}) \\ \vdots \\ f(x_n) \end{pmatrix}$$

2.2 Second Order Approximation

$$\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \mathcal{O}\big(h^4\big) \\
f(x-h) &= f(x) - hf'(x) + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \mathcal{O}\big(h^4\big) \\
f(x+h) + f(x-h) &= 2f(x) + 2\frac{f''(x)}{2}h^2 + \mathcal{O}\big(h^4\big) \\
h^2 f''(x) &= +f(x+h) + f(x-h) - 2f(x) + \mathcal{O}\big(h^4\big) \\
f''(x) &\approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}\big(h^2\big)
\end{aligned}$$

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

$$B_{\mathrm{C}} f(x) = \frac{1}{h^2}\begin{pmatrix}
-2 & 1 & & & & & & 0 \\
1 & -2 & 1 & & & & & \\
 & \ddots & \ddots & \ddots & & & & \\
 & & 1 & -2 & 1 & & & \\
 & & & \ddots & \ddots & \ddots & & \\
 & & & & 1 & -2 & 1 & \\
 & & & & & 1 & -2 & 1 \\
0 & & & & & & 1 & -2
\end{pmatrix}\begin{pmatrix}
f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{i-1}) \\ f(x_i) \\ f(x_{i+1}) \\ \vdots \\ f(x_n)
\end{pmatrix}$$

3 Two Dimensional Problems

In class you solved the 1D Laplacian, namely

$$\begin{cases} -\Delta u = 0 & \in \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{4}$$

This was doable because $\Omega = [0, 1]$, so you would discretize it with a uniform mesh, and since it was only 1D

$$\begin{aligned}
-\Delta u &= -\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} \\
&\approx \frac{-u(x+h) + 2u(x) - u(x-h)}{h^2}.
\end{aligned}$$

But how can this generalize to 2 or higher dimensions?

$$-\Delta u = -\frac{\partial^2 u}{\partial x_1^2} - \frac{\partial^2 u}{\partial x_2^2} - \cdots - \frac{\partial^2 u}{\partial x_n^2} \tag{5}$$

So for $d = 2$, we see

$$-\Delta u = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2}$$

But observe,

$$\frac{\partial^2 u(x,y)}{\partial x^2} \approx \frac{u(x-h,y) - 2u(x,y) + u(x+h,y)}{h^2}$$
$$\frac{\partial^2 u(x,y)}{\partial y^2} \approx \frac{u(x,y-h) - 2u(x,y) + u(x,y+h)}{h^2}$$

Combining these into the Laplacian, we see

$$u_{i,j} = \frac{1}{4}\left(u_{i,j-1} + u_{i-1,j} + u_{i,j+1} + u_{i+1,j}\right) \tag{6}$$

3.1 Finite Difference Stencil

Sometimes indexing is confusing, so we will pictorially illustrate these schemes.

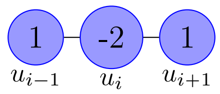

Figure 1: The three point stencil in 1D.

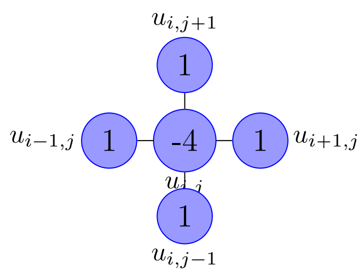

Figure 2: The five point stencil in 2D.

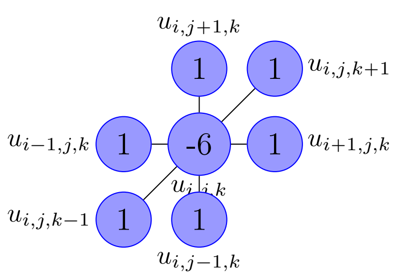

Figure 3: The seven point stencil in 3D.

But what does the matrix look like for this set up? We will leverage what we know about the 3 point stencil to solve this. First for adjacent nodes along the same row, we essentially have the 1,-4,1 stencil coming from nodes $u_{i-1,j}, u_{i,j}$, and $u_{i+1,j}$.

$$\mathbf{T} = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{pmatrix} \tag{7}$$

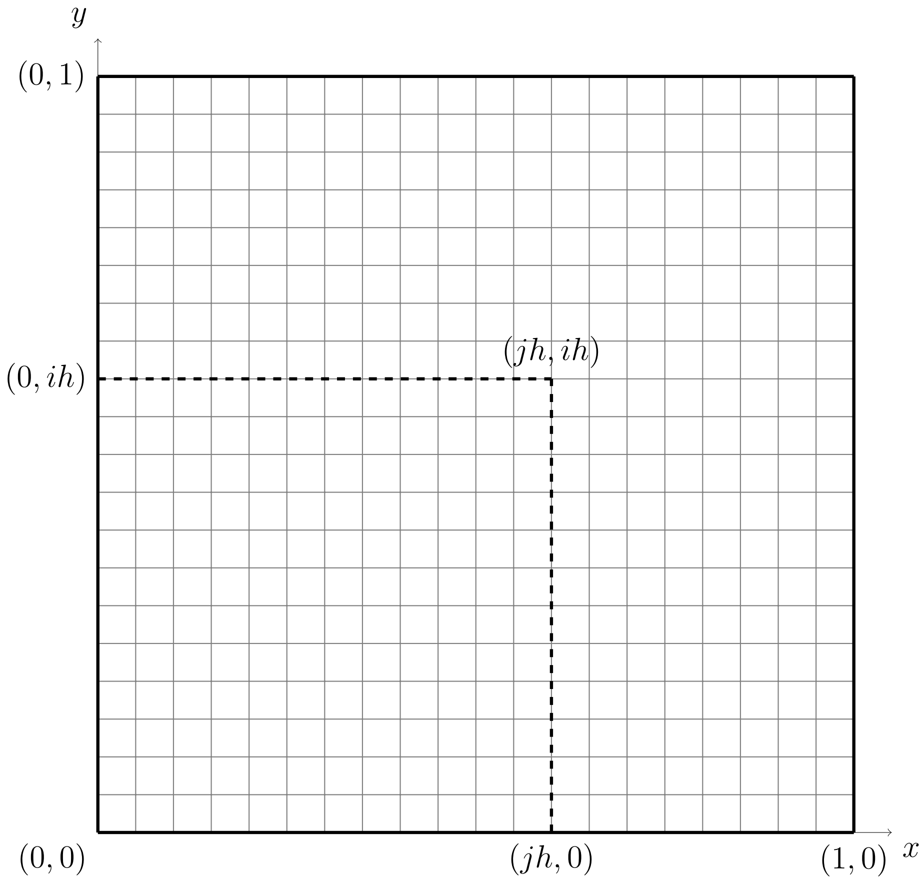

Figure 4: A 2D uniform grid for solving Laplace's equation.

Notice if there are m interior nodes ($m+2$ total nodes per row including the boundary), then $\mathbf{T} \in \mathbb{R}^{m\times m}$. But where do we put the values for $u_{i,j-1}, u_{i,j+1}$? We need these values to be at least m nodes away from the point $u_{i,j}$ because of how we order the nodes. So we need a -1 in the $((i+m), j)$ position. Since $\mathbf{T}$ is $m \times m$, we know it will be outside of the $\mathbf{T}$ matrix, but only by i nodes. This is true for all i, j. Similarly this is true if we examined the $(i, (j+m))$ position. So we end up with a matrix that has this form:

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & -\mathbf{I} & & \\ -\mathbf{I} & \mathbf{T} & \ddots & \\ & \ddots & \ddots & -\mathbf{I} \\ & & -\mathbf{I} & \mathbf{T} \end{pmatrix} \tag{8}$$

This type of matrix is known to have block tri-diagonal structure.
Maybe it would be beneficial to think of the nodes columns at a time, so

$$\mathbf{u}_j = \begin{pmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{m,j} \end{pmatrix}, \qquad \forall j = 1, 2, \cdots, m.$$

Then we can write the 5 point stencil as

$$-\mathbf{u}_{j-1} + \mathbf{T}\mathbf{u}_j - \mathbf{u}_{j+1} = \mathbf{f} \tag{9}$$

Then if we stack these $\mathbf{u}_j$ vectors of nodes on top of each other, we see

$$\mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_m \end{pmatrix},$$

so we have $n = m \times m$ linear equations for n unknowns, we again arrive at

$$\mathbf{A}\mathbf{u} = \mathbf{f} \tag{10}$$

4 Sparsity and Solving These Linear Systems

Typically the LHS can be used multiple times against multiple RHS. This leads us to believe that $\mathbf{A} = \mathbf{LU}$ might be a helpful in this problem.

Definition 4.1 ((p,q) banded matrices)**.** Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ and let p and q be integers between 0 and $n-1$. We call $\mathbf{A}$ a band matrix of upper bandwidth p and lower bandwidth q if $a_{ij} = 0$ for $j > i + p$ or $i > j + q$. In shorthand, $\mathbf{A}$ is a (p,q) *banded matrix.*

Example 4.1. *For a diagonal matrix* $\mathbf{D}$*,* $p = q = 0$*. For the* $[1, -2, 1]$ *tridiagonal matrix from finite differences in 1D, we have* $p = q = 1$*. Can anyone tell me what the bandwidth of the banded matrix for finite differences in 2D is?*

Theorem 4.2 (LU Factorization fro Banded Matrices.)**.** *If* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *is an invertible* (p,q) *banded matrix then performing LU factorization* with no pivoting*, then* $\mathbf{U}$ *is an upper triangular matrix with upper bandwidth* p*. Similarly,* $\mathbf{L}$ *is a unit lower triangular matrix with lower bandwidth* q*.*

Proof. Carry out the LU factorization precedure. □

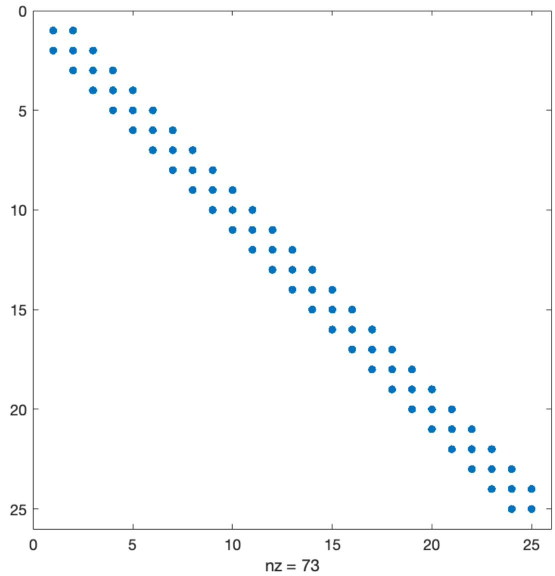

Figure 5: Sparsity pattern for 1D finite difference.

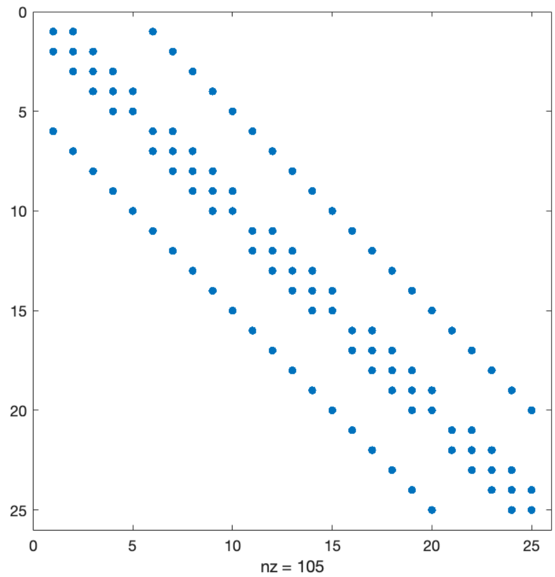

Figure 6: Sparsity pattern for 2D finite difference.

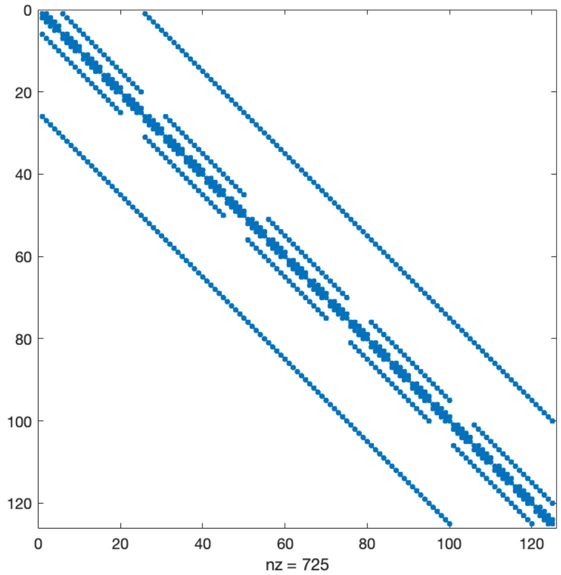

Figure 7: Sparsity pattern for 3D finite difference.

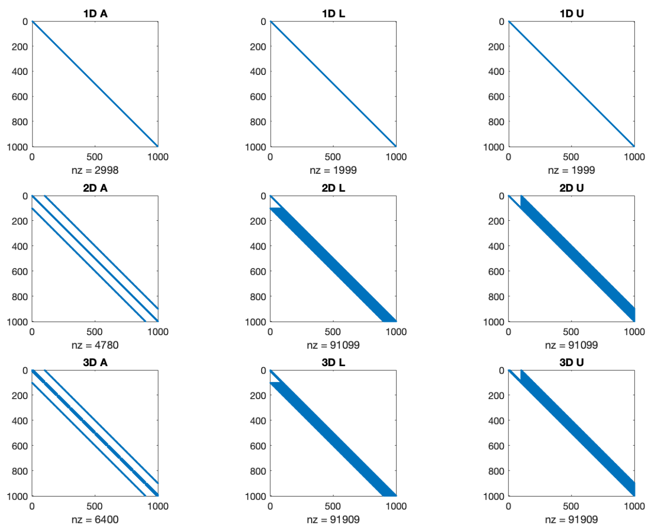

Figure 8: Sparsity pattern for finite differences, and their LU factors.