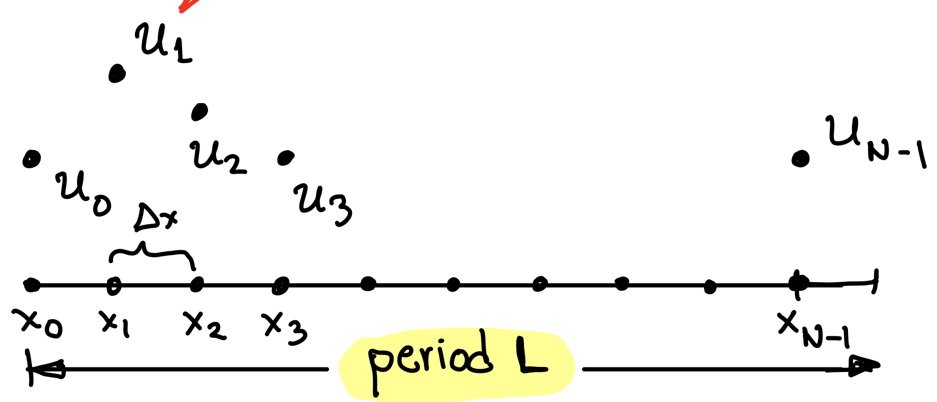
Trigonometic Interpolation + Differentiation

- periodic discrete function



$\Delta x = \text{constant}$

Discrete Fourier Transform:

$$\hat{u}_n = \sum_{i=0}^{N-1} u_i e^{-\underline{i} k_n x_i} \qquad \text{where: } k_n = n \frac{2\pi}{L}$$

Forward $u_i \rightarrow \hat{u}_n$

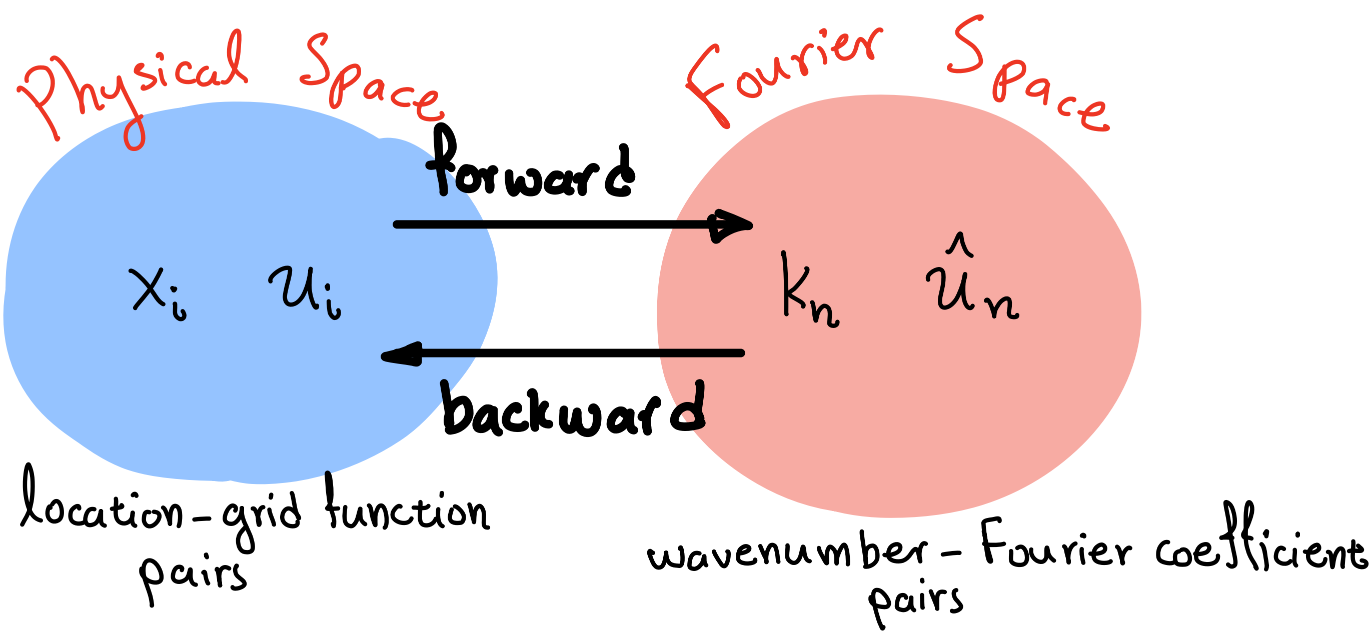
Important:

- $i = \sqrt{-1}$ imaginary unit
- $e^{-i k_n x_j} = \cos(k_n x_j) + i \sin(k_n x_j)$
- $\hat{u}_n$ are complex
- When u_i is real $\hat{u}_n = \hat{u}^{\star}_{N-n}$ complex conjugate
- Aliasing: $\hat{u}_n$ are the same for $n \to n \pm mN$ integer
- **CHECK IMPLEMENTATION on ordering of $\hat{u}_n$, k_n**

Backward DFT:

$$u_i = \frac{1}{N} \sum_{n=0}^{N-1} \hat{u}_n e^{i k_n x_i}$$

This is the expression to find u_i. However, in applications the transform will take as input all Fourier coefficients and return all values of u_i



Spectral Derivative

We will utilize the discrete Fourier transform to estimate the derivatives of u_i at locations x_i:

u_i written using expression for inverse Fourier Transform:

$$u_i = \frac{1}{N} \sum_{n=0}^{N} \hat{u}_n e^{ik_n x_i}$$

differentiate in x both sides:

$$\frac{du_i}{dx} = \frac{d}{dx}\left[\frac{1}{N} \sum_{n=0}^{N} \hat{u}_n e^{ik_n x_i}\right]$$

$$\frac{du_i}{dx} = \frac{1}{N} \sum_{n=0}^{N}\left[\hat{u}_n \frac{d}{dx}\left(e^{ik_n x_i}\right)\right]$$

$$\frac{du_i}{dx} = \frac{1}{N} \sum_{n=0}^{N}\left[\hat{u}_n i k_n e^{ik_n x_i}\right]$$

Remember: This is a sum over n

This is now in the form:

$$\frac{du_i}{dx} = \frac{1}{N} \sum_{n=0}^{N}\left[\left(\text{Fourier Coefficients}\right) e^{ik_n x_i}\right]$$

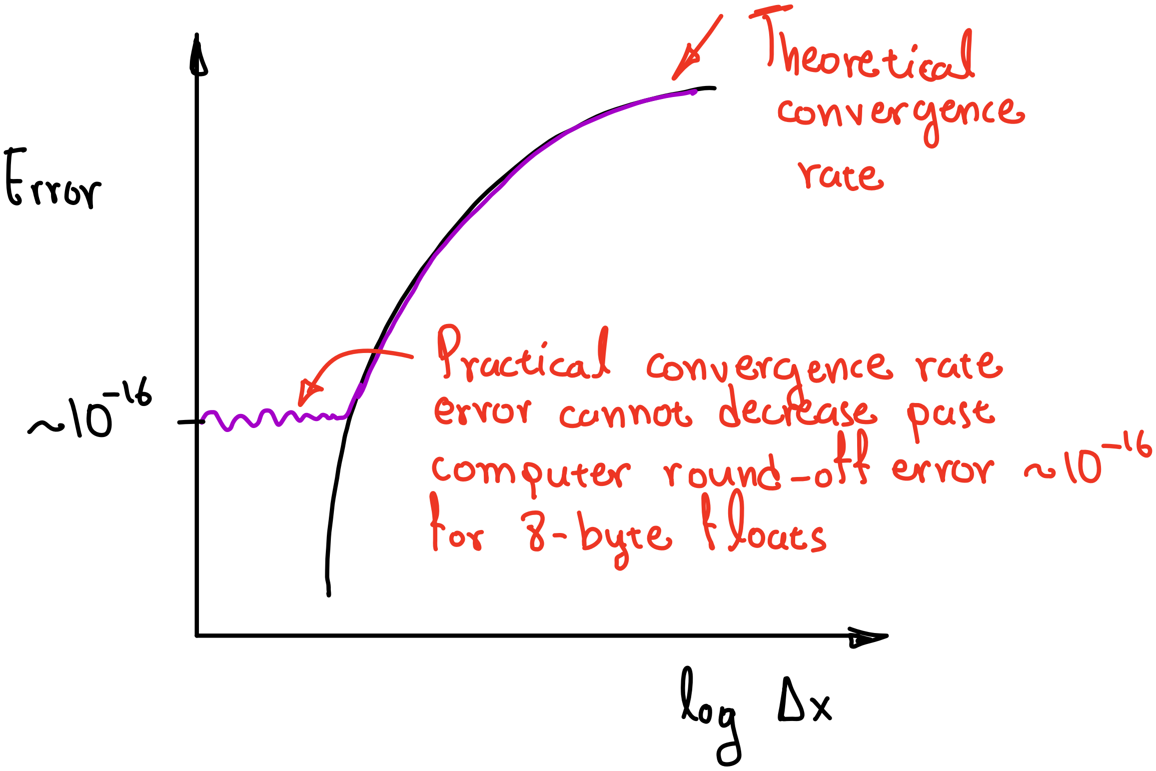
By the uniqness property of the Fourier Transform we have shown that $ik_n\hat{u}_n$ are the coefficients of the Fourier transform of $\frac{du_i}{dx}$ ← The derivative of u_i at x_i

Similarly: $(\underline{i}k_n)^m \hat{u}_n$ are the Fourier coefficients of the m-th derivative

For example: second derivative $m=2$: $(\underline{i}k_n)^2 \hat{u}_n = -k_n^2 \hat{u}_n$

Important:
- **ONLY periodic functions**
- **ONLY constant Δx**

Order of accuracy of the spectral derivative is "infinite"
This means error decreses faster than any power of Δx^n
if $u(x)$ is infinitly differentiable



Recipe:

How to apply this in practice:

We have u_i at x_i locations and we want to find $\frac{du}{dx}$ at x_i

Steps:
1. Compute wavenumbers k_n
2. $\hat{u}_n = DFT(u_i)$ compute Fourier coefficients $\hat{u}_n$
3. Form Fourier coefficients of $\frac{du}{dx}$

$$\widehat{\frac{du}{dx}}_n = \underline{i} k_n \hat{u}_n$$

multiply the corresponding k_n and u_n times $\underline{i}$ (imaginary unit)

4. $\frac{du_i}{dx} = \text{inverse DFT}(\underline{i} k_n \hat{u}_n)$

take the inverse transform to get back to physical space and find $\frac{du}{dx}$ at x_i

Finite Difference Approximation (Lomax 3.2-3.4)

Taylor series

$$u_{i+j} = u_i + (j\Delta x)\frac{\partial u}{\partial x}\Big|_i + \frac{1}{2}(j\Delta x)^2\frac{\partial^2 u}{\partial x^2}\Big|_i + \cdots + \frac{1}{n!}(j\Delta x)^n\frac{\partial^n u}{\partial x^n}\Big|_i + \cdots$$

expanding at x_i

to distance $x_i - x_j$

Example $j=1$

$$u_{i+1} = u_i + \Delta x\frac{\partial u}{\partial x}\Big|_i + \frac{1}{2}\Delta x^2\frac{\partial^2 u}{\partial x^2}\Big|_i + \cdots$$

$$\underbrace{\frac{u_{i+1}-u_i}{\Delta x} - \frac{\partial u}{\partial x}\Big|_i}_{\text{appoximating } \frac{\partial u}{\partial x}\big|_i \text{ with error}} = \underbrace{\frac{1}{2}\Delta x\frac{\partial^2 u}{\partial x^2}\Big|_i}_{\text{leading error term}} + \cdots \text{ infinite terms}$$

$$u_{i-1} = u_i - \Delta x\frac{\partial u}{\partial x}\Big|_i + \frac{1}{2}\Delta x^2\frac{\partial^2 u}{\partial x^2}\Big|_i - \frac{1}{6}\Delta x^3\frac{\partial^3 u}{\partial x^3} + \cdots$$

$$\frac{u_{i+1}-u_{i-1}}{2\Delta x} - \frac{\partial u}{\partial x}\Big|_i = \underbrace{\frac{1}{6}\Delta x^2\frac{\partial^3 u}{\partial x^3}\Big|_i}_{\text{leading error term}} + \cdots$$

point operator

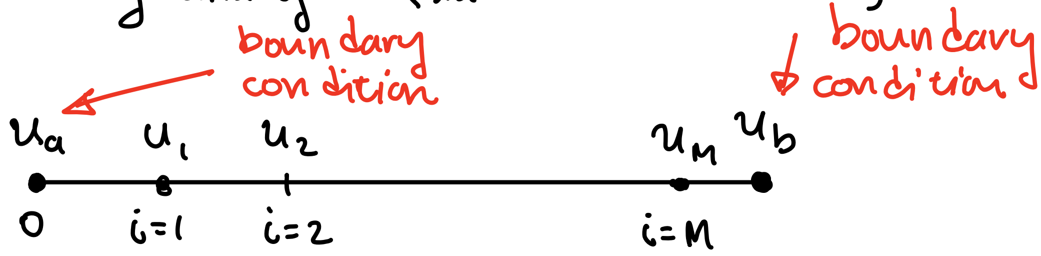
ORDER OF ACCURACY $= 2$

Move from <u>point</u> operators to <u>matrix</u> operators

Why? 1. Boundary conditions

2. Stability analysis (later this semester)

<u>Example</u>



$\frac{\partial^2 u}{\partial x^2}$? approximation is $(\delta_{xx} u)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2)$

$$\delta_{xx} u_1 = \frac{1}{\Delta x^2}(u_a - 2u_1 + u_2)$$

$$\delta_{xx} u_2 = \frac{1}{\Delta x^2}(u_1 - 2u_2 + u_3)$$

$$\vdots$$

$$\delta_{xx} u_M = \frac{1}{\Delta x^2}(u_{M-1} - 2u_M + u_b)$$

diagonal

boundary conditions

$$\delta_{xx}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_M \end{bmatrix} = \frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & & \ddots & & \\ 0 & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_M \end{bmatrix} + \begin{bmatrix} u_a \\ 0 \\ \vdots \\ \vdots \\ u_b \end{bmatrix}$$

$$\delta_{xx}\vec{u} = A\vec{u} + \vec{b}$$

vector $\vec{u}$ is only a function of <u>time</u>

$$\delta_{xx}\vec{u} = \frac{1}{\Delta x^2} B(M : 1, -2, 1)\,\vec{u} + \vec{b}$$

General FD approximation:

$$\sum_{j=-r}^{s} b_j \frac{\partial^m u}{\partial x^m}\bigg|_{i+j} - \sum_{j=-p}^{q} a_j u_{i+j} = \text{error}$$

r+s+1 points — implicit, Hermitian, Padé, compact

p+q+1 points — explicit difference

Stencil width = max(s, q) + max(r, p) + 1

Example: Implicit Finite difference:

$$\frac{\partial u}{\partial x}\bigg|_{i-1} + 4\frac{\partial u}{\partial x}\bigg|_{i} + \frac{\partial u}{\partial x}\bigg|_{i+1} - \frac{3}{\Delta x}\left(u_{i+1} - u_{i-1}\right) = \frac{\Delta x^4}{120}\frac{\partial^5 u}{\partial x^5} + \dots$$

Order = 4 stencil width = 3

Matrix operator:

$$\frac{1}{6} B(1,4,1)\, \delta_x \vec{u} = \frac{1}{2\Delta x} B(-1,0,1)\vec{u} + \vec{b}$$

$$\delta_x \vec{u} = 6\, B(1,4,1)^{-1}\left[\frac{1}{2\Delta x} B(-1,0,1)\vec{u} + \vec{b}\right]$$