Advanced Computation:
Computational Electromagnetics

The Finite-Difference Method

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Outline

- Finite-Difference Approximations
- Finite-Difference Method
- Numerical Boundary Conditions
- Matrix Operators

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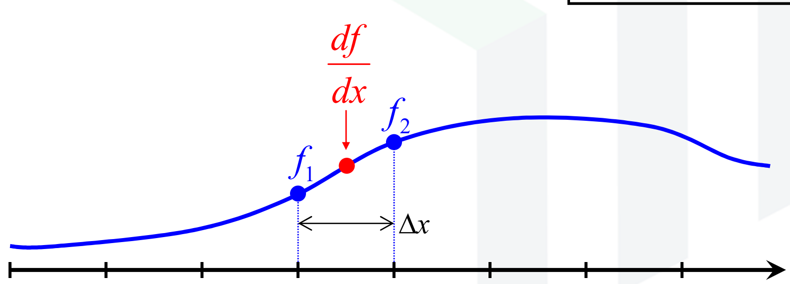
Finite Difference Approximations

The Basic Finite-Difference Approximation

$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

second-order accurate first-order derivative



This is the only finite-difference approximation we will use in this course!

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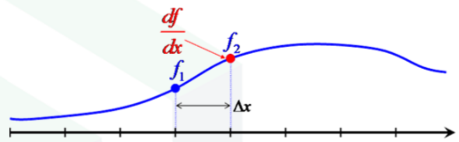
Types of Finite-Difference Approximations

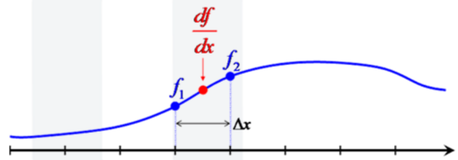
Backward Finite-Difference

$$\frac{df_2}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$



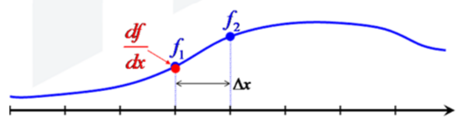
Central Finite-Difference

$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$



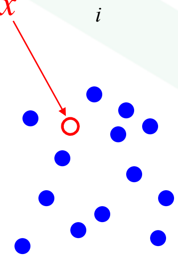
Forward Finite-Difference

$$\frac{df_1}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$



The Generalized Finite-Difference

$$\frac{d^n f}{dx^n} \cong \sum_i a_i f_i$$



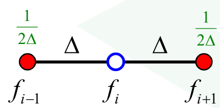
The derivative of any order of a function at any position can be approximated as a linear sum of known points of that function.

$$L\{f\} \cong \sum_i a_i f_i$$

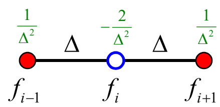
In fact, any linear operation on the function can be approximated as a linear sum of known points of that function.

Finite-Difference "Atoms"

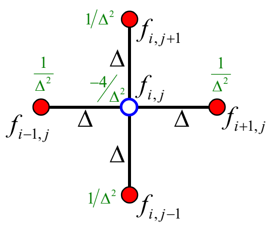
Any finite-difference approximation can be summarized graphically as an "atom."



$$\frac{d}{dx}f\left(x_i\right) \cong \frac{f_{i+1}-f_{i-1}}{2\Delta}$$



$$\frac{d^2}{dx^2}f\left(x_i\right) \cong \frac{f_{i+1}-2f_i+f_{i-1}}{\Delta^2}$$



$$\nabla^2 f\left(x_i\right) \cong \frac{f_{i+1,j}-2f_{i,j}+f_{i-1,j}}{\Delta^2}+\frac{f_{i,j+1}-2f_{i,j}+f_{i,j-1}}{\Delta^2}$$

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Finite-Difference Method

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Overview of Our Approach to FDM

1. Identify and write the governing equation(s).

$$a(x)\frac{\partial^2}{\partial x^2}f(x)+\gamma b(x)\frac{\partial}{\partial x}f(x)+c(x)f(x)=g(x)$$

2. Write the matrix form of this equation going term-by-term.

$$a(x)\frac{\partial^2}{\partial x^2}f(x)+\gamma b(x)\frac{\partial}{\partial x}f(x)+c(x)f(x)=g(x)$$

$$[A]\left[D_x^2\right][f]+\gamma[B][D_x][f]+[C][f]=[g]$$

3. Put matrix equation in the standard form of $[L][f] = [g]$.

$$[L][f]=[g] \qquad \text{where} \quad [L]=[A]\left[D_x^2\right]+\gamma[B][D_x]+[C]$$

```
L = A*D2X + y*B*DX + C;
```

4. Solve $[L][f] = [g]$.

$$[f]=[L]^{-1}[g]$$

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What's the Catch?

$$[L]=[A]\left[D_x^2\right]+\gamma[B][D_x]+[C]$$

How are these matrices constructed? What is their meaning?

$$\gamma \qquad [A] \quad [B] \quad [C] \qquad [D_x] \quad \left[D_x^2\right]$$

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Functions Vs. Operations (1 of 2)

$$a(x)\frac{\partial^2}{\partial x^2}f(x)+\gamma b(x)\frac{\partial}{\partial x}f(x)+c(x)f(x)=g(x)$$

Operations

Everything else in a differential equation is something that operates on a function.

$a(x),b(x),c(x) \equiv$ point-by-point multiplication on $f(x)$

$\frac{\partial}{\partial x},\frac{\partial^2}{\partial x^2} \equiv$ calculates derivatives of $f(x)$

$\gamma \equiv$ scales entire $f(x)$

Functions

The only time functions appear in a differential equation is as the unknown or as the excitation.

$f(x) \equiv$ unknown

$g(x) \equiv$ excitation

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Functions Vs. Operations (2 of 2)

$$[A]\left[D_x^2\right][f]+\gamma[B][D_x][f]+[C][f]=[g]$$

Operations

Operations are always stored in square matrices. Any linear operation can be put into matrix form.

$$[L]=\begin{bmatrix} l_{11} & l_{12} & & l_{1M} \\ l_{21} & l_{22} & \cdots & l_{2M} \\ & \vdots & & \\ l_{M1} & l_{M2} & & l_{MM} \end{bmatrix}$$

Functions

Functions are stored as column vectors.

$$[f]=\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_M \end{bmatrix} \qquad [g]=\begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_M \end{bmatrix}$$

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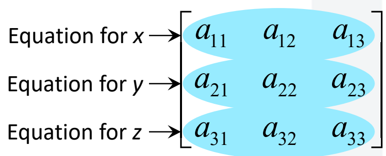
Interpretation of Matrices

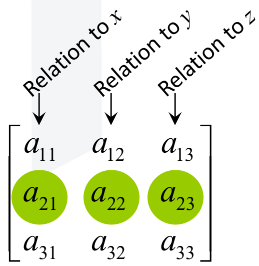
$$a_{11}x + a_{12}y + a_{13}z = b_1$$
$$a_{21}x + a_{22}y + a_{23}z = b_2$$
$$a_{31}x + a_{32}y + a_{33}z = b_3$$

$$\Rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

EQUATION FOR…



RELATION TO…



From a purely mathematical perspective, this interpretation does not make sense. This interpretation will be highly useful and insightful because of how we derive the equations.

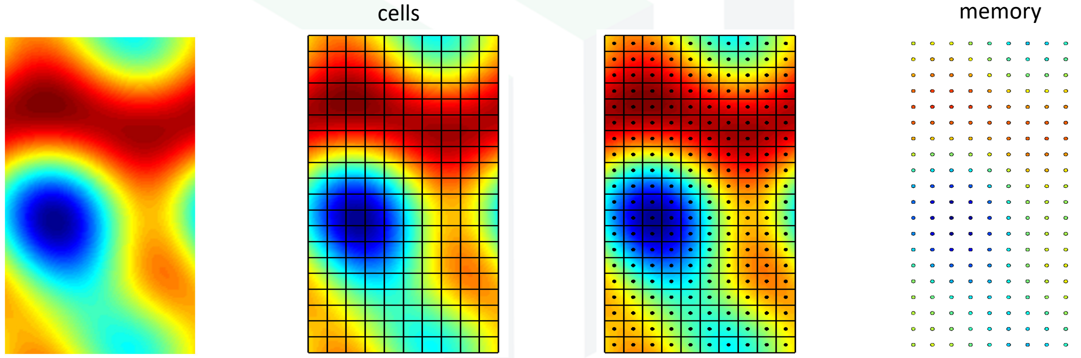
Representing Functions on a Grid

Example physical (continuous) 2D function

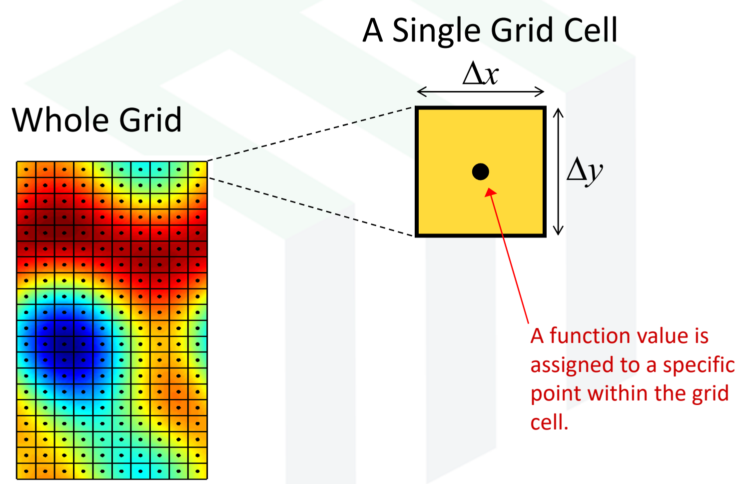
A grid is constructed by dividing space into discrete cells

Function is known only at discrete points

Representation of what is actually stored in memory



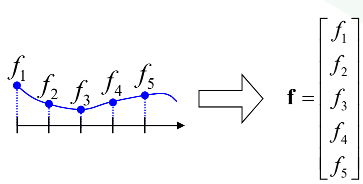
Grid Cells



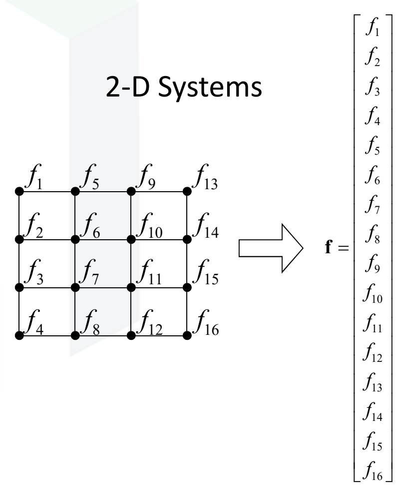
$$\Delta x, \Delta y \equiv \text{grid resolution parameters}$$

Functions are Put Into Column Vectors

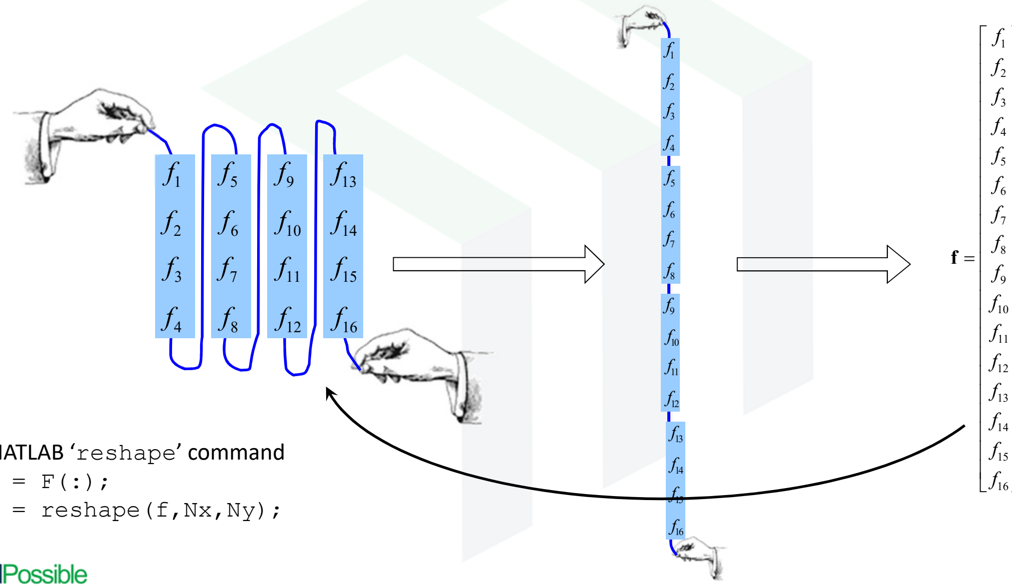
1-D Systems



2-D Systems



Putting Functions into Column Vectors



MATLAB ‘`reshape`’ command

```
f = F(:);
F = reshape(f,Nx,Ny);
```

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Locating Points in Column Vectors

1D Grids

Node located at `nx` → `m = nx`

2D Grids

Node located at `nx,ny` → `m = (ny – 1)*Nx + nx`

3D Grids

Node located at `nx,ny,nz`

→ `m = (nz – 1)*Nx*Ny + (ny – 1)*Nx + nx`

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The Finite-Difference Method

Differential Equation to Solve

$$\frac{df(x)}{dx} - a(x) f(x) = g(x)$$

Conventional FDM

Tedious, but not difficult.

$$\frac{f(k+1) - f(k-1)}{2\Delta x} - a(k) f(k) = g(k)$$

Very difficult and tedious.

$$[L][f] = [g]$$

Easy.

Improved FDM

Almost effortless.

$$[D_x][f] - [a][f] = [g]$$

Very easy and clean

$$[L][f] = [g]$$
$$[L] = [D_x] - [a]$$

Easy.

$$[f] = [L]^{-1}[g]$$

Most time consuming step.

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Conventional FDM (1 of 3)

Step 1 – Start with a differential equation to be solved.

$$\frac{d^2 f}{dx^2} - a\frac{df}{dx} - bf = c$$

Step 2 – Approximate the derivatives with finite differences.

$$\frac{f(k+1) - 2f(k) + f(k-1)}{\Delta^2} - a(k)\frac{f(k+1) - f(k-1)}{2\Delta} - b(k) f(k) = c(k)$$

IMPORTANT RULE: Every term in a finite-difference equation must exist at the same point.

Step 3 – Expand equation and collect common terms.

$$\frac{1}{\Delta^2} f(k+1) - \frac{2}{\Delta^2} f(k) + \frac{1}{\Delta^2} f(k-1) - \frac{a(k)}{2\Delta} f(k+1) + \frac{a(k)}{2\Delta} f(k-1) - b(k) f(k) = c(k)$$

$$\left[\frac{1}{\Delta^2} - \frac{a(k)}{2\Delta}\right] f(k+1) - \left[b(k) + \frac{2}{\Delta^2}\right] f(k) + \left[\frac{1}{\Delta^2} + \frac{a(k)}{2\Delta}\right] f(k-1) = c(k)$$

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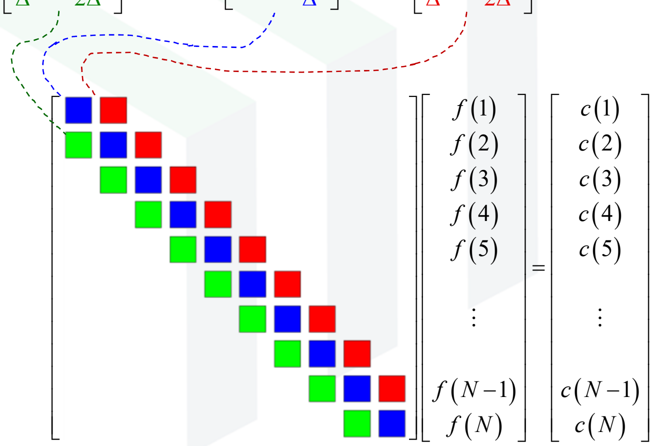
Conventional FDM (2 of 3)

Step 4 – The final equation is used to populate a matrix equation.

$$\left[\frac{1}{\Delta^2}+\frac{a(k)}{2\Delta}\right]f(k-1)-\left[b(k)+\frac{2}{\Delta^2}\right]f(k)+\left[\frac{1}{\Delta^2}-\frac{a(k)}{2\Delta}\right]f(k+1)=c(k)$$

Filling in the matrix like this can be a very difficult and tedious task for more complicated differential equations or for systems of differential equations.



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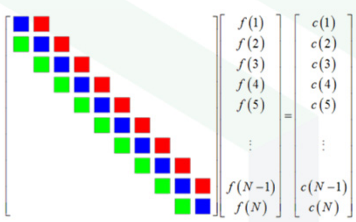
Conventional FDM (3 of 3)

Step 5 – The matrix equation is solved for the unknown function $f(x)$



$\Longrightarrow$

$$[L][f]=[c]$$

$$\mathbf{L}\mathbf{f}=\mathbf{c}$$

$\Downarrow$

$$[f]=[L]^{-1}[c]$$

$$\mathbf{f}=\mathbf{L}^{-1}\mathbf{c}$$

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Improved FDM

We want a very easy way to immediately write differential equations in matrix form. Starting with the same differential equation…

$$\frac{\partial^2 f}{\partial x^2} - a\frac{\partial f}{\partial x} - bf = c$$

We will develop a procedure by which this will be directly written in matrix form without having to explicitly handle any finite-differences.

$$\frac{\partial^2}{\partial x^2} f - a\frac{\partial}{\partial x} f - bf = c$$

$\mathbf{D}_x^{(2)}$, $\mathbf{A}$, $\mathbf{D}_x^{(1)}$, and $\mathbf{B}$ are square matrices that perform linear operations on the vector **f**.

$$\Downarrow$$

$$\mathbf{D}_x^{(2)}\mathbf{f} - \mathbf{A}\mathbf{D}_x^{(1)}\mathbf{f} - \mathbf{B}\mathbf{f} = \mathbf{c} \quad \Rightarrow \quad \underbrace{\left[\mathbf{D}_x^{(2)} - \mathbf{A}\mathbf{D}_x^{(1)} - \mathbf{B}\right]}_{\mathbf{L}=[L]}\mathbf{f} = \mathbf{c}$$

$$\mathbf{f} = \mathbf{L}^{-1}\mathbf{c}$$

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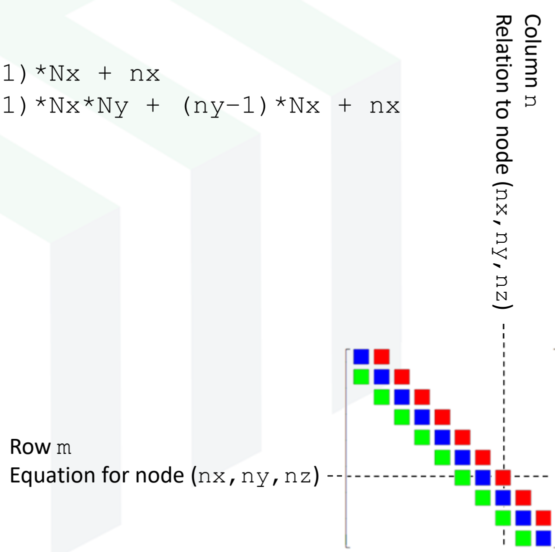
Locating Points in Matrices

1D → `m or n = nx`
2D → `m or n = (ny-1)*Nx + nx`
3D → `m or n = (nz-1)*Nx*Ny + (ny-1)*Nx + nx`



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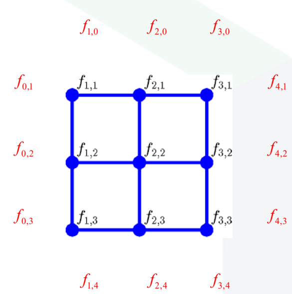
Numerical Boundary Conditions

The Problem at the Boundaries

Suppose it is desired to solve the following differential equation on a 3×3 grid.

$$\frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} = g(x,y) \quad \rightarrow \quad \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{\Delta x^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{\Delta y^2} = g_{i,j}$$



$$\frac{f_{2,1} - 2f_{1,1} + f_{0,1}}{\Delta x^2} + \frac{f_{1,2} - 2f_{1,1} + f_{1,0}}{\Delta y^2} = g_{1,1}$$

$$\frac{f_{3,1} - 2f_{2,1} + f_{1,1}}{\Delta x^2} + \frac{f_{2,2} - 2f_{2,1} + f_{2,0}}{\Delta y^2} = g_{2,1}$$

$$\frac{f_{4,1} - 2f_{3,1} + f_{2,1}}{\Delta x^2} + \frac{f_{3,2} - 2f_{3,1} + f_{3,0}}{\Delta y^2} = g_{3,1}$$

$$\frac{f_{2,2} - 2f_{1,2} + f_{0,2}}{\Delta x^2} + \frac{f_{1,3} - 2f_{1,2} + f_{1,1}}{\Delta y^2} = g_{1,2}$$

$$\frac{f_{3,2} - 2f_{2,2} + f_{1,2}}{\Delta x^2} + \frac{f_{2,3} - 2f_{2,2} + f_{2,1}}{\Delta y^2} = g_{2,2}$$

$$\frac{f_{4,2} - 2f_{3,2} + f_{2,2}}{\Delta x^2} + \frac{f_{3,3} - 2f_{3,2} + f_{3,1}}{\Delta y^2} = g_{3,2}$$

$$\frac{f_{2,3} - 2f_{1,3} + f_{0,3}}{\Delta x^2} + \frac{f_{1,4} - 2f_{1,3} + f_{1,2}}{\Delta y^2} = g_{1,3}$$

$$\frac{f_{3,3} - 2f_{2,3} + f_{1,3}}{\Delta x^2} + \frac{f_{2,4} - 2f_{2,3} + f_{2,2}}{\Delta y^2} = g_{2,3}$$

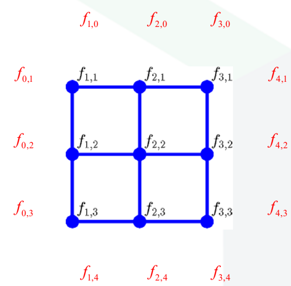
$$\frac{f_{4,3} - 2f_{3,3} + f_{2,3}}{\Delta x^2} + \frac{f_{3,4} - 2f_{3,3} + f_{3,2}}{\Delta y^2} = g_{3,3}$$

The terms in red exist outside of the grid.

How this is handled is called a *boundary condition*.

Dirichlet Boundary Conditions (1 of 2)

The simplest boundary condition is to assume that all values of $f(x, y)$ outside of the grid are zero.



$$\frac{f_{2,1}-2f_{1,1}+0}{\Delta x^2}+\frac{f_{1,2}-2f_{1,1}+0}{\Delta y^2}=g_{1,1}$$
$$\frac{f_{3,1}-2f_{2,1}+f_{1,1}}{\Delta x^2}+\frac{f_{2,2}-2f_{2,1}+0}{\Delta y^2}=g_{2,1}$$
$$\frac{0-2f_{3,1}+f_{2,1}}{\Delta x^2}+\frac{f_{3,2}-2f_{3,1}+0}{\Delta y^2}=g_{3,1}$$
$$\frac{f_{2,2}-2f_{1,2}+0}{\Delta x^2}+\frac{f_{1,3}-2f_{1,2}+f_{1,1}}{\Delta y^2}=g_{1,2}$$
$$\frac{f_{3,2}-2f_{2,2}+f_{1,2}}{\Delta x^2}+\frac{f_{2,3}-2f_{2,2}+f_{2,1}}{\Delta y^2}=g_{2,2}$$
$$\frac{0-2f_{3,2}+f_{2,2}}{\Delta x^2}+\frac{f_{3,3}-2f_{3,2}+f_{3,1}}{\Delta y^2}=g_{3,2}$$
$$\frac{f_{2,3}-2f_{1,3}+0}{\Delta x^2}+\frac{0-2f_{1,3}+f_{1,2}}{\Delta y^2}=g_{1,3}$$
$$\frac{f_{3,3}-2f_{2,3}+f_{1,3}}{\Delta x^2}+\frac{0-2f_{2,3}+f_{2,2}}{\Delta y^2}=g_{2,3}$$
$$\frac{0-2f_{3,3}+f_{2,3}}{\Delta x^2}+\frac{0-2f_{3,3}+f_{3,2}}{\Delta y^2}=g_{3,3}$$

Dirichlet Boundary Conditions (2 of 2)

Dirichlet boundary conditions assume function values from outside of the grid are zero.

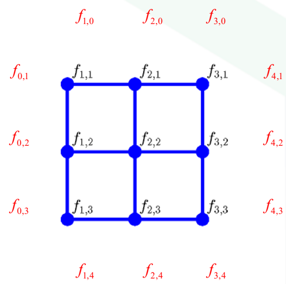
$$\frac{\partial f(x_1, y_i)}{\partial x} \cong \frac{f(x_2, y_i) - 0}{2\Delta_x}$$
$$\frac{\partial f(x_{N_x}, y_i)}{\partial x} \cong \frac{0 - f(x_{N_x-1}, y_i)}{2\Delta_x}$$
$$\frac{\partial f(x_i, y_1)}{\partial y} \cong \frac{f(x_i, y_2) - 0}{2\Delta_y}$$
$$\frac{\partial f(x_i, y_{N_y})}{\partial y} \cong \frac{0 - f(x_i, y_{N_y-1})}{2\Delta_y}$$

$$\frac{\partial^2 f(x_1, y_i)}{\partial x^2} \cong \frac{f(x_2, y_i) - 2f(x_1, y_i) + 0}{\Delta_x^2}$$
$$\frac{\partial^2 f(x_{N_x}, y_i)}{\partial x^2} \cong \frac{0 - 2f(x_{N_x}, y_i) + f(x_{N_x-1}, y_i)}{\Delta_x^2}$$
$$\frac{\partial^2 f(x_i, y_1)}{\partial y^2} \cong \frac{f(x_i, y_2) - 2f(x_i, y_1) + 0}{\Delta_y^2}$$
$$\frac{\partial^2 f(x_i, y_{N_y})}{\partial y^2} \cong \frac{0 - 2f(x_i, y_{N_y}) + f(x_i, y_{N_y-1})}{\Delta_y^2}$$

Periodic Boundary Conditions (1 of 2)

If the function $f(x,y)$ is periodic, then the values from outside of the grid can be mapped to a value from inside the grid at the other side.

$$f_{0,j} = f_{3,j},\ f_{4,j} = f_{1,j},\ f_{i,0} = f_{i,3},\ \text{and}\ f_{i,4} = f_{i,1}$$



$$\frac{f_{2,1} - 2f_{1,1} + f_{3,1}}{\Delta x^2} + \frac{f_{1,2} - 2f_{1,1} + f_{1,3}}{\Delta y^2} = g_{1,1}$$

$$\frac{f_{3,1} - 2f_{2,1} + f_{1,1}}{\Delta x^2} + \frac{f_{2,2} - 2f_{2,1} + f_{2,3}}{\Delta y^2} = g_{2,1}$$

$$\frac{f_{1,1} - 2f_{3,1} + f_{2,1}}{\Delta x^2} + \frac{f_{3,2} - 2f_{3,1} + f_{3,3}}{\Delta y^2} = g_{3,1}$$

$$\frac{f_{2,2} - 2f_{1,2} + f_{3,2}}{\Delta x^2} + \frac{f_{1,3} - 2f_{1,2} + f_{1,1}}{\Delta y^2} = g_{1,2}$$

$$\frac{f_{3,2} - 2f_{2,2} + f_{1,2}}{\Delta x^2} + \frac{f_{2,3} - 2f_{2,2} + f_{2,1}}{\Delta y^2} = g_{2,2}$$

$$\frac{f_{1,2} - 2f_{3,2} + f_{2,2}}{\Delta x^2} + \frac{f_{3,3} - 2f_{3,2} + f_{3,1}}{\Delta y^2} = g_{3,2}$$

$$\frac{f_{2,3} - 2f_{1,3} + f_{3,3}}{\Delta x^2} + \frac{f_{1,1} - 2f_{1,3} + f_{1,2}}{\Delta y^2} = g_{1,3}$$

$$\frac{f_{3,3} - 2f_{2,3} + f_{1,3}}{\Delta x^2} + \frac{f_{2,1} - 2f_{2,3} + f_{2,2}}{\Delta y^2} = g_{2,3}$$

$$\frac{f_{1,3} - 2f_{3,3} + f_{2,3}}{\Delta x^2} + \frac{f_{3,1} - 2f_{3,3} + f_{3,2}}{\Delta y^2} = g_{3,3}$$

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Periodic Boundary Conditions (2 of 2)

Periodic boundary conditions assume function values from outside of the grid can be taken from the opposite side of the grid.

$$\frac{\partial f(x_1, y_i)}{\partial x} \cong \frac{f(x_2, y_i) - f(x_{N_x}, y_i)}{2\Delta_x}$$

$$\frac{\partial f(x_{N_x}, y_i)}{\partial x} \cong \frac{f(x_1, y_i) - f(x_{N_x-1}, y_i)}{2\Delta_x}$$

$$\frac{\partial f(x_i, y_1)}{\partial y} \cong \frac{f(x_i, y_2) - f(x_i, y_{N_y})}{2\Delta_y}$$

$$\frac{\partial f(x_i, y_{N_y})}{\partial y} \cong \frac{f(x_i, y_1) - f(x_i, y_{N_y-1})}{2\Delta_y}$$

$$\frac{\partial^2 f(x_1, y_i)}{\partial x^2} \cong \frac{f(x_2, y_i) - 2f(x_1, y_i) + f(x_{N_x}, y_i)}{\Delta_x^2}$$

$$\frac{\partial^2 f(x_{N_x}, y_i)}{\partial x^2} \cong \frac{f(x_1, y_i) - 2f(x_{N_x}, y_i) + f(x_{N_x-1}, y_i)}{\Delta_x^2}$$

$$\frac{\partial^2 f(x_i, y_1)}{\partial y^2} \cong \frac{f(x_i, y_2) - 2f(x_i, y_1) + f(x_i, y_{N_y})}{\Delta_y^2}$$

$$\frac{\partial^2 f(x_i, y_{N_y})}{\partial y^2} \cong \frac{f(x_i, y_1) - 2f(x_i, y_{N_y}) + f(x_i, y_{N_y-1})}{\Delta_y^2}$$

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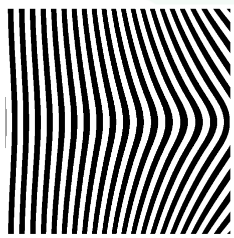
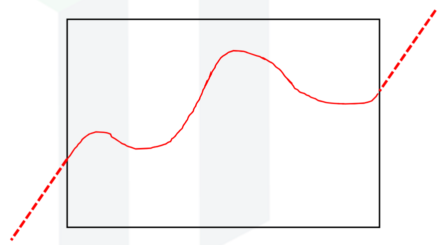
Neumann Boundary Conditions

We use Neumann boundary conditions for non-periodic functions or functions that are not zero at the boundary. Here the function continues linearly outside of the grid.



Spatially variant grating that is not periodic and not zero at the boundaries.



Here is a 1D function with Neumann boundaries

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Neumann BC's for 1D Function

The finite-difference approximation for a 1D function is

$$\left.\frac{df}{dx}\right|_i \cong \frac{f_{i+1} - f_{i-1}}{2\Delta_x}$$

At i=1, we have a problem…

$$\left.\frac{df}{dx}\right|_{i=1} \cong \frac{f_2 - f_0}{2\Delta_x}$$

This term doesn't exist!

$$\left.\frac{df}{dx}\right|_{i=1} \cong \frac{f_2 - f_1}{\Delta_x}$$

At $i=N_x$, we have another problem…

$$\left.\frac{df}{dx}\right|_{i=N_x} \cong \frac{f_{N_x+1} - f_{N_x-1}}{2\Delta_x}$$

This term doesn't exist!

$$\left.\frac{df}{dx}\right|_{i=N_x} \cong \frac{f_{N_x} - f_{N_x-1}}{\Delta_x}$$

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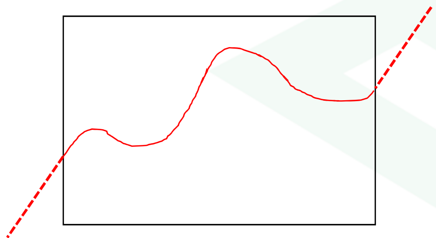
What About the 2nd-Order Derivatives for the Neumann Boundary Condition?



In order for the function to continue in a straight line, the second-order derivate should be set to zero at the boundary.

IMPORTANT: This is NOT Dirichlet boundary conditions. A Dirichlet BC sets the function itself to zero outside of the grid, not the derivative. Here, the 2nd-order derivative is set to zero.

$$\left.\frac{d^2 f}{dx^2}\right|_{i=1} \cong \frac{f_2 - f_1 + f_0}{\Delta_x^2} \rightarrow \left.\frac{d^2 f}{dx^2}\right|_{i=1} \cong 0$$

$$\left.\frac{d^2 f}{dx^2}\right|_{i=N_x} \cong \frac{f_{N_x+1} - f_{N_x} + f_{N_x-1}}{\Delta_x^2} \rightarrow \left.\frac{d^2 f}{dx^2}\right|_{i=N_x} \cong 0$$

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Neumann Boundary Conditions for 2D Functions

Neumann boundary conditions are used when a function should be continuous at the boundary. That is, the first-order derivative is continuous and the second-order derivative is zero.

$$\frac{\partial f(x_1, y_i)}{\partial x} \cong \frac{f(x_2, y_i) - f(x_1, y_i)}{\Delta_x} \qquad \frac{\partial^2 f(x_1, y_i)}{\partial x^2} = 0$$

$$\frac{\partial f(x_{N_x}, y_i)}{\partial x} \cong \frac{f(x_{N_x}, y_i) - f(x_{N_x-1}, y_i)}{\Delta_x} \qquad \frac{\partial^2 f(x_{N_x}, y_i)}{\partial x^2} = 0$$

$$\frac{\partial f(x_i, y_1)}{\partial y} \cong \frac{f(x_i, y_2) - f(x_i, y_1)}{\Delta_y} \qquad \frac{\partial^2 f(x_i, y_1)}{\partial y^2} = 0$$

$$\frac{\partial f(x_i, y_{N_y})}{\partial y} \cong \frac{f(x_i, y_{N_y}) - f(x_i, y_{N_y-1})}{\Delta_y} \qquad \frac{\partial^2 f(x_i, y_{N_y})}{\partial y^2} = 0$$

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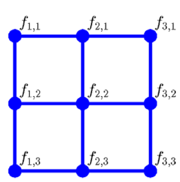
Matrix Operators

Origin of Matrix Operators

We start with a governing equation.

$$\frac{d^2 f(x,y)}{dx^2} = g(x,y)$$



We construct a grid to store the functions.

We approximate the governing equation with finite-differences and then write the finite-difference equation at each point the grid.

$$\frac{f_{2,1} - 2f_{1,1} + 0}{\Delta x^2} = g_{1,1}$$
$$\frac{f_{3,1} - 2f_{2,1} + f_{1,1}}{\Delta x^2} = g_{2,1}$$
$$\frac{0 - 2f_{3,1} + f_{2,1}}{\Delta x^2} = g_{3,1}$$
$$\frac{f_{2,2} - 2f_{1,2} + 0}{\Delta x^2} = g_{1,2}$$
$$\frac{f_{3,2} - 2f_{2,2} + f_{1,2}}{\Delta x^2} = g_{2,2}$$
$$\frac{0 - 2f_{3,2} + f_{2,2}}{\Delta x^2} = g_{3,2}$$
$$\frac{f_{2,3} - 2f_{1,3} + 0}{\Delta x^2} = g_{1,3}$$
$$\frac{f_{3,3} - 2f_{2,3} + f_{1,3}}{\Delta x^2} = g_{2,3}$$
$$\frac{0 - 2f_{3,3} + f_{2,3}}{\Delta x^2} = g_{3,3}$$

We collect the large set of equations into a single matrix equation.

$$\underbrace{\frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{\mathbf{D}_x^2} \cdot \begin{bmatrix} f_{1,1} \\ f_{2,1} \\ f_{3,1} \\ f_{1,2} \\ f_{2,2} \\ f_{3,2} \\ f_{1,3} \\ f_{2,3} \\ f_{3,3} \end{bmatrix} = \begin{bmatrix} g_{1,1} \\ g_{2,1} \\ g_{3,1} \\ g_{1,2} \\ g_{2,2} \\ g_{3,2} \\ g_{1,3} \\ g_{2,3} \\ g_{3,3} \end{bmatrix}$$

This matrix calculates the derivative of $f(x,y)$ and puts the answer in $g(x,y)$. This is a matrix operator.

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Other Matrix Operators

A square matrix can ***always*** be constructed to perform ***any*** linear operation on a function that is stored in a column vector.

$$\frac{d}{dx} f(x) \rightarrow \mathbf{D}_x \mathbf{f} = \underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{\mathbf{D}_x} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_N \end{bmatrix}$$

$$\text{FFT}\left[f(x)\right] \rightarrow \mathbf{Ff} \qquad g(x)f(x) \rightarrow \mathbf{Gf}$$

$$\int \left[f(x)\right] dx \rightarrow \left[\int\right]\mathbf{f} \qquad h(x) * f(x) \rightarrow \mathbf{Hf}$$

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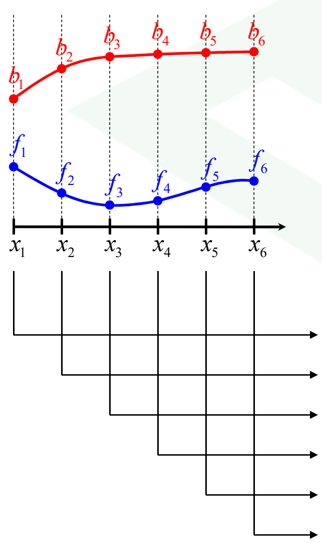
Point-by-Point Multiplication (1 of 2)



Since we are storing our "functions" in vector form, how do we perform a point-by-point multiplication using a square matrix?

$$b(x) f(x) \rightarrow \mathbf{Bf}$$

$$\underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}}_{\mathbf{Bf}}$$

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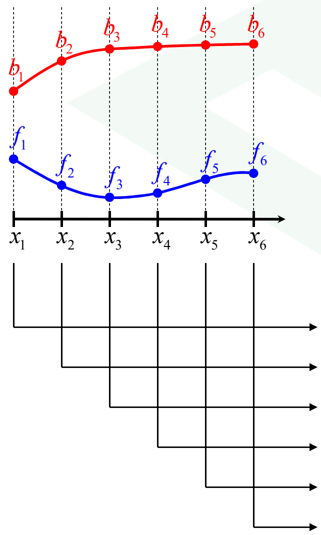
Point-by-Point Multiplication (2 of 2)



Since we are storing our "functions" in vector form, how do we perform a point-by-point multiplication using a square matrix?

$$b(x)\,f(x) \quad \rightarrow \quad \mathbf{Bf}$$

$$\underbrace{\begin{bmatrix} b_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_6 \end{bmatrix}}_{\mathbf{B}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}}_{\mathbf{Bf}}$$

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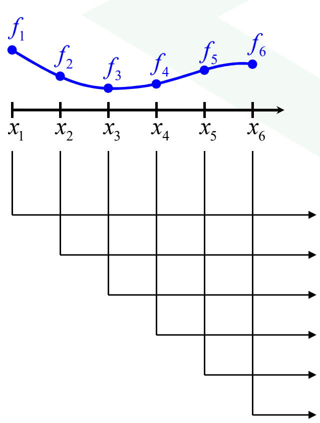
First-Order Partial Derivative (1 of 2)

How do we construct a square matrix so that when it premultiplies a vector, we get a vector containing the first-order partial derivative?

$$\frac{\partial}{\partial x} f(x) \quad \rightarrow \quad \mathbf{D}_x^{(1)}\mathbf{f}$$



$$\underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{\mathbf{D}_x^{(1)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_2 - f_0)/2\Delta_x \\ (f_3 - f_1)/2\Delta_x \\ (f_4 - f_2)/2\Delta_x \\ (f_5 - f_3)/2\Delta_x \\ (f_6 - f_4)/2\Delta_x \\ (f_7 - f_5)/2\Delta_x \end{bmatrix}}_{\mathbf{D}_x^{(1)}\mathbf{f}}$$

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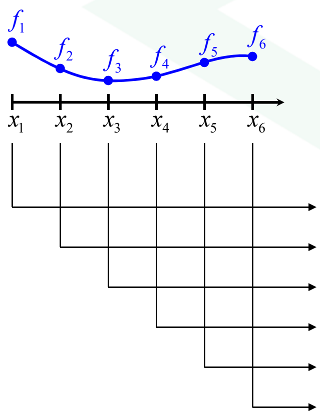
First-Order Partial Derivative (2 of 2)

How do we construct a square matrix so that when it premultiplies a vector, we get a vector containing the first-order partial derivative?

$$\frac{\partial}{\partial x} f(x) \rightarrow \mathbf{D}_x^{(1)} \mathbf{f}$$



$$\underbrace{\frac{1}{2\Delta_x}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}}_{\mathbf{D}_x^{(1)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_2 - f_0)/2\Delta_x \\ (f_3 - f_1)/2\Delta_x \\ (f_4 - f_2)/2\Delta_x \\ (f_5 - f_3)/2\Delta_x \\ (f_6 - f_4)/2\Delta_x \\ (f_7 - f_5)/2\Delta_x \end{bmatrix}}_{\mathbf{D}_x^{(1)}\mathbf{f}}$$

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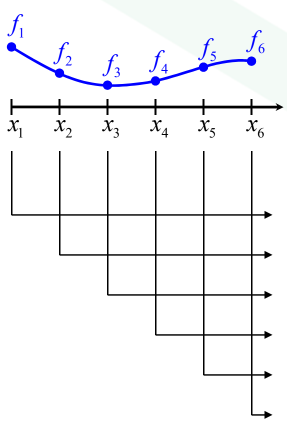
Second-Order Partial Derivative (1 of 2)

How do we construct a square matrix so that when it premultiplies a vector, we get a vector containing the second-order partial derivative?

$$\frac{\partial^2}{\partial x^2} f(x) \rightarrow \mathbf{D}_x^{(2)} \mathbf{f}$$



$$\underbrace{\begin{bmatrix} \\ & & ? & & \\ \\ \end{bmatrix}}_{\mathbf{D}_x^{(2)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_2 - 2f_1 + f_0)/\Delta_x^2 \\ (f_3 - 2f_2 + f_1)/\Delta_x^2 \\ (f_4 - 2f_3 + f_2)/\Delta_x^2 \\ (f_5 - 2f_4 + f_3)/\Delta_x^2 \\ (f_6 - 2f_5 + f_4)/\Delta_x^2 \\ (f_7 - 2f_6 + f_5)/\Delta_x^2 \end{bmatrix}}_{\mathbf{D}_x^{(2)}\mathbf{f}}$$

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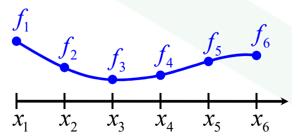
Second-Order Partial Derivative (2 of 2)

How do we construct a square matrix so that when it premultiplies a vector, we get a vector containing the second-order partial derivative?

$$\frac{\partial^2}{\partial x^2} f(x) \quad \rightarrow \quad \mathbf{D}_x^{(2)} \mathbf{f}$$



$$\underbrace{\frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{\mathbf{D}_x^{(2)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_2 - 2f_1 + f_0)/\Delta_x^2 \\ (f_3 - 2f_2 + f_1)/\Delta_x^2 \\ (f_4 - 2f_3 + f_2)/\Delta_x^2 \\ (f_5 - 2f_4 + f_3)/\Delta_x^2 \\ (f_6 - 2f_5 + f_4)/\Delta_x^2 \\ (f_7 - 2f_6 + f_5)/\Delta_x^2 \end{bmatrix}}_{\mathbf{D}_x^{(2)}\mathbf{f}}$$

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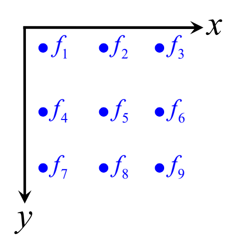
What About 2D Grids (1 of 2)?

Two-dimensional grids are a little more difficult

$$\frac{\partial^2}{\partial x^2} f(x,y) \quad \rightarrow \quad \mathbf{D}_x^{(2)} \mathbf{f}$$



$$\underbrace{\frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & & & & & & & \\ 1 & -2 & 1 & & & & & & \\ & 1 & -2 & 0 & & & & & \\ & & 0 & -2 & 1 & & & & \\ & & & 1 & -2 & 1 & & & \\ & & & & 1 & -2 & 0 & & \\ & & & & & 0 & -2 & 1 & \\ & & & & & & 1 & -2 & 1 \\ & & & & & & & 1 & -2 \end{bmatrix}}_{\mathbf{D}_x^{(2)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \\ f_9 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_2 - 2f_1 + f_{???})/\Delta_x^2 \\ (f_3 - 2f_2 + f_1)/\Delta_x^2 \\ (f_{???} - 2f_3 + f_2)/\Delta_x^2 \\ (f_5 - 2f_4 + f_{???})/\Delta_x^2 \\ (f_6 - 2f_5 + f_4)/\Delta_x^2 \\ (f_{???} - 2f_6 + f_5)/\Delta_x^2 \\ (f_8 - 2f_7 + f_{???})/\Delta_x^2 \\ (f_9 - 2f_8 + f_7)/\Delta_x^2 \\ (f_{???} - 2f_9 + f_8)/\Delta_x^2 \end{bmatrix}}_{\mathbf{D}_x^{(2)}\mathbf{f}}$$

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What About 2D Grids (2 of 2)?

Two-dimensional grids are a little more difficult

$$\frac{\partial^2}{\partial x^2} f(x,y) \rightarrow \mathbf{D}_x^{(2)}\mathbf{f}$$

$$\begin{array}{c} x \rightarrow \\ y \downarrow \end{array} \quad \begin{array}{ccc} \bullet f_1 & \bullet f_2 & \bullet f_3 \\ \bullet f_4 & \bullet f_5 & \bullet f_6 \\ \bullet f_7 & \bullet f_8 & \bullet f_9 \end{array}$$

$$\underbrace{\frac{1}{\Delta_y^2}\begin{bmatrix} -2 & 0 & 0 & 1 & & & & & \\ 0 & -2 & 0 & 0 & 1 & & & & \\ 0 & 0 & -2 & 0 & 0 & 1 & & & \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & & \\ & 1 & 0 & 0 & -2 & 0 & 0 & 1 & \\ & & 1 & 0 & 0 & -2 & 0 & 0 & 1 \\ & & & 1 & 0 & 0 & -2 & 0 & 0 \\ & & & & 1 & 0 & 0 & -2 & 0 \\ & & & & & 1 & 0 & 0 & -2 \end{bmatrix}}_{\mathbf{D}_y^{(2)}} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \\ f_9 \end{bmatrix}}_{\mathbf{f}} = \underbrace{\begin{bmatrix} (f_4 - 2f_1 + f_{???})/\Delta_y^2 \\ (f_5 - 2f_2 + f_{???})/\Delta_y^2 \\ (f_6 - 2f_3 + f_{???})/\Delta_y^2 \\ (f_7 - 2f_4 + f_1)/\Delta_y^2 \\ (f_8 - 2f_5 + f_2)/\Delta_y^2 \\ (f_9 - 2f_6 + f_3)/\Delta_y^2 \\ (f_{???} - 2f_7 + f_4)/\Delta_y^2 \\ (f_{???} - 2f_8 + f_5)/\Delta_y^2 \\ (f_{???} - 2f_9 + f_6)/\Delta_y^2 \end{bmatrix}}_{\mathbf{D}_y^{(2)}\mathbf{f}}$$

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Derivative Operators with Dirichlet Boundary Conditions

$$\mathbf{D}_x^{(2)} = \frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

Both of these matrices only have numbers along three of their diagonals.

This is called tridiagonal.

This suggests a fast way to construct these matrices.

$\mathbf{D}_x^{(2)}$ has some corrections shown in blue along two of its diagonals.

$$\mathbf{D}_y^{(2)} = \frac{1}{\Delta_y^2}\begin{bmatrix} -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 \end{bmatrix}$$

These matrices contain mostly zeros.

These are called a sparse matrices.

See MATLAB `sparse()` command.

Also see MATLAB `spdiags()` command.

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Why Do We Need Separate Matrix Operators for First- and Second-Order Derivatives?

It is known that

$$\frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial}{\partial x} \qquad \frac{\partial^2}{\partial y^2} = \frac{\partial}{\partial y}\frac{\partial}{\partial y}$$

Can we just calculate $\mathbf{D}^{(2)}$ from $\mathbf{D}^{(1)}$?

$$\mathbf{D}_x^{(2)} \stackrel{?}{=} \mathbf{D}_x^{(1)}\mathbf{D}_x^{(1)} \qquad \mathbf{D}_y^{(2)} \stackrel{?}{=} \mathbf{D}_y^{(1)}\mathbf{D}_y^{(1)}$$

Yes, but this does not make efficient use of the grid. For a 5-point, 1D grid, we have

$$\mathbf{D}_x^{(1)}\mathbf{D}_x^{(1)} = \frac{1}{(2\Delta_x)^2}\begin{bmatrix} -1 & 0 & 1 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ 0 & 1 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

This is not as accurate because it calculates the derivative with poorer grid resolution than is available.

$$\mathbf{D}_x^{(2)} = \frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

This matrix operator makes optimal use of the available grid resolution.

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2D Derivative Operators for 1D Grids

When `Nx=1` and `Ny>1`

$\mathbf{D}_x = \mathbf{Z}$ zero matrix

$\mathbf{D}_y$ is standard for 1D grid

$$\mathbf{D}_x = \begin{bmatrix} 0 & & 0 \\ & 0 & \\ & & \ddots \\ 0 & & 0 \end{bmatrix}$$

When `Nx>1` and `Ny=1`

$\mathbf{D}_x$ is standard for 1D grid

$\mathbf{D}_y = \mathbf{Z}$ zero matrix

$$\mathbf{D}_y = \begin{bmatrix} 0 & & 0 \\ & 0 & \\ & & \ddots \\ 0 & & 0 \end{bmatrix}$$

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USE SPARSE MATRICES!!!!!!!

WARNING !!

The derivative operators will be **EXTREMELY** large matrices.

For a small grid that is just 100×200 points:

Total Number of Points:	20,000
Size of Derivate Operators:	20,000 × 20,000
Total Elements in Matrices:	400,000,000
Memory to Store One Full Matrix:	6 Gb
Memory to Store One Sparse Matrix:	1 Mb

NEVER AT ANY POINT should you use **FULL MATRICES** in the finite-difference method.
Not even for intermediate steps. **NEVER*!***

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