Ch. 6. Discrete Transform methods : Spectral method

6.1 Fourier series

$$f(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ikx}$$

k: wavenumber

↑ continuous ft. ↑ Fourier coefficient

$$f'(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k (ik) e^{ikx} = \sum_{k=-\infty}^{\infty} ik\hat{f}_k e^{ikx}$$

↳ Fourier coeff. of f'

$$f(x) \xrightarrow{FT} \hat{f}_k \longrightarrow ik\hat{f}_k \xrightarrow{IFT} f'(x)$$

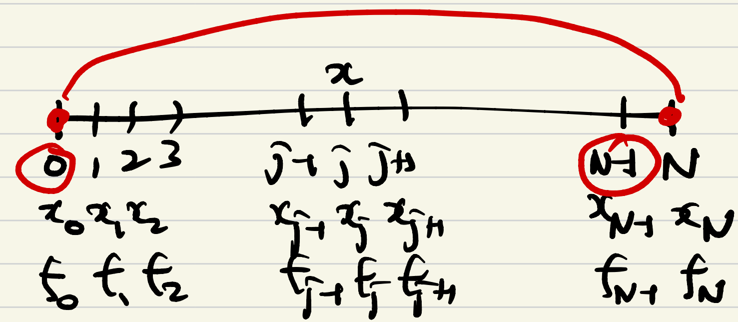
6.1.1 Discrete Fourier Series

f : periodic ft.

$f_0 = f_N$

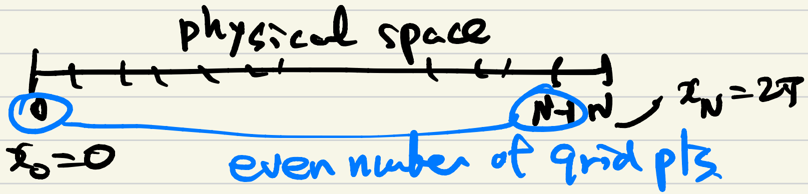
N gridpts.

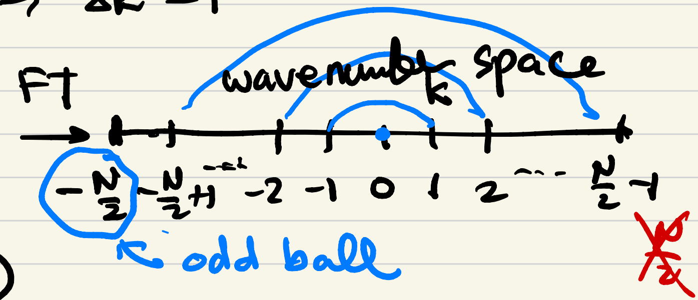
N : even number



Let us take N to be even number and period of f to be 2π.

e^{ikx} $\Delta k \cdot L = \Delta k \cdot 2\pi = 2\pi \Rightarrow \Delta k = 1$





$x_j = jh \quad h = \frac{2\pi}{N}$ (grid spacing)

uniform grids

- Discrete Fourier transformation (DFT)

$$f_j = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{ikx_j} \qquad . \; j = 0, 1, 2, \cdots, N-1$$

$\hat{f}_k$ → discrete Fourier coeff. of f_j

$O(N^2)$ operation

(If a period of f is L, $\Delta k \cdot L = 2\pi \rightarrow \Delta k = 2\pi / L$)

$f_j \xrightarrow{DFT} \hat{f}_k \Rightarrow A\hat{f}_k = f_j$ To obtain $\hat{f}_k$, $O(N^3)$ operations. too expensive!

↑ full matrix

So, we use orthogonality,

$x_j = \frac{2\pi}{N} j$ ← $e^{imNx_j} = e^{im2\pi j}$

$$I = \sum_{j=0}^{N-1} e^{ikx_j} e^{-ik'x_j} = \sum_{j=0}^{N-1} e^{i(k-k')x_j} = \begin{cases} N & \text{if } k = k' \pm mN \\ 0 & \text{otherwise} \end{cases}$$

$m = 0, \pm 1, \pm 2, \pm 3, \cdots$

$$\boxed{f_j = \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{ikx_j}}$$

$$\sum_{j=0}^{N-1} f_j e^{-ik'x_j} = \sum_{j=0}^{N-1} \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{ikx_j} e^{-ik'x_j}$$

$$= \sum_{k=-N/2}^{N/2-1} \sum_{j=0}^{N-1} \hat{f}_k e^{i(k-k')x_j} = N \hat{f}_{k'}$$

$$\rightarrow \boxed{\hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}}$$

$k = -\frac{N}{2}, -\frac{N}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{N}{2}-1$

→ $O(N^2)$ operations

FFT (fast FT) → $O(N \log_2 N)$ operations ('Numerical Recipes' for subroutine)

DFT:

$$\begin{cases} f_j = \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{ikx_j} & j = 0, 1, 2, \cdots, N-1 \quad N \\ \hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j} & k = -\frac{N}{2}, \cdots, 0, \cdots, \frac{N}{2}-1 \quad N \end{cases}$$

f_j: real (N)

$\hat{f}_k$: complex number (2N) $a + ib$

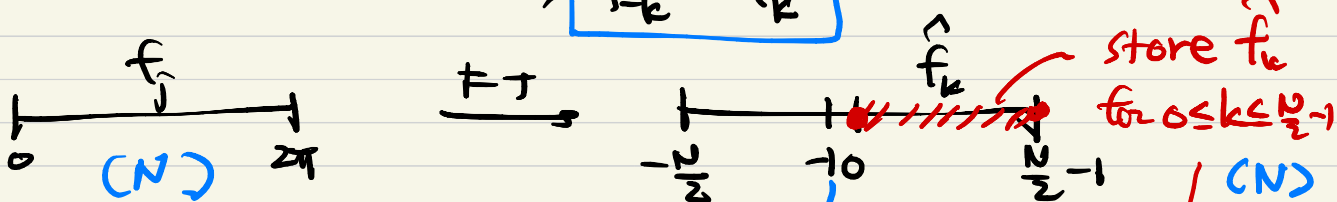
- FT of a real ft.

f: real ft. $\xrightarrow{FT}$ $\hat{f}_k$: complex

$$\left(\hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j} \right)^* \rightarrow \hat{f}_k^* = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{+ikx_j} = \hat{f}_{-k}$$

$$e^{+ikx_j} = e^{-i(-k)x_j}$$

$$\Rightarrow \boxed{\hat{f}_{-k} = \hat{f}_k^*}$$



$\hookrightarrow \hat{f}_{-k} = \hat{f}_k^*$

No need to store $\hat{f}_{-k}$ when f is real.

- Higher dimensions

$f(x,y)$: doubly periodic in x & y directions

$$f(x_m, y_\ell) = \sum_{k_1=-\frac{N_1}{2}}^{\frac{N_1}{2}-1} \sum_{k_2=-\frac{N_2}{2}}^{\frac{N_2}{2}-1} \hat{f}_{k_1,k_2} e^{ik_1 x_m} e^{ik_2 y_\ell}$$

$m = 0, 1, 2, \cdots, N_1 - 1$

$\ell = 0, 1, 2, \cdots, N_2 - 1$

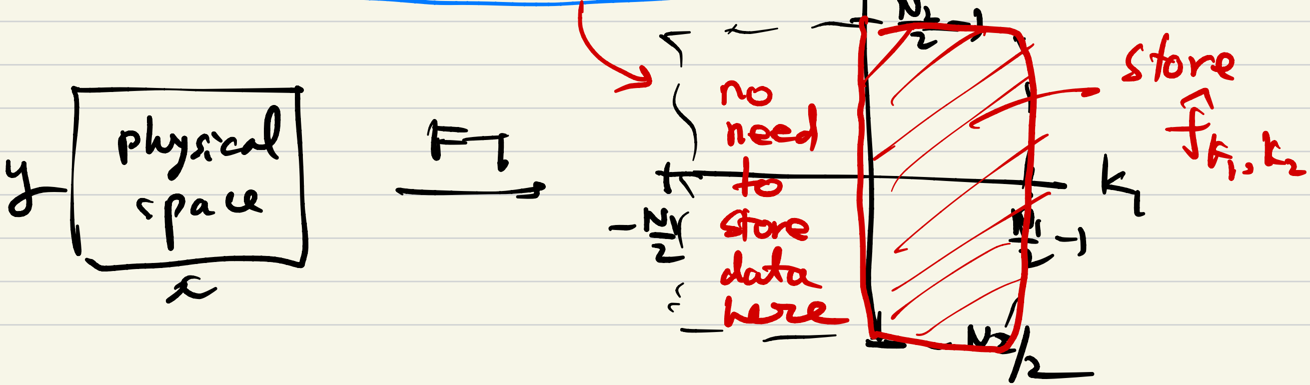
Use orthogonality

$$\hat{f}_{k_1,k_2} = \frac{1}{N_1} \frac{1}{N_2} \sum_{m=0}^{N_1-1} \sum_{\ell=0}^{N_2-1} f_{m,\ell} e^{-ik_1 x_m} e^{-ik_2 y_\ell}$$

$k_1 = -\frac{N_1}{2}, \cdots, 0, \cdots \frac{N_1}{2} - 1$

$k_2 = -\frac{N_2}{2}, \cdots, 0, \cdots \frac{N_2}{2} - 1$

If f is real, $\hat{f}_{-k_1,-k_2} = \hat{f}^*_{k_1,k_2}$



- DFT of a product of two fts.

Let $H(x) = f(x)\,g(x)$

$$\hat{H}_m = \widehat{fg}_m = \frac{1}{N}\sum_{j=0}^{N-1} f_j g_j e^{-imx_j}, \quad m = -\frac{N}{2}, \cdots, 0, \cdots, \frac{N}{2}-1$$

$$= \frac{1}{N}\sum_{j=0}^{N-1}\left(\sum_k \hat{f}_k e^{ikx_j}\right)\left(\sum_{k'} \hat{g}_{k'} e^{ik'x_j}\right) e^{-imx_j}$$

$$= \frac{1}{N}\sum_{j=0}^{N-1}\sum_k\sum_{k'} \hat{f}_k \hat{g}_{k'} e^{i(k+k'-m)x_j}$$

(orthogonality

$$\frac{1}{N}\sum_{j=0}^{N-1} e^{i(k+k'-m)x_j} = \begin{cases} 1 & \text{if } k+k'-m = \pm\alpha N \\ & (\alpha = 0, 1, 2, \cdots) \\ 0 & \text{otherwise} \end{cases}$$
)

Sum over j is non-zero only if $k+k' = m$ or $m \pm N$ $(\alpha=1)$

because $-N/2 \le k, k', m \le \frac{N}{2}-1$.

$\downarrow$ $k' = m-k$? $k' = m-k\pm N$

$$\hat{H}_m = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \hat{g}_{m-k}$$

convolution sum of $\hat{f}$ and $\hat{g}$

$\hookrightarrow O(N^2)$ operations. expensive

The part of summation corresponding to $k+k' = m \pm N$ is known as the aliasing error and should be discarded because Fourier exponentials corresponding to those wavenumbers cannot be resolved on the grid size N.

If we simply multiply f and g at each grid point, the resulting discrete ft. will be contaminated by the aliasing error and not be equal to the inverse FT of $\hat{H}_m$.

ex) $f(x) = \sin 2x$, $g(x) = \sin 3x$, $0 \le x \le 2\pi$

$k=2$ $\qquad$ $k=3$

$x_j = \frac{2\pi}{N} j$, $j = 0, 1, 2, \cdots, N-1$ $\qquad$ $\hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}$

For $N=8 \Rightarrow k = 0, \pm 1, \pm 2, \pm 3, -4$

$$\hat{f}_k = \begin{cases} \pm i\frac{1}{2} & \text{for } k = \pm 2 \\ 0 & \text{otherwise} \end{cases} \qquad \hat{g}_k = \begin{cases} \pm i\frac{1}{2} & \text{for } k = \pm 3 \\ 0 & \text{otherwise} \end{cases}$$

$$H(x) = f(x)\,g(x) = \sin 2x \sin 3x = \frac{1}{2}(\cos x - \cos 5x)$$

↳ $k=1$ ↳ $k=5$

$$\hat{H}_k = \begin{cases} \frac{1}{4} & \text{for } k=\pm 1 \\ -\frac{1}{4} & \text{for } k=\pm 5 \\ 0 & \text{otherwise} \end{cases}$$ exact sol.

→ we need $k = 0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5, -6 \Rightarrow$ we need $N = 12$ to get exact sol.

$N_H \geq \frac{3}{2} N_f$ (or N_g) $\frac{3}{2} \times 8 = \underline{12}$

With $N = 16$ ($k = 0, \pm 1, \cdots, \pm 7, -8$)

$$\hat{H}_m = \sum_{k=-8}^{7} \hat{f}_k \hat{g}_{m-k}$$

$$\hat{H}_5 = \sum_{k=-8}^{7} \hat{f}_k \hat{g}_{5-k} = \hat{f}_2 \hat{g}_3 = -\frac{1}{4}$$

$$\hat{H}_1 = \sum \hat{f}_k \hat{g}_{1-k} = \hat{f}_{-2} \hat{g}_3 = \frac{1}{4}$$

$$\rightarrow \hat{H}_m = \begin{cases} \frac{1}{4} & \text{for } m=\pm 1 \\ -\frac{1}{4} & \text{for } m \pm 5 \\ 0 & \text{otherwise} \end{cases}$$ accurate

with $N=8$ $(k=0, \pm1, \pm2, \pm3, -4)$

$$\hat{H}_m = \sum_{k=-4}^{3} \hat{f}_k \hat{g}_{m-k} \qquad \hat{H}_1 = \sum \hat{f}_k \hat{g}_{1-k} = \hat{f}_{-2}\hat{g}_3 = \frac{1}{4}$$

$$\rightarrow \hat{H}_m = \begin{cases} \frac{1}{4} & \text{for } m=\pm1 \\ 0 & \text{otherwise} \end{cases}$$

⇐ accurate for $m=\pm1$ but lose $\cos 5x$.

the result is ok within the number of grid pts.

Now, multiplying f and g at each grid pt w/ $N=8$ and FT. what happen?

$$\hat{H}_m = \frac{1}{N}\sum_{j=0}^{N} f_j g_j e^{-imx_j}$$

$f_j g_j$ → contains $-\frac{1}{2}\cos 5x_j \rightarrow -\frac{1}{2}e^{\pm i5x_j}$

orthogonality : $\pm5 - m = \alpha N = 8\alpha$

$\alpha=0$: $m=\pm5$ ✗ $(m=0, \pm1, \pm2, \pm3, -4)$

$\alpha=1$: $m=\pm5-8 = -3$ or -13 → $\hat{H}_{-3} = -1/4$

$\alpha=-1$: $m=\pm5+8 = +13$ or 3 → $\hat{H}_3 = -1/4$

$$\Rightarrow \hat{H}_m = \begin{cases} \frac{1}{4} & \text{for } m = \pm 1 \\ -\frac{1}{4} & \text{for } m = \pm 3 \\ 0 & \text{otherwise} \end{cases}$$

Not good!

Exact sol. : $0.5(\cos x - \cos 5x)$

$\rightarrow 0.5(\cos x - \cos 3x)$

aliasing error