- Lax - Wendroff scheme

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0$$

$$\phi(x, t+\Delta t) = \phi(x,t) + \Delta t \underbrace{\frac{\partial \phi}{\partial t}(x,t)}_{= -c\frac{\partial \phi}{\partial x}} + \frac{1}{2}\Delta t^2 \underbrace{\frac{\partial^2 \phi}{\partial t^2}(x,t)}_{= \frac{\partial}{\partial t}\left(\frac{\partial \phi}{\partial t}\right) = \frac{\partial}{\partial t}\left(-c\frac{\partial \phi}{\partial x}\right) = -c\frac{\partial}{\partial x}\frac{\partial \phi}{\partial t} = c^2\frac{\partial^2 \phi}{\partial x^2}} + \frac{1}{6}\Delta t^3 \frac{\partial^3 \phi}{\partial t^3}(x,t) + \cdots$$

CD2 :

$$\boxed{\phi_j^{n+1} = \phi_j^n - c\Delta t\,\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} + \frac{1}{2}c^2\Delta t^2\,\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}} + \underbrace{O(\Delta t^3)}_{\Delta t^3 \frac{\partial^3 \phi}{\partial t^3}}$$

Lax-Wendroff scheme

$\downarrow$

dispersive error

explicit

stable for CFL < 1

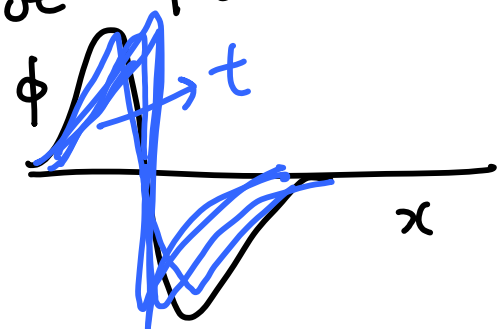
2nd-order accurate in space & time

disadvantage : c is not constant
nonlinear $c = c(\phi)$
higher dimension
$\Big] \longrightarrow$ difficulty

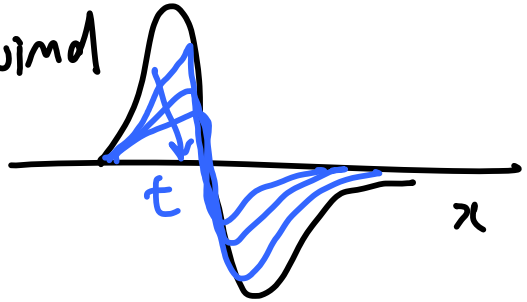
this method can be applied to

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2} \longrightarrow \begin{cases} \dfrac{\partial u}{\partial t} = c \dfrac{\partial w}{\partial x} \\ \dfrac{\partial w}{\partial t} = c \dfrac{\partial u}{\partial x} \end{cases}$$

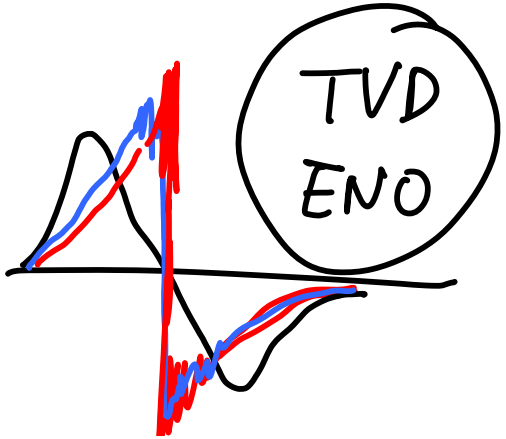
- $\dfrac{\partial \phi}{\partial t} + \phi \dfrac{\partial \phi}{\partial x} = 0$ nonlinear



upwind



CD2



- Implicit method for hyperbolic eqs.

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0$$

CD2 + CN $\rightarrow$ $$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + c \cdot \frac{1}{2}\left[\frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} + \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x}\right] = 0$$

- no amplitude error (no dissipation)
- dispersive error
- stable

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}$$

① splitting into two eqs. u & w and applying CN to two eqs.

② applying CN directly to wave eq.

② : $$\frac{\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}}{\Delta t^2} = \frac{1}{2} c^2 \left[\frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2} + \frac{\phi_{j+1}^{n} - 2\phi_j^{n} + \phi_{j-1}^{n}}{\Delta x^2} \right]$$

stable

a little more accurate than the method applied to two splitted eqs.

spurious root

higher dimension (2D/3D) $\rightarrow$ ADI

nonlinear eq $\frac{\partial \phi}{\partial t} + \phi \frac{\partial \phi}{\partial x} = 0$ $\rightarrow$ iterative method for implicit scheme.

- MacCormack scheme – very popular

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0 \rightarrow \begin{cases} \phi_j^* = \phi_j^n - \frac{c\Delta t}{\Delta x}(\phi_{j+1}^n - \phi_j^n) & \text{predictor} \\ \phi_j^{n+1} = \frac{1}{2}(\phi_j + \phi_j^*) - \frac{c\Delta t}{2\Delta x}(\phi_j^* - \phi_{j-1}^*) & \text{corrector} \end{cases}$$

equivalent to Lax-Wendroff scheme for linear prob.

$\hookrightarrow O(\Delta x^2)$ & $O(\Delta t^2)$

CFL < 1

readily extended to 2D & 3D

accurate & easier to program

desirable nonlinear properties

Ch. 6 Discrete Transform methods : Spectral method

6.1 Fourier Series

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

k : wave number

$f(x)$ ↑ continuous f-t.

$\hat{f}_k$ → Fourier coeff.

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

$ik\hat{f}_k$ → Fourier coeff. of f'

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

6.1.1 Discrete Fourier Series

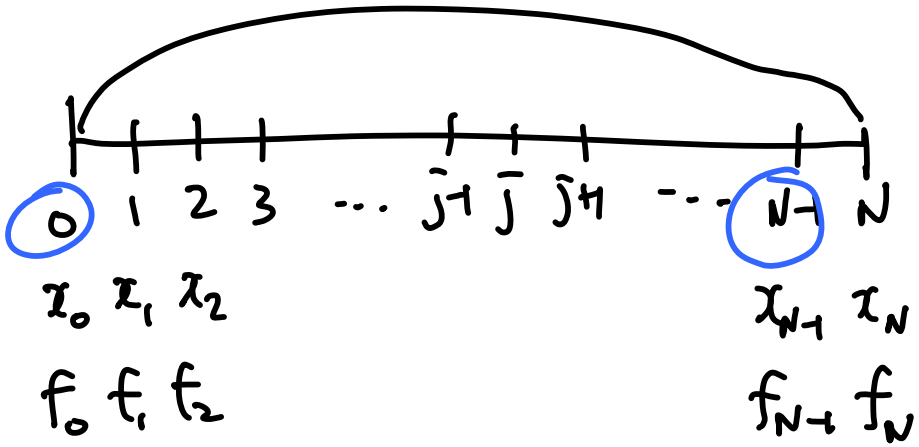
f : periodic ft.

$\downarrow$

$f_N = f_0$

N grid pts

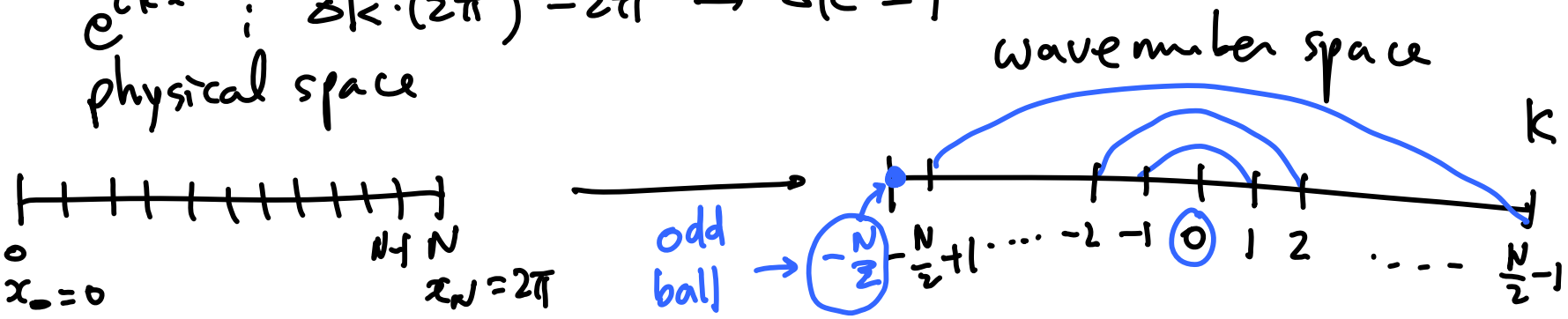
N : even number



Let us take N to be even number and <u>period of f to be 2π</u>.

e^{ikx} ; $\alpha k \cdot (2\pi) = 2\pi \rightarrow \alpha k = 1$

physical space



$x_j = jh$, $h = 2\pi/N$ (grid spacing) uniform!

<u>Discrete Fourier transformation</u> (DFT)

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

$\mathcal{O}(4N^2)$ operations

discrete Fourier coeff. of f_j.

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

$$f_j \xrightarrow{\text{DFT}} \hat{f}_k \Rightarrow \underbrace{A}_{\text{full matrix}} \hat{f}_k = f_j$$

Then, to get $\hat{f}_k$, $\mathcal{O}(N^3)$ operations too expensive!

use orthogonality

$$I = \sum_{j=0}^{N-1} e^{ikx_j} e^{-ik'x_j} = \sum_{j=0}^{N-1} e^{i(k-k')x_j} = \begin{cases} N & \text{if } k = k' + mN \\ & (m = 0, \pm 1, \pm 2, \ldots) \\ 0 & \text{otherwise} \end{cases}$$

$$f_j = \sum \hat{f}_k e^{ikx_j}$$

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

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

$$\rightarrow \boxed{\hat{f}_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}} \qquad k = -\frac{N}{2}, \ldots, -1, 0, 1, \ldots, \frac{N}{2} - 1$$

$\rightarrow O(N^2)$ operations.

FFT $\longrightarrow$ $\mathcal{O}(N\log_2 N)$ operations

(fast FT) See 'Numerical Recipes' for this routine.

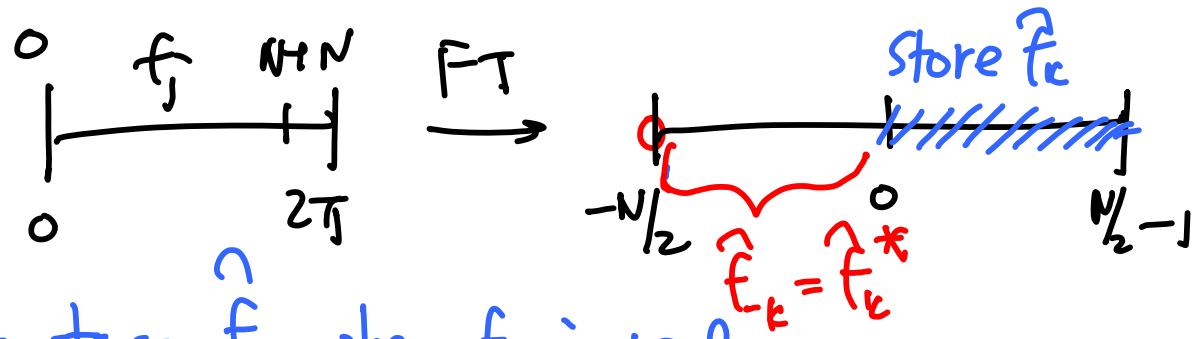
DFT :
$$\begin{cases} f_j = \sum_{k=-N/2}^{N/2-1} \hat{f}_k e^{ikx_j}, & j=0,1,2,\cdots,N-1 \\ \hat{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f_j e^{-ikx_j}, & k=-N/2,\cdots,-1,0,1,\cdots,N/2-1 \end{cases}$$

. FT of a real ft.

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

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

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



No need to store $\hat{f}_k$ when f is real.

- Higher dimensions

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

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

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

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

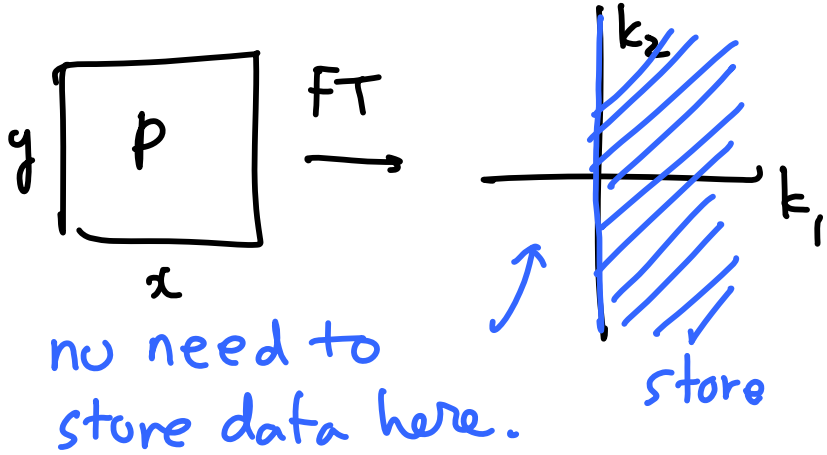
Use orthogonality

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

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

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

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



- DFT of a product of two fts

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

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

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

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

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

sum over j is non-zero only if $k+k'=m$ or $m \pm N$

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

$\rightarrow k' = m - k$

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

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

↳ $O(N^2)$ operation

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 these wavenumbers cannot be resolved on the grid size N.

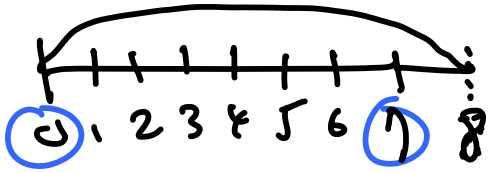
If we simply multiply f and g at each grid point, the resulting discrete f.t. will be contaminated by the aliasing error and not be equal to the inverse FT of $\widehat{H_m}$.

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

$k=2$ $\quad k=3$ $\quad dk = 1$

$x_j = \frac{2\pi}{N} j$. $j = 0, 1, \cdots, N-1$

For $N=8$



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

$\hookrightarrow$ $k = 0, \pm1, \pm2, \pm3, -4$

$$\hat{f}_k = \begin{cases} \pm i\frac{1}{2} & \text{for } k=\pm2 \\ 0 & \text{otherwise} \end{cases}$$

$\rightarrow$ $0, \pm1, \pm2, -3 \rightarrow N=6$

$N=6 \rightarrow k = 0, \pm1, \pm2, -3$

$$\hat{g}_k = \begin{cases} \pm i\frac{1}{2} & \text{for } k=\pm3 \\ 0 & \text{otherwise} \end{cases}$$

$\rightarrow$ $0, \pm1, \pm2, \pm3, -4 \rightarrow N=8$

$k=\pm1$ $\quad$ $k=\pm5$

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

$$\hat{H}_k = \begin{cases} \frac{1}{4} & \text{for } k=\pm1 \\ -\frac{1}{4} & \text{for } k=\pm5 \\ 0 & \text{otherwise} \end{cases}$$

exact sol.

$\rightarrow$ We need $k = 0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5, -6$

" " $N = 12 \Rightarrow N_H = \frac{3}{2} N_{f \text{ or } g}$ $\left(\frac{3}{2} \times \underset{N_g}{8} = \underset{N_H}{12}\right)$

with $N = 16$ $(k = 0, \pm 1, \pm 2, \dots, \pm 7, -8)$

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

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

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

$$\vdots$$

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

accurate!

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

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

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

$\leftarrow$ accurate for $m=\pm1$ but lose $\cos 5x$!

the result is o/k within # of grid pts.

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

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

$e^{-i(m\pm5)x_j}$

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

orthogonality : $\pm 5 - m = \alpha N = 8\alpha$

$\alpha = 0$: $m = \pm 5$ X $(m = 0, \pm 1, \pm 2, \pm 3, -4)$

$\alpha = 1$: $m = \pm 5 - 8 = -3$ or $\cancel{-13}$

$\hat{H}_{-3} = -\frac{1}{4}$

$\alpha = -1$: $m = \pm 5 + 8 = \cancel{+13}$ or $+3$

$\hat{H}_3 = -\frac{1}{4}$

$$\Rightarrow \hat{H}_m = \begin{cases} \frac{1}{4} & \text{for } m = \pm 1 \\ -\frac{1}{4} & \text{for } m = \pm 3 \\ 0 & \text{otherwise} \end{cases} \rightarrow 0.5(\cos x - \cos 3x)$$

aliasing error

- what should we do for $f \times g$?

① $f_j \xrightarrow{FT} \hat{f}_k$, $g_j \xrightarrow{FT} \hat{g}_k$ $\Big\rangle$ $\sum_m \hat{f}_k \hat{g}_{m-k} \xrightarrow{IFT} h_j = f_j g_j$

$\Theta(N \log_2 N)$ $\quad$ $\Theta(N^2)$ most expensive $\quad$ $\Theta(N \log_2 N)$

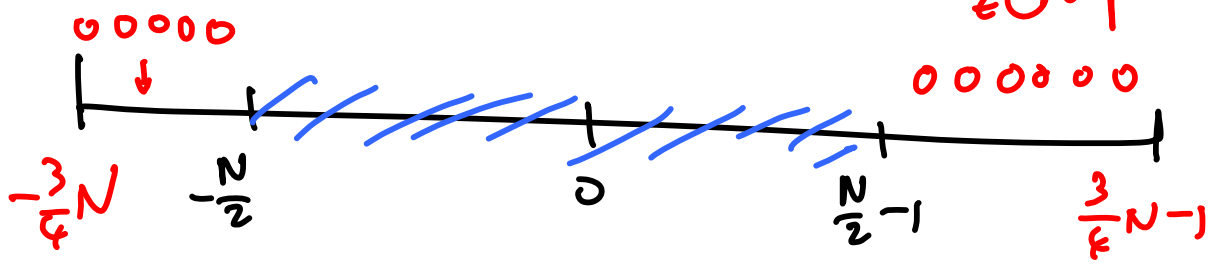
② $f_j \xrightarrow{FT} \hat{f}_k$, $g_j \xrightarrow{FT} \hat{g}_k$ $\Big\rangle$ add zeros to $\hat{f}_k$ & $\hat{g}_k$ on $\frac{N}{2}-1 \le k \le \frac{3}{4}N-1$, $-\frac{3}{4}N \le k \le -\frac{N}{2}$

N

$\Theta(N \log_2 N)$

$\frac{3}{2}N$

zero padding



$$\mathcal{O}\left(\tfrac{3}{2}N\log\left(\tfrac{3}{2}N\right)\right) \downarrow \text{IFT}$$

$$\hat{H}_m \xleftarrow{\text{FT}} H_j = f_j g_j \longleftrightarrow f_j \text{ and } g_j \quad \tfrac{3}{2}N$$

$$\mathcal{O}\left(\tfrac{3}{2}N\log_2\left(\tfrac{3}{2}N\right)\right) \qquad \mathcal{O}\left(\tfrac{3}{2}N\right)$$

Spectral interpolation

$\downarrow$

remove values at $\frac{N}{2}-1 \le k \le \frac{3}{4}N-1$

$$-\tfrac{3}{4}N \le k \le -\tfrac{N}{2}$$

$\downarrow$ IFT $\mathcal{O}(N\log_2 N)$

H_j

② is cheaper than ① and has no aliasing error $\rightarrow$ called "aliasing control". $N_H = \frac{3}{2}(N_f \text{ or } N_g)$