Fourier transform and its applications

A Tuesday in 2024 Winter

9:50-12:15
三教1200

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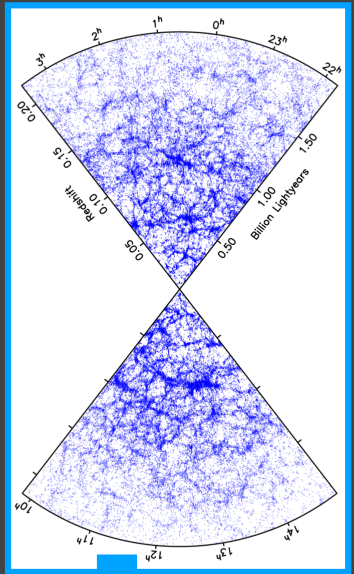
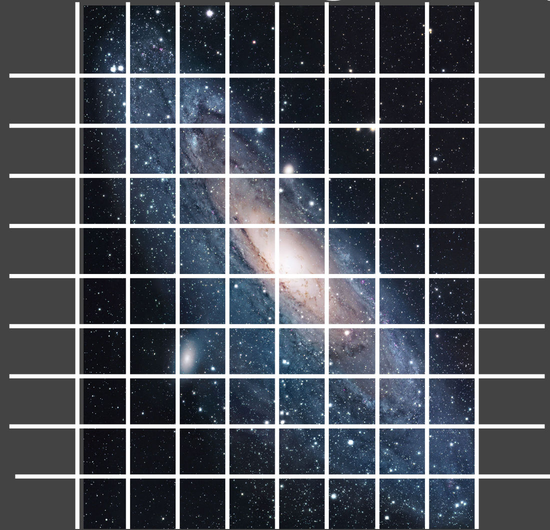
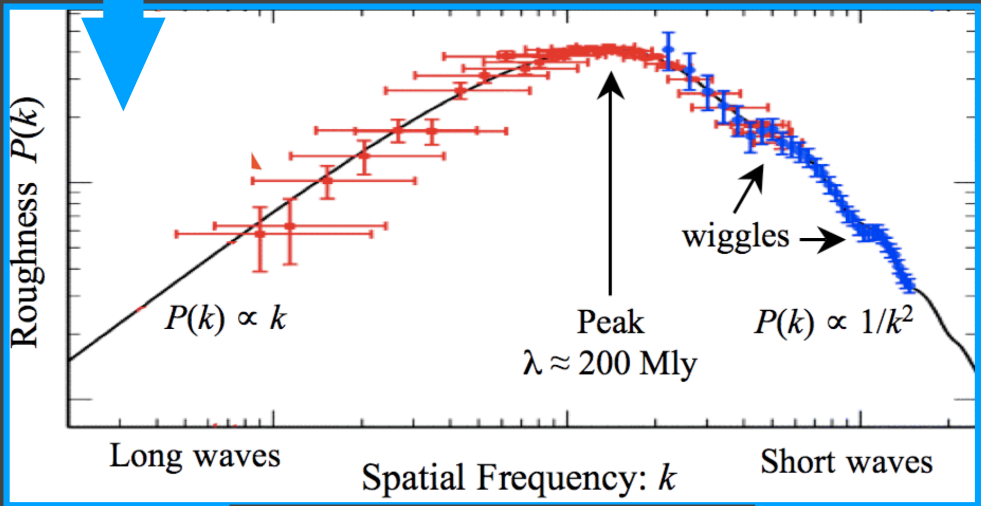


Image deconvolution

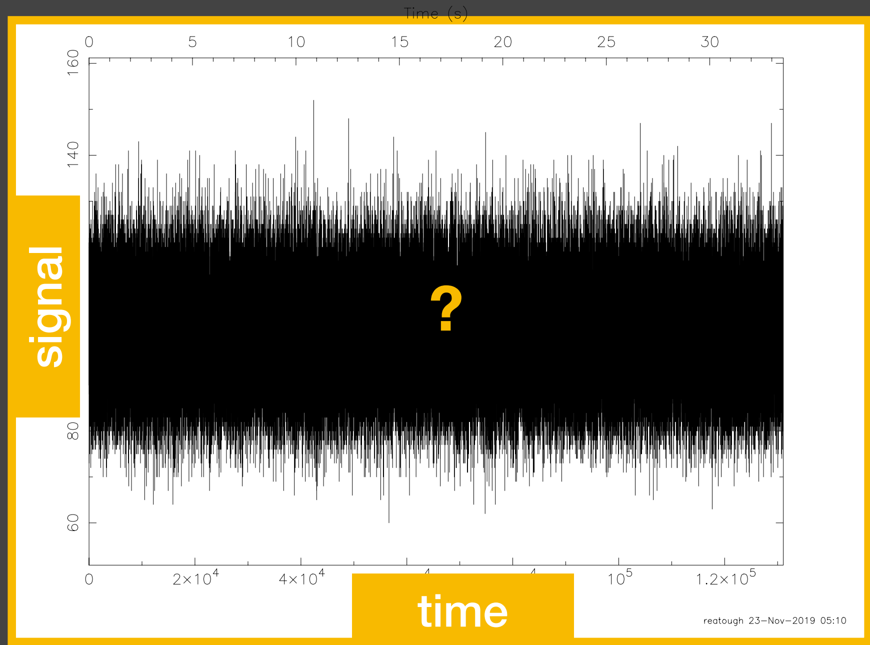
Green's function ⊗ Density field



Gravitational field calculation



LSS power spectrum



$$h(x) = \Sigma_k H_k \exp(ikx)$$
$$H_k = \frac{1}{L}\int_{-L/2}^{L/2} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

Fourier series

$$L \to \infty$$
$$\frac{2\pi}{L}\Sigma_k \to \int \mathrm{d}k$$
$$LH_k = H(k)$$

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k$$
$$H(k) = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

Fourier integral

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k$$
$$H(k) = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

$H(k)$ is the Fourier transform of $h(x)$,
$k = 2\pi\xi$ is the *angular* spatial frequency (wavenumber).

$$h(x) = \int_{-\infty}^{\infty} H(\xi)\ \exp(i2\pi\xi x)\,\mathrm{d}\xi$$
$$H(\xi) = \int_{-\infty}^{\infty} h(x)\ \exp(-i2\pi\xi x)\,\mathrm{d}x$$

$H(\xi)$ is the Fourier transform of $h(x)$,
ξ is spatial frequency, x is position.

Spatial domain

$$h(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(\omega)\ \exp(i\omega t)\,\mathrm{d}\omega$$
$$H(\omega) = \int_{-\infty}^{\infty} h(t)\ \exp(-i\omega t)\,\mathrm{d}t$$

Time domain

$$h(t) = \int_{-\infty}^{\infty} H(f)\ \exp(i2\pi ft)\,\mathrm{d}f$$
$$H(f) = \int_{-\infty}^{\infty} h(t)\ \exp(-i2\pi ft)\,\mathrm{d}t$$

$H(\omega)$ is the Fourier transform of $h(t)$,
$\omega = 2\pi f$ is the *angular* frequency.

$H(f)$ is the Fourier transform of $h(t)$,
f is time frequency, t is time.

Fourier transform (FT)

The Fourier pairs may have the following integral forms:

Spatial domain

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k$$
$$H(k) = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

$H(k)$ is the Fourier transform of $h(x)$, $k = 2\pi\xi$ is the *angular* spatial frequency (wavenumber).

$$h(x) = \int_{-\infty}^{\infty} H(\xi)\ \exp(i2\pi\xi x)\,\mathrm{d}\xi$$
$$H(\xi) = \int_{-\infty}^{\infty} h(x)\ \exp(-i2\pi\xi x)\,\mathrm{d}x$$

$H(\xi)$ is the Fourier transform of $h(x)$, ξ is spatial frequency, x is position.

Time domain

$$h(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(\omega)\ \exp(i\omega t)\,\mathrm{d}\omega$$
$$H(\omega) = \int_{-\infty}^{\infty} h(t)\ \exp(-i\omega t)\,\mathrm{d}t$$

$H(\omega)$ is the Fourier transform of $h(t)$, $\omega = 2\pi f$ is the *angular* frequency.

$$h(t) = \int_{-\infty}^{\infty} H(f)\ \exp(i2\pi f t)\,\mathrm{d}f$$
$$H(f) = \int_{-\infty}^{\infty} h(t)\ \exp(-i2\pi f t)\,\mathrm{d}t$$

$H(f)$ is the Fourier transform of $h(t)$, f is time frequency, t is time.

Note: t, x, f, ω, ξ, k are real numbers; the transform pairs can be complex functions!

$$H(\xi_x, \xi_y) = \iint h(x, y)\, e^{-i2\pi(\xi_x x + \xi_y y)}\,\mathrm{d}x\mathrm{d}y, \quad h(x, y) = \iint H(\xi_x, \xi_y)\, e^{i2\pi(\xi_x x + \xi_y y)}\,\mathrm{d}\xi_x\mathrm{d}\xi_y$$

Basic properties

A while ago we learnt a slightly different form of the Fourier transform:

$$h(x) = \frac{1}{2\pi}\int_0^{\infty} [a_k \cos(kx) + b_k \sin(kx)]\,\mathrm{d}k,$$ for which, the Fourier cosine transform is:

$$\boxed{a_k} = \int_{-\infty}^{\infty} h(x)\ \cos(kx)\,\mathrm{d}x;$$ the Fourier sine transform is: $$\boxed{b_k} = \int_{-\infty}^{\infty} h(x)\ \sin(kx)\,\mathrm{d}x.$$

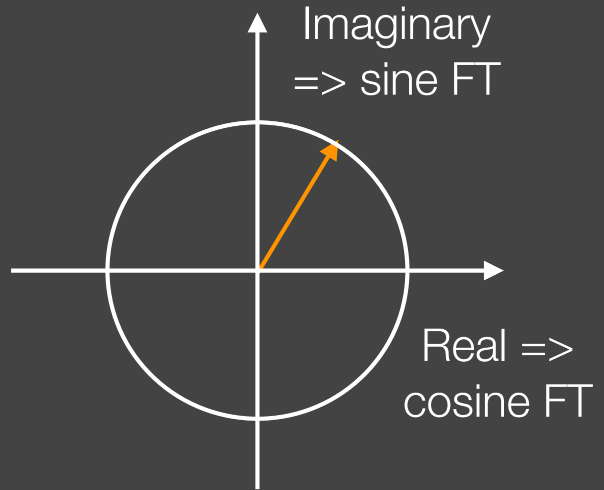
What's the relation between the two forms?

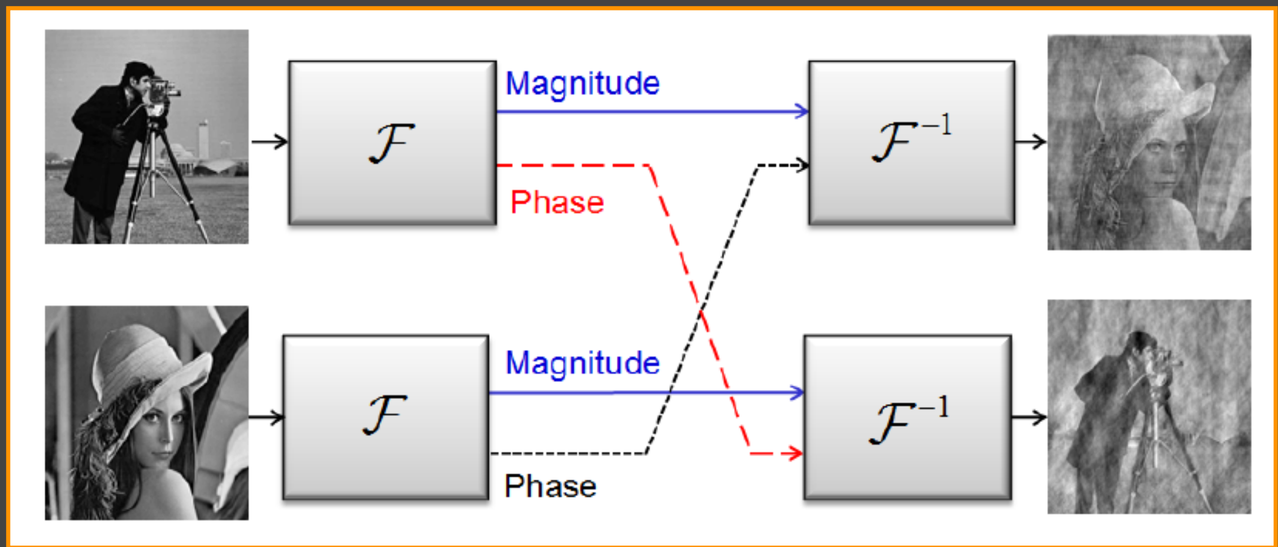
$$\boxed{H(k)} = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x = \underbrace{\int_{-\infty}^{\infty} h(x)\ \cos(kx)\,\mathrm{d}x}_{a_k} - i\underbrace{\int_{-\infty}^{\infty} h(x)\ \sin(kx)\,\mathrm{d}x}_{b_k}$$

Relations above suggest: $H(k) = a_k - ib_k$, $a_k = \mathrm{Re}\{H(k)\}$, $b_k = -\,\mathrm{Im}\{H(k)\}$

The complex FT is simply to use a complex plane to express the cosine and sine Fourier transforms.

Magnitude $r_k = \sqrt{a_k^2 + b_k^2}$ Phase $\phi_k = \tan^{-1}(-b_k/a_k)$





Basic properties

$$H(k) = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x = \int_{-\infty}^{\infty} h(x)\ \cos(kx)\,\mathrm{d}x - i\int_{-\infty}^{\infty} h(x)\ \sin(kx)\,\mathrm{d}x$$

Can be complex function of *k*

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \cos(kx)\,\mathrm{d}k + \frac{i}{2\pi}\int_{-\infty}^{\infty} H(k)\ \sin(kx)\,\mathrm{d}k$$

Can be complex function of *x*

- In general, both $h(x)$ and $H(k)$ can be complex functions. Even for real function $h(x)$, $H(k)$ in general is a complex function of k.
- If $h(x)$ is a real function, then it is easy to see that $H(k\_) = H^*(k_+)$ [i.e., the reality condition, linking negative and positive frequencies, $*$ indicates complex conjugate.
- If $h(x)$ is a pure imaginary function, then $H(k\_) = -H^*(k_+)$.
- For real function $h(x)$, $H(k=0) = \int_{-\infty}^{\infty} h(x)\,\mathrm{d}x$ => area under function $h(x)$,

  — the "DC component."
  - When $h(x)$ is real and even, $H(k)$ is also real and an even function of k; while if $h(x)$ is real and odd, then $H(k)$ is pure imaginary and an odd function of k.

Basic properties

$$h(x) = \underbrace{\frac{1}{2\pi}\int_0^\infty a_k \cos(kx)\,\mathrm{d}k}_{\text{even function of } x} + \underbrace{\cancel{\frac{1}{2\pi}\int_0^\infty b_k \sin(kx)\,\mathrm{d}k}}_{\text{odd function of } x}$$

★ If $h(x)$ is a real and even function of x,

then $b_k = 0$, $a_k = \int_{-\infty}^{\infty} \underbrace{h(x)\ \cos(kx)}_{\text{even function of x}}\,\mathrm{d}x = 2\int_0^\infty h(x)\ \cos(kx)\,\mathrm{d}x$

then $b_k = 0$, $H(k) = a_k - ib_k = a_k = 2\int_0^\infty h(x)\ \cos(kx)\,\mathrm{d}x$

$H(k)$ is also a real and even function of k

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k = \underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \cos(kx)\,\mathrm{d}k}_{\text{even function of } x} + \underbrace{\cancel{\frac{i}{2\pi}\int_{-\infty}^{\infty} H(k)\ \sin(kx)\,\mathrm{d}k}}_{\text{odd function of } x}$$

then $h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^{\infty} \underbrace{H(k)\ \cos(kx)}_{\text{real and even function of } k}\,\mathrm{d}k = \frac{1}{\pi}\int_0^\infty H(k)\ \cos(kx)\,\mathrm{d}k$

Check $h(x)$ is a real and even function of x

Basic properties

$$h(x) = \underbrace{\frac{1}{2\pi}\int_0^{\infty} \cancel{a_k \cos(kx)\,\mathrm{d}k}}_{\text{even function of } x} + \underbrace{\frac{1}{2\pi}\int_0^{\infty} b_k \sin(kx)\,\mathrm{d}k}_{\text{odd function of } x}$$

★ If $h(x)$ is a real and odd function of x,

then $a_k = 0,\ b_k = \int_{-\infty}^{\infty} \underbrace{h(x)\ \sin(kx)\,\mathrm{d}x}_{\text{even function of x}} = 2\int_0^{\infty} h(x)\ \sin(kx)\,\mathrm{d}x$

then $a_k = 0,\ H(k) = a_k - ib_k = -ib_k = -2i\int_0^{\infty} h(x)\ \sin(kx)\,\mathrm{d}x$ $H(k)$ is pure imaginary and odd function of k

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k = \underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty} \cancel{H(k)\ \cos(kx)\,\mathrm{d}k}}_{\text{even function of } x} + \underbrace{\frac{i}{2\pi}\int_{-\infty}^{\infty} H(k)\ \sin(kx)\,\mathrm{d}k}_{\text{odd function of } x}$$

then $h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k = \frac{i}{2\pi}\int_{-\infty}^{\infty} H(k)\ \sin(kx)\,\mathrm{d}k = \frac{i}{\pi}\int_0^{\infty} H(k)\ \sin(kx)\,\mathrm{d}k$

With i, this part is real and even function of k

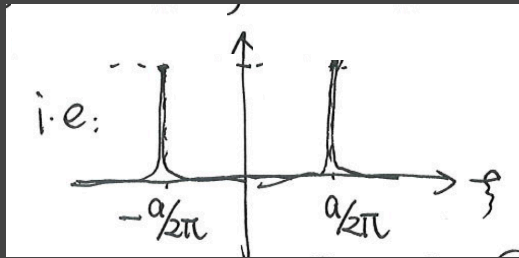
Check $h(x)$ is a real and odd function of x

Basic properties

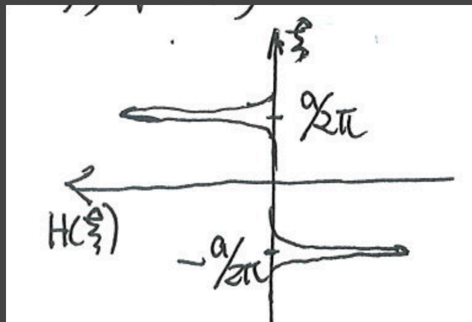
$$h(x) = \int_{-\infty}^{\infty} H(\xi)\, \exp(i2\pi\xi x)\, \mathrm{d}\xi \qquad H(\xi) = \int_{-\infty}^{\infty} h(x)\, \exp(-i2\pi\xi x)\, \mathrm{d}x$$

★ $h(x) = 1\,[\sim \cos(0)]$, $H(\xi) = \delta(\xi)$, i.e., only zero frequency mode!
Certain frequency (in momentum space) has broadest uncertainty in configuration space.

★ $h(x) = \cos(ax), H(\xi) = \frac{1}{2}\left[\delta(\xi - \frac{a}{2\pi}) + \delta(\xi + \frac{a}{2\pi})\right]$



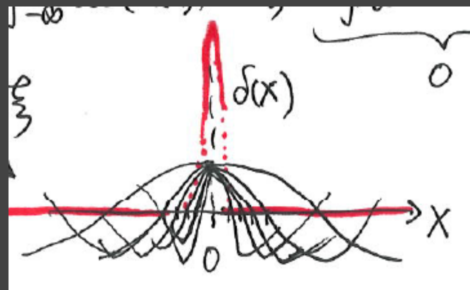
★ $h(x) = \sin(ax), H(\xi) = \frac{1}{2i}\left[\delta(\xi - \frac{a}{2\pi}) - \delta(\xi + \frac{a}{2\pi})\right]$



★ $h(x) = \delta(x)\,[\sim \Sigma_k e^{i2\pi\xi_k x}]$, $H(\xi) = 1$,
i.e., exact position is made of plane waves of all frequency modes.
Certain position in configuration space has broadest uncertainty in momentum space.

$$\delta(x) = \int_{-\infty}^{\infty} \exp(i2\pi\xi x)\, \mathrm{d}\xi = \int_{-\infty}^{\infty} [\cos(2\pi\xi x) + \cancel{i \sin(2\pi\xi x)}]\, \mathrm{d}\xi$$

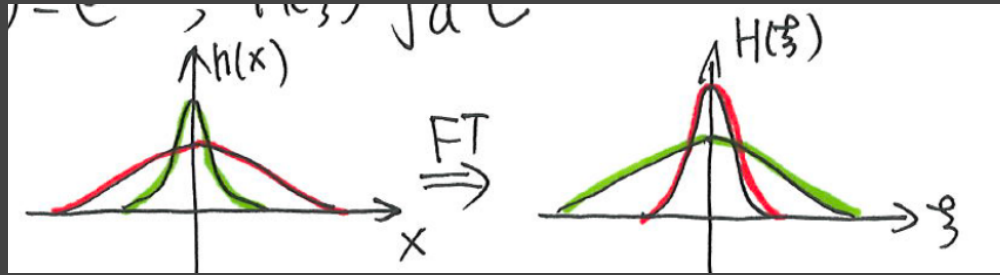
$$= \int_{-\infty}^{\infty} \cos(2\pi\xi x)\, \mathrm{d}\xi = \Sigma_k \cos(2\pi\xi_k x)$$



Basic properties

$$h(x) = \int_{-\infty}^{\infty} H(\xi)\, \exp(i2\pi\xi x)\, \mathrm{d}\xi \quad H(\xi) = \int_{-\infty}^{\infty} h(x)\, \exp(-i2\pi\xi x)\, \mathrm{d}x$$

★ $h(x) = e^{-ax^2}, H(\xi) = \sqrt{\frac{\pi}{a}} \exp\left(- \frac{(\pi\xi)^2}{a} \right)$



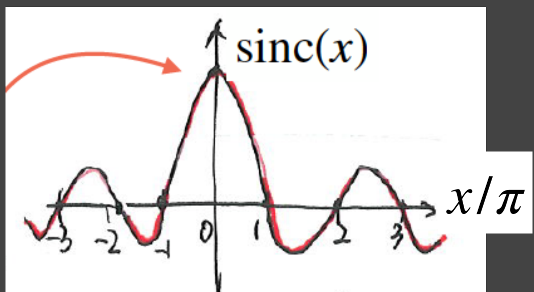
★ $h(x) = \mathrm{rect}(ax), H(\xi) = \frac{1}{|a|} \mathrm{sinc}\left(\frac{\xi}{a} \right)$

Gaussian function ⟷ Gaussian function
(In one domain) (In the other domain)

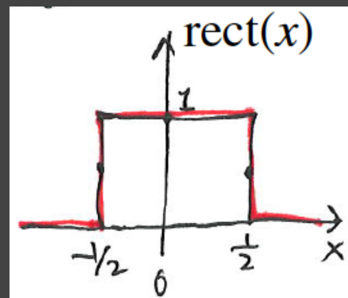
★ $h(x) = \mathrm{sinc}(ax), H(\xi) = \frac{1}{|a|} \mathrm{rect}\left(\frac{\xi}{a} \right)$

Sinc function ⟷ "Top hat"
(In one domain) (In the other domain)

$$\mathrm{sinc}(x) = \frac{\sin(x)}{x}$$



$$\mathrm{rect}(x) = \begin{cases} 0 & \text{if } |x| > 1/2 \\ 1/2 \text{ or } 0 & \text{if } |x| = 1/2 \\ 1 & \text{if } |x| < 1/2 \end{cases}$$



★ **Stretch (scaling) theorem:** $h(ax) \leftrightarrow \frac{1}{|a|} H(\frac{\xi}{a})$**,** for real non-zero a.

i.e., compress (stretch) in one domain, expand (shrink) in the other domain.

Basic properties

★ **Linearity theorem:** $h(x) = af(x) + bg(x) \rightarrow H(\xi) = aF(\xi) + bG(\xi)$

★ **Shifting theorem (time shifting):** $h(x) = \underbrace{f(x - x_0)}_{\text{shifting}} \rightarrow H(\xi) = F(\xi)\, \underbrace{\exp(-i2\pi\xi x_0)}_{\text{phase rotation}}$

★ **Modulation theorem (frequency shifting):** $h(x) = f(x)\underbrace{e^{i2\pi x\xi_0}}_{\text{phase rotation}} \rightarrow H(\xi) = \underbrace{F(\xi - \xi_0)}_{\text{shifting}}$

phase rotation ⟷ shifting
(In one domain) (In the other domain)

$$h(x) = e^{i2\pi x\xi_0}, H(\xi) = \delta(\xi - \xi_0)$$

$$h(x) = \delta(x - x_0), H(\xi) = \exp(-i2\pi\xi x_0)$$

★ **Derivative theorem:** $H^{(n)}(\xi) \leftarrow \mathrm{FT} \rightarrow \dfrac{\mathrm{d}^n\, h(x)}{\mathrm{d}x^n}$ then $H^{(n)}(\xi) = (i2\pi\xi)^n H(\xi)$

Basic properties

Piecewise multiplication (In one domain) $\longleftrightarrow$ Convolution/correlation (In the other domain)

★ **Convolution theorem:** $h(x) = (f \circledast g)(x) \equiv \int_{\infty}^{\infty} f(x')g(x-x')\,\mathrm{d}x'$ then $H(\xi) = F(\xi)\cdot G(\xi)$

★ **Correlation theorem:** $h(x) = (f \boxtimes g)(x) \equiv \int_{\infty}^{\infty} f^*(x')g(x+x')\,\mathrm{d}x'$ then $H(\xi) = F^*(\xi)\cdot G(\xi)$

1. Only if $H(\xi)$ is a real function , then $(f \boxtimes g)(x) = (g \boxtimes f)(x)$.
2. For auto-correlation, $g(x) = f(x)$, then $H(\xi) = |F(\xi)|^2$

Autocorrelation $\longleftrightarrow$ Power spectrum
(in one domain) (in the other domain)

— essentially PSD of field $f(x)$!

Parseval's theorem (*total power of signal, in 1d case*)

$$P_{\rm tot} = \int_{-\infty}^{\infty} |h(x)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} |H(\xi)|^2\,\mathrm{d}\xi \quad \text{or} \quad \int_{-\infty}^{\infty} |h(x)|^2\,\mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{\infty} |H(k)|^2\,\mathrm{d}k$$

$\mathrm{PSD}(\xi) \equiv |H(\xi)|^2 + |H(-\xi)|^2$ being power spectrum density, $P_{\rm tot} = \int_0^{\infty} \mathrm{PSD}(\xi)\,\mathrm{d}\xi$.

Discrete Fourier transform

DFT: Discrete Fourier Transform

Discretization is a nature of measurements!

Continuous FT

$$\boxed{H(\xi)} = \int_{-\infty}^{\infty} h(x)\ \exp(-i2\pi\xi x)\,\mathrm{d}x \qquad \boxed{H(k)} = \int_{-\infty}^{\infty} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

$$\boxed{h(x)} = \int_{-\infty}^{\infty} H(\xi)\ \exp(i2\pi\xi x)\,\mathrm{d}\xi \qquad \boxed{h(x)} = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(k)\ \exp(ikx)\,\mathrm{d}k$$

$k = 2\pi\xi$ is the *angular* spatial frequency (wavenumber).

DFT on *N* point

$$\boxed{H_k} = \Sigma_{j=0}^{N-1} h_j \exp\left(-i\frac{2\pi jk}{N}\right)$$

$$\boxed{h_j} = \frac{1}{N}\Sigma_{k=-\frac{N}{2}}^{\frac{N}{2}-1} H_k \exp\left(i\frac{2\pi jk}{N}\right)$$

H_k is the DFT of h_j, note: H_k here differs from Fourier series by N! *j*, *k* are integers!

$$\int \mathrm{d}\vec{k} = \left(\frac{2\pi}{L}\right)^{\mathrm{d}} \Sigma_{\vec{k}} = \frac{(2\pi)^{\mathrm{d}}}{V}\Sigma_{\vec{k}}$$

$$\int \mathrm{d}\vec{x} = \left(\frac{L}{N}\right)^{\mathrm{d}} \Sigma_{\vec{j}} = \frac{V}{N^{\mathrm{d}}}\Sigma_{\vec{j}}$$

$$\boxed{|H(\xi_k)| = |H(k)| = \Delta |H_k|}$$

$$\boxed{h(x_j) = h_j}$$

$x_0 \quad x_j = x_0 + \Delta j \quad h_j = h(x_j)$

Sampling resolution $\Delta = L/N$

DFT: Discrete Fourier Transform

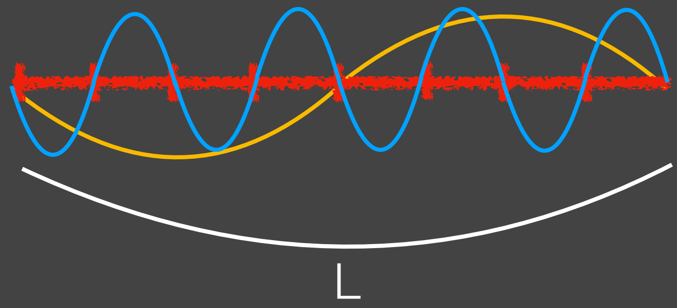
Discretization is a nature of measurements!

$$H_k = \Sigma_{j=0}^{N-1} h_j \exp\left(-i\frac{2\pi jk}{N}\right)$$

$$h_j = \frac{1}{N}\Sigma_{k=-\frac{N}{2}}^{\frac{N}{2}-1} H_k \exp\left(i\frac{2\pi jk}{N}\right)$$

DFT on *N* point

Nyquist-Shannon sampling theory tells:

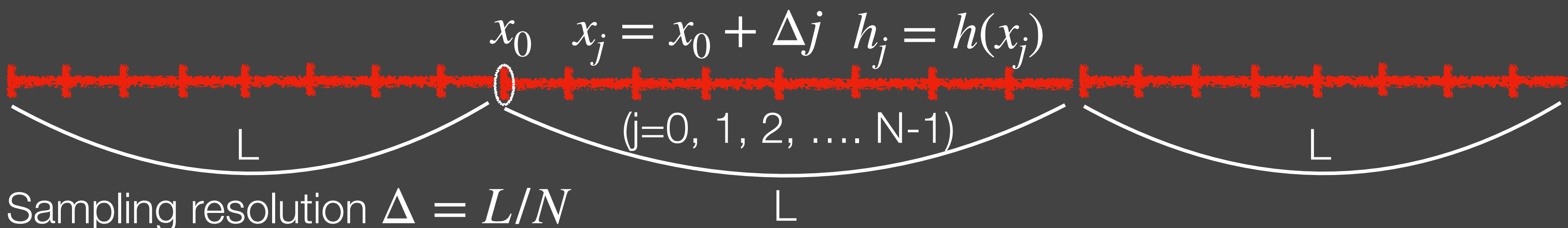


Lowest frequency $\xi_0 = 1/L$

Highest frequency $\xi_{\mathrm{Nyquist}} = N/(2L) = 1/(2\Delta)$

Frequency $\xi_k = k\xi_0 = k/L$, where $k = 0, \pm 1, \pm 2, \ldots \pm N/2$

Periodicity: $h_{j\pm mN} = h_j$ and $H_{k\pm mN} = H_k$, $m = 0, \pm 1, \pm 2, \ldots.$



Sampling resolution $\Delta = L/N$

DFT: Discrete Fourier Transform

Basic properties

$$H_k = \Sigma_{j=0}^{N-1} h_j \exp\left(-i\frac{2\pi jk}{N}\right)$$

$$h_j = \frac{1}{N}\Sigma_{k=-\frac{N}{2}}^{\frac{N}{2}-1} H_k \exp\left(i\frac{2\pi jk}{N}\right)$$

DFT on *N* point

Periodicity:

- $h_{j\pm mN} = h_j$
- $H_{k\pm mN} = H_k$

The zeroth mode:

- $H_{k=0} = \Sigma_{j=0}^{N-1} h_j$

The $\pm N/2$ modes:

- $H_{k=N/2} = \Sigma_{j=0}^{N-1} h_j \cos(\pi j) - i\Sigma_{j=0}^{N-1} h_j \sin(\pi j) = \Sigma_{j=0}^{N-1} h_j \cos(\pi j)$
- $H_{k=-N/2} = \Sigma_{j=0}^{N-1} h_j \cos(\pi j) + i\Sigma_{j=0}^{N-1} h_j \sin(\pi j) = \Sigma_{j=0}^{N-1} h_j \cos(\pi j)$

  => $H_{k=-N/2} = H_{k=N/2} = \Sigma_{j=0}^{N-1} h_j \cos(\pi j)$

For real function $h(t)$:

- Consider the degree of freedom for a N-real-number series $\{h_j\}$, then after Fourier transform (DFT), there are N complex components in $\{H_k\}$, i.e., $2N$ real numbers. Are there really $2N$ degree of freedom in Fourier domain?

  No, because *if $\{h_j\}$ are real, then $H_{k_-} = H^*_{k_+}$*, i.e., the negative frequency modes do NOT provide extra information other than what have already been carried in the positive modes! => Complex modes $k = 1,2...\frac{N}{2} - 1$, plus two real modes $k = 0,\frac{N}{2}$, total of $2\left(\frac{N}{2} - 1\right) + 1 + 1 = N$ d.o.f.

DFT: Discrete Fourier Transform

Basic properties

$$H_k = \Sigma_{j=0}^{N-1} h_j \exp\left(-i\frac{2\pi jk}{N}\right)$$
$$h_j = \frac{1}{N}\Sigma_{k=-\frac{N}{2}}^{\frac{N}{2}-1} H_k \exp\left(i\frac{2\pi jk}{N}\right)$$

DFT on *N* point

To estimate power spectrum density with DFT:

$$\mathrm{PSD}(\xi_k) \equiv |H(\xi_k)|^2 + |H(-\xi_k)|^2 = \Delta^2(|H_k|^2 + |H_{N-k}|^2)$$

Sampling resolution $\Delta = L/N$, $k = 0, 1, 2, \ldots N/2$

If $h(x)$ is a real function, then

$$\mathrm{PSD}(\xi_k) = 2\left(\frac{L}{N}\right)^2\left[\left(\Sigma_{j=0}^{N-1} h_j \cos\left(\frac{2\pi jk}{N}\right)\right)^2 + \left(\Sigma_{j=0}^{N-1} h_j \sin\left(\frac{2\pi jk}{N}\right)\right)^2\right]$$

Parseval's theorem for CFT:

$$\int_{-\infty}^{\infty} |h(x)|^2 \,\mathrm{d}x = \int_{-\infty}^{\infty} |H(\xi)|^2 \,\mathrm{d}\xi$$
$$\int_{-\infty}^{\infty} |h(x)|^2 \,\mathrm{d}x = \frac{1}{2\pi}\int_{-\infty}^{\infty} |H(k)|^2 \,\mathrm{d}k$$

Parseval's theorem for DFT:

$$\Sigma_{j=0}^{N-1} |h_j(x_j = x_0 + \Delta j)|^2 = \frac{1}{N}\Sigma_{k=0}^{N-1} |H_k|^2$$

DFT: Discrete Fourier Transform

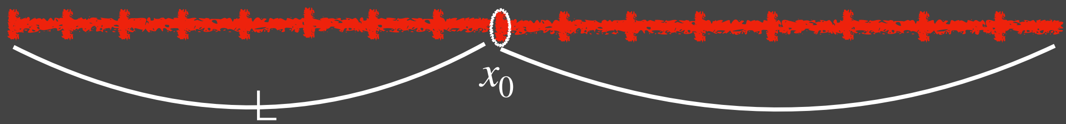
What's the relation and difference between Fourier series and Fourier integral, between CFT and DFT?

If the period of a signal extends to infinity, i.e., $L \to \infty$, then $h(x)$ expressed as Fourier series becomes Fourier integral.

DFT is more for finite period signal analysis. The frequency sampling is determined by the Nyquist-Shannon theory.

Nyquist-Shannon sampling theory tells:

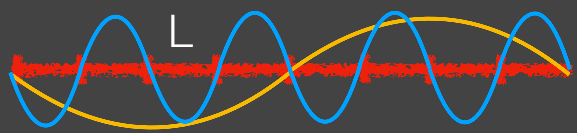
$x_j = x_0 + \Delta j \quad h_j = h(x_j)$ (j=0, 1, 2, ... N-1)



Lowest frequency $\xi_0 = 1/L$

Highest frequency

$\xi_{\mathrm{Nyquist}} = N/(2L) = 1/(2\Delta)$



Fourier series

$$h(x) = \Sigma_k H_k \exp(ikx)$$

$$H_k = \frac{1}{L}\int_{-L/2}^{L/2} h(x)\ \exp(-ikx)\,\mathrm{d}x$$

Continuous FT

$$h(x) = \int_{-\infty}^{\infty} H(\xi)\ \exp(i2\pi\xi x)\,\mathrm{d}\xi$$

$$H(\xi) = \int_{-\infty}^{\infty} h(x)\ \exp(-i2\pi\xi x)\,\mathrm{d}x$$

DFT on *N* point

$$h_j = \frac{1}{N}\Sigma_{k=-\frac{N}{2}}^{\frac{N}{2}-1} H_k \exp\left(i\frac{2\pi jk}{N}\right)$$

$$H_k = \Sigma_{j=0}^{N-1} h_j \exp\left(-i\frac{2\pi jk}{N}\right)$$

Can the DFT of a discretized sampling of the underlying function $h(x)$ provide exact Fourier transforms of $h(x)$? In other words, are we 100% sure that we can reconstruct signal $h(x)$ from a DFT?

We are going to switch to time and frequency domains for a change…

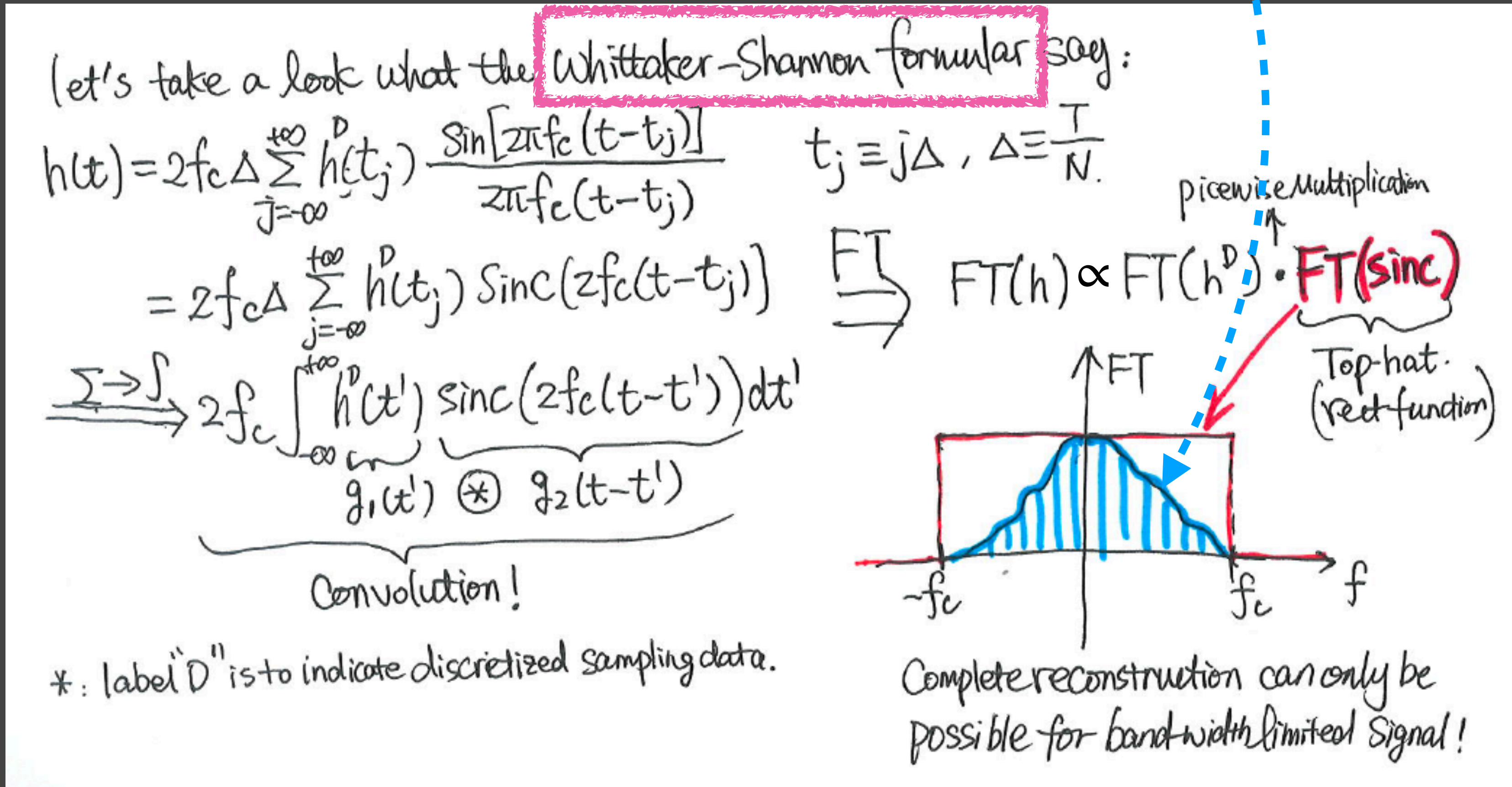
It is possible to reconstruct the real underlying signal $h(t)$ from the DFT of a discretized sampling of $h(t)$, only if $h(t)$ is "bandwidth-limited", i.e., $H(f) = 0$ for $|f| > f_c$ — via Whittaker-Shannon formula.

When $h(t)$ is not band limited, "aliasing" happens.

Whittaker-Shannon sampling and the aliasing problem of DFT

For a bandwidth-limited signal $h(t)$, i.e., $H(f) = 0$ for $|f| > f_c$, we have the following:

$$h(t) = 2f_c\Delta\Sigma_{j=\infty}^{+\infty} h^{\mathrm{D}}(t_j)\frac{\sin[2\pi f_c(t - j\Delta)]}{2\pi f_c(t - j\Delta)}$$ - ***Whittaker-Shannon formular***

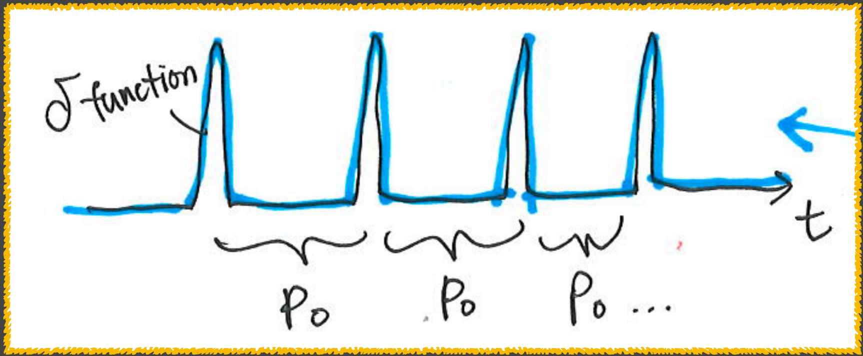


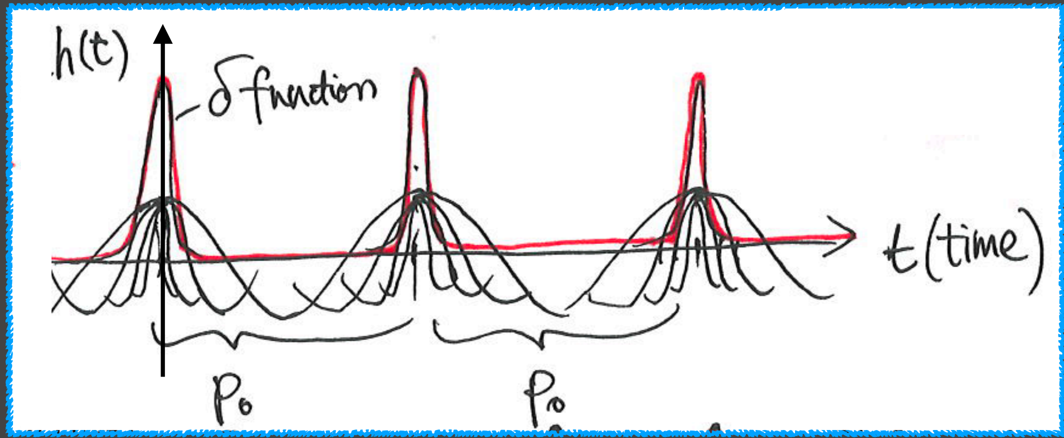
The theorem tells us: if the sample resolution $\Delta = T/N$ is such that the corresponding to the highest sampling frequency $f_{\mathrm{Nyq}} = 1/(2\Delta)$ is higher than the band-width threshold frequency f_c, then the original signal $h(t)$ can be exactly reconstructed from ***evenly sampled data*** $\{h^{\mathrm{D}}(t_j)\}$ with such sample resolution $\Delta = T/N$!

Whittaker-Shannon sampling and the aliasing problem of DFT

When the signal is not band-width limited, i.e., $H(f) \neq 0$ for $|f| > f_c$.

Let's first consider a periodic time-domain signal, made of a series of delta pulses $\Sigma_{j=-\infty}^{\infty}\delta(t-jP_0)$, where j is integer, P_0 is the pulse period, frequency of $\omega_0 = 2\pi/P_0$.





This is also called a "Shah function", defined as: $III(t) \equiv \Sigma_{j=-\infty}^{+\infty}\delta(t-j)$,

with $FT(III) = \Sigma_{n=-\infty}^{+\infty}\delta(f-n)$, or the "*Dirac comb function*", defined as:

$$III_{P_0}(t) \equiv \Sigma_{j=-\infty}^{+\infty}\delta(t-jP_0)\left[=\frac{1}{P_0}III\left(\frac{t}{P_0}\right)\right], \text{ with } FT[III_{P_0}(f)] = \frac{1}{P_0}\Sigma_{n=-\infty}^{+\infty}\delta\left(f-\frac{n}{P_0}\right).$$

Therefore write out $III_{P_0}(t)$ using Fourier series:

$$III_{P_0}(t) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\exp\left(i\frac{2\pi kt}{P_0}\right) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\left[\cos\left(\frac{2\pi kt}{P_0}\right) + \underline{i\sin\left(\frac{2\pi kt}{P_0}\right)}\right]$$

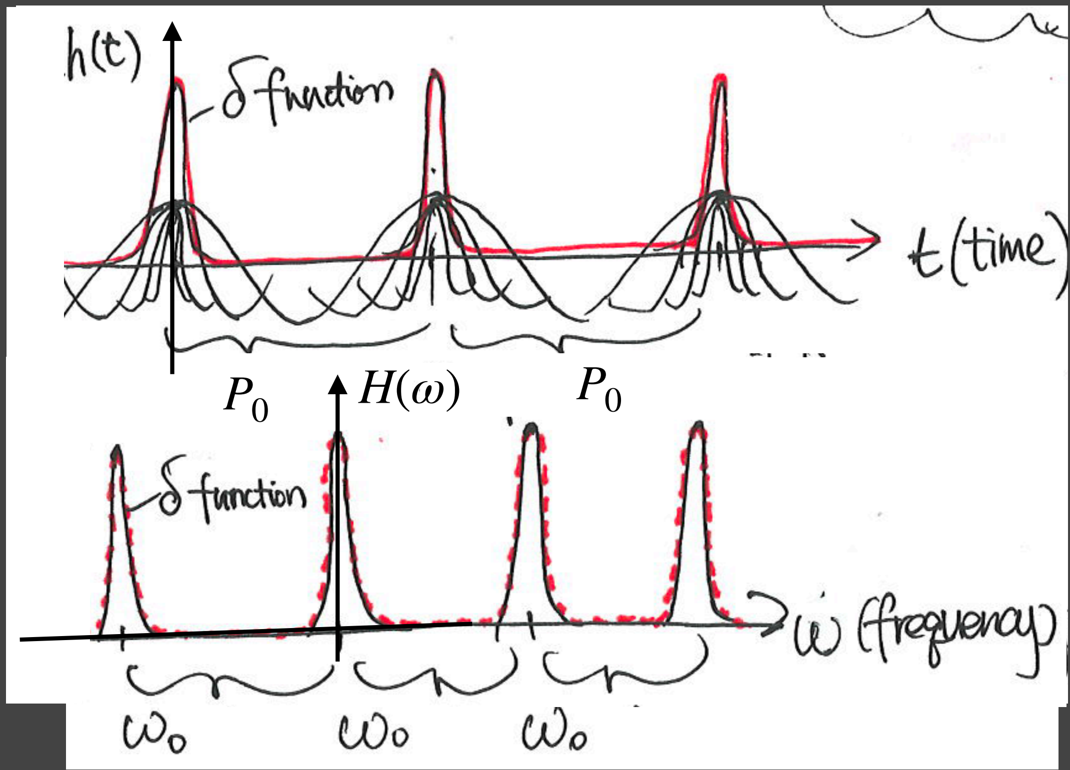
odd function of *k*, *sum going to zero.*

i.e., $$\boxed{III_{P_0}(t) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\cos\left(\frac{2\pi kt}{P_0}\right) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\cos(k\omega_0 t)}$$

Very important and fun!

$$III_{P_0}(t) \equiv \Sigma_{j=-\infty}^{+\infty}\delta(t - jP_0) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\cos\left(\frac{2\pi kt}{P_0}\right) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\cos(k\omega_0 t)$$

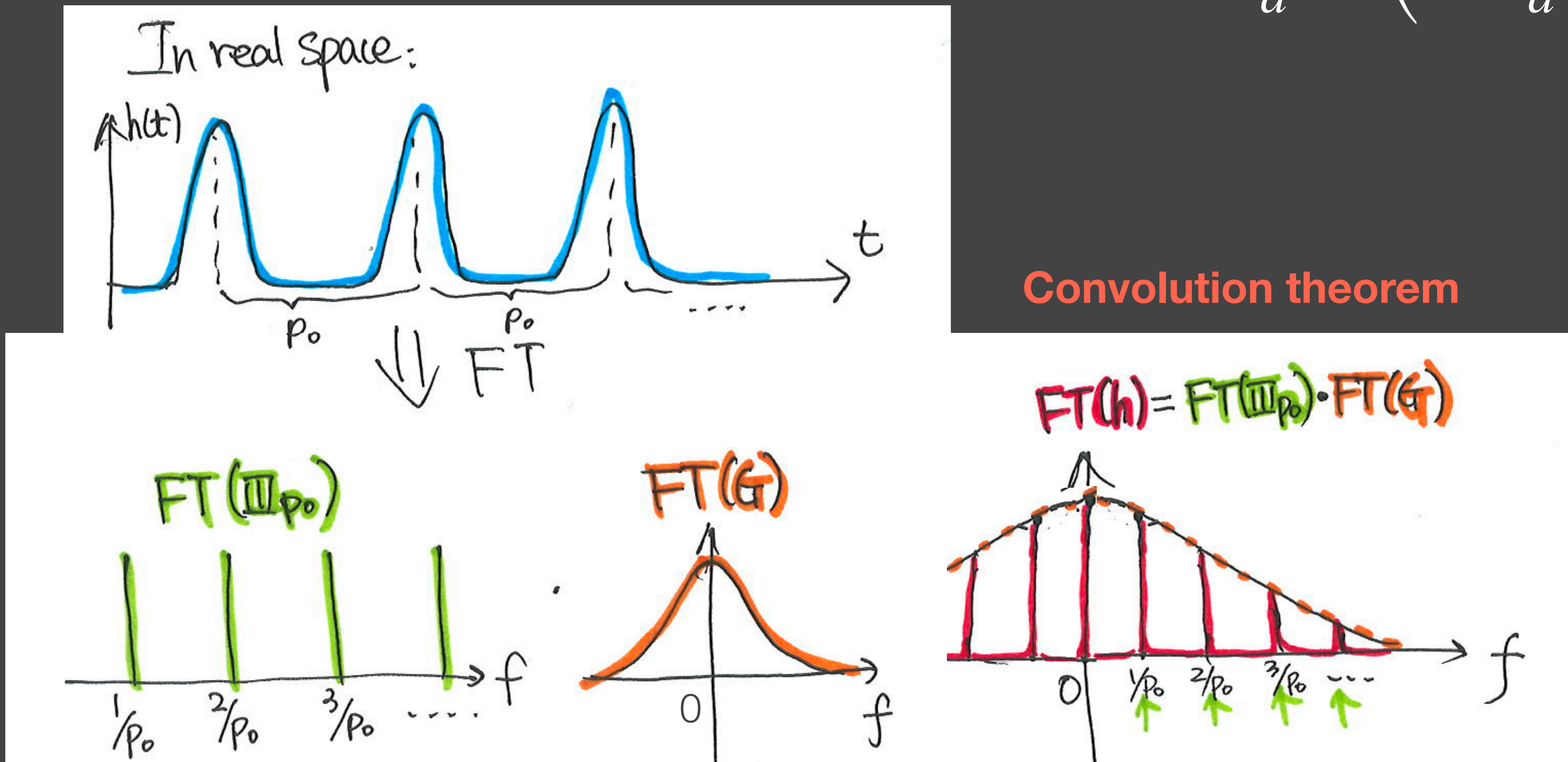
$$\mathrm{FT}[III_{P_0}(f)] = \frac{1}{P_0}\Sigma_{n=-\infty}^{+\infty}\delta(f - \frac{n}{P_0}) \quad \mathrm{FT}[III_{P_0}](\omega) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\delta(\omega - k\omega_0) \quad \omega_0 = 2\pi/P_0$$



With the Dirac Comb, we can study periodic signals!

$$III_{P_0}(t) \equiv \Sigma_{j=-\infty}^{+\infty}\delta(t - jP_0) \quad FT(III_{P_0}) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\delta(\omega - k\omega_0)$$

Now consider a series of Gaussian pulse with period P_0, the signal can be described by $h(t) = (III_{P_0} \circledast g)(t)$, where $g(t) = \exp(-at^2)$ with FT $G(f) = \frac{\pi}{a}\exp\left(-\frac{(\pi f)^2}{a}\right)$.



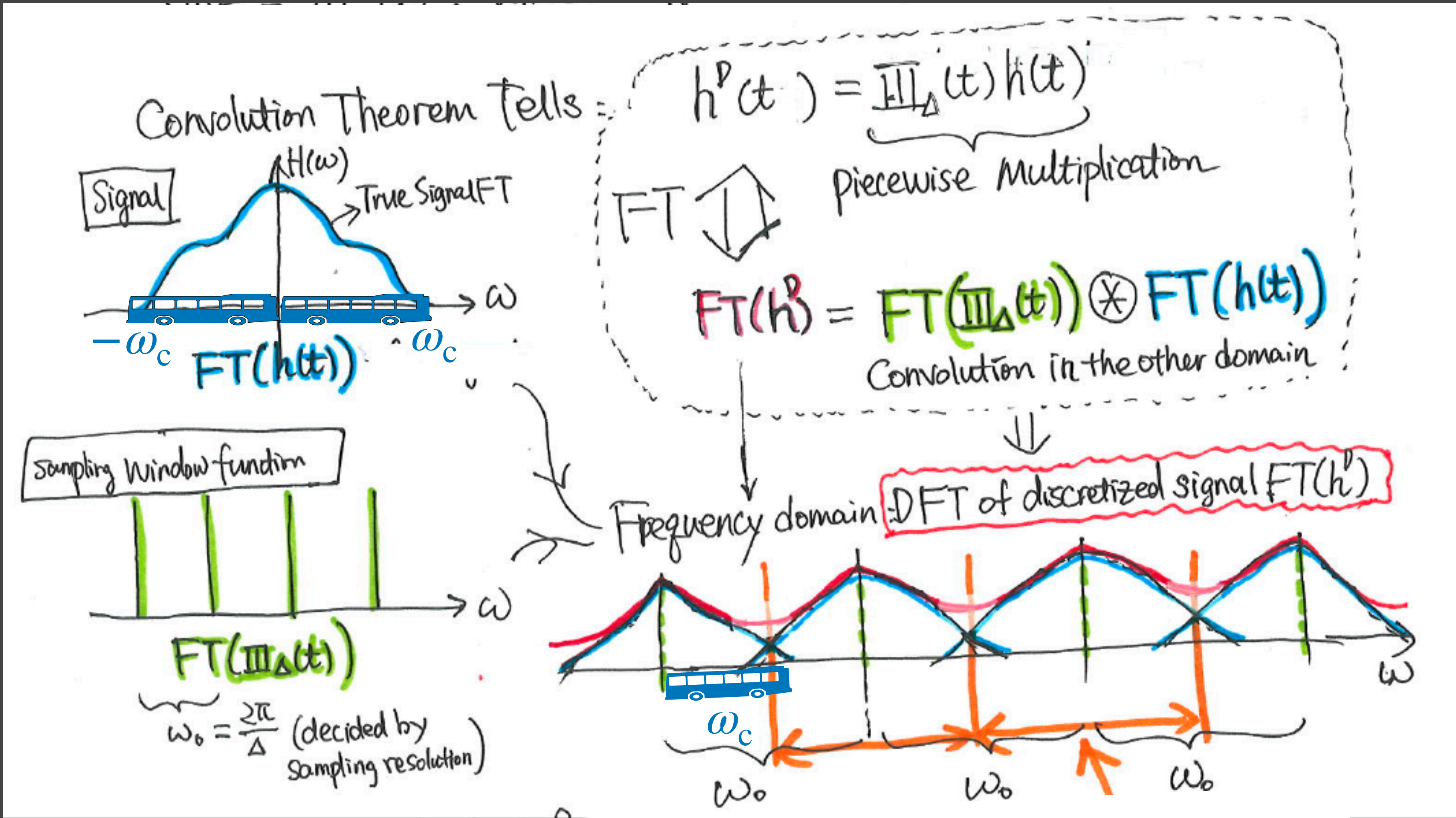
With the Dirac Comb, we can study periodic signals!

$$\boxed{III_{P_0}(t) \equiv \Sigma_{j=-\infty}^{+\infty}\delta(t - jP_0) \quad FT(III_{P_0}) = \frac{1}{P_0}\Sigma_{k=-\infty}^{+\infty}\delta(\omega - k\omega_0)}$$

Now consider a discrete time series to sample a signal $h(t)$, the sampled data are given by $h_{\mathrm{D}}(t_j) = \underbrace{\Sigma_j\delta(t - t_j)}_{\text{Sampling window function (SWF)}} \cdot h(t)$

1. The signal has an actual bandwidth of $[-\omega_{\mathrm{c}}, \omega_{\mathrm{c}}]$
2. The signal is sampled by $\mathrm{SWF} \equiv III_\Delta(t)$, where $\Delta = T/N$ is the sampling resolution. Its Fourier transform has period in frequency domain of $\omega_0 = 2\pi/\Delta$.
3. For a DFT sampling with resolution $\Delta = T/N$, the highest angular frequency is given by $\omega_{\mathrm{Nyq}} = \pi/\Delta = \omega_0/2$. Therefore the angular frequency domain of DFT is in range of $[-\omega_0/2, \omega_0/2]$.
4. We have studied that only if $\omega_{\mathrm{Nyq}} = \omega_0/2 \geqslant \omega_{\mathrm{c}}$, then the true signal can be reconstructed with the DFT measured from the discrete time series $h_{\mathrm{D}}(t_j)$.
5. What if $\omega_{\mathrm{Nyq}} = \omega_0/2 < \omega_{\mathrm{c}}$? ***the aliasing problem of DFT!***

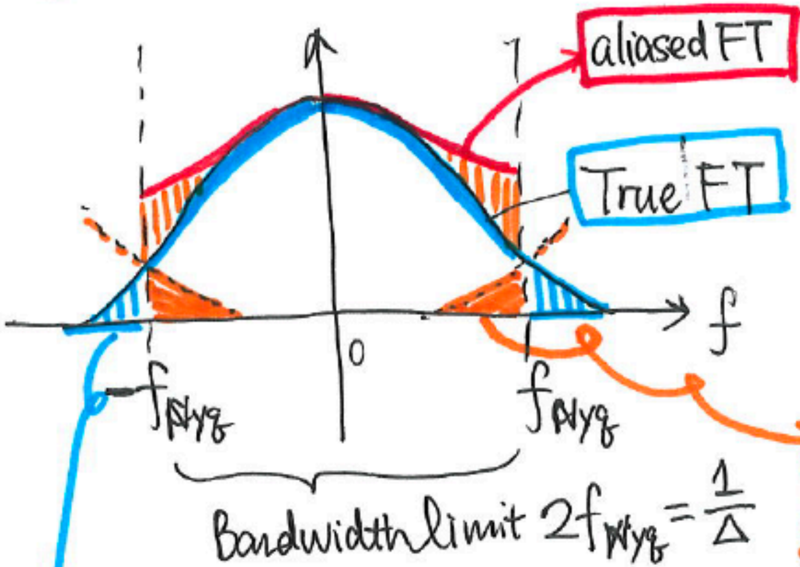
With Dirac Comb, we can describe discretized data.

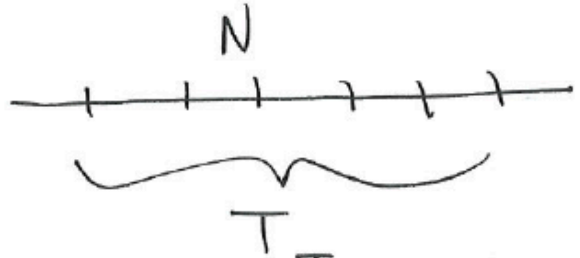


If the sampling resolution resulting in $\omega_{\mathrm{Nyq}} = \omega_0/2 < \omega_{\mathrm{c}}$, the DFT of the discrete time series will start overlapping across different neighboring images.

The "aliasing" problem of DFT

So, why this bandwidth limit matters?





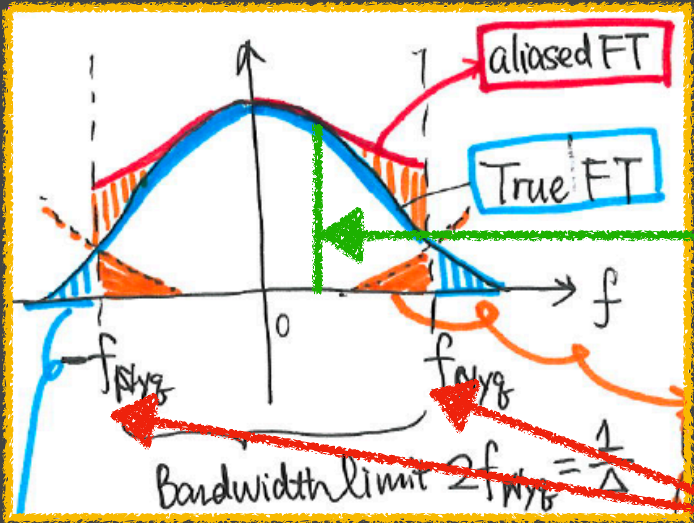
$\Delta = \frac{T}{N}$ Sampling resolution

When "Spill over" happens, any frequency component outside $(-f_{Nyq}, f_{Nyq})$ is aliased – falsely translated – into the range. This is called "Aliasing".

This means: the signal has higher frequency features, which can not be presented using the given sampling resolution $\Delta = T/N$.

DFT Aliasing is due to (1) inability to resolve details in a time series beyond $|f_{\mathrm{Nyq}}|$; and (2) the periodicity nature of FT.

The "aliasing" problem of DFT



The total data length T (of a periodic signal) decides the lowest frequency $f_0 = 1/T$

The sampling resolution $\Delta \equiv T/N$ essentially decides the bandwidth $f_{\mathrm{Nyq}} = N/(2T) = 1/(2\Delta)$

What can I do about Aliasing?

Increasing sampling frequency and thus resolution by increasing N, thus the Nyquist frequency is increased in order to present finer details of the time series.

Always make sure:

$\lim_{f \to f_{\mathrm{Nyq}}^{+}} |H(f)| \approx 0$ and $\lim_{f \to -f_{\mathrm{Nyq}}^{-}} |H(f)| \approx 0$

The "aliasing" problem of DFT

A related phenomenon is the **Gibbs phenomenon:**

Fourier coefficients of smoother functions will more rapidly decay at higher frequencies (resulting in faster convergence), whereas Fourier coefficients of discontinuous functions will slowly decay (resulting in slower convergence).

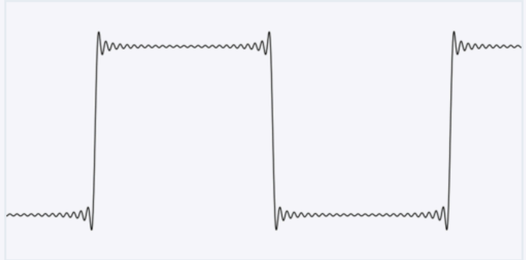
e.g., a square wave function can be expressed as a sum:

$$\Sigma_{k=1}^{\infty}\frac{1}{k}\sin(kx).$$

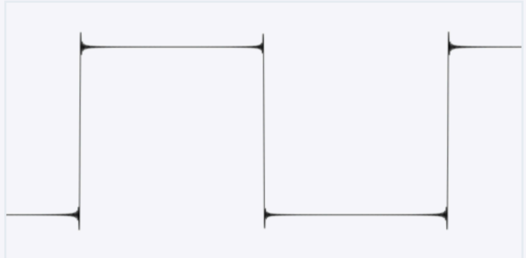
When the summation is truncated at a finite N (e.g., 5, 25, 125 in figure), there is a remarkable oscillation behavior (with an amplitude of 9% of the jump magnitude) around a jump discontinuity. Only when $N \to \infty$, the summation converges to the mid-point around the jump discontinuity.

The Gibbs Phenomenon can be alleviated by using a smoother method of Fourier series summation (e.g., Fejér summation or Riesz summation) or continuous wavelet transformation.

Functional approximation of square wave using 5 harmonics

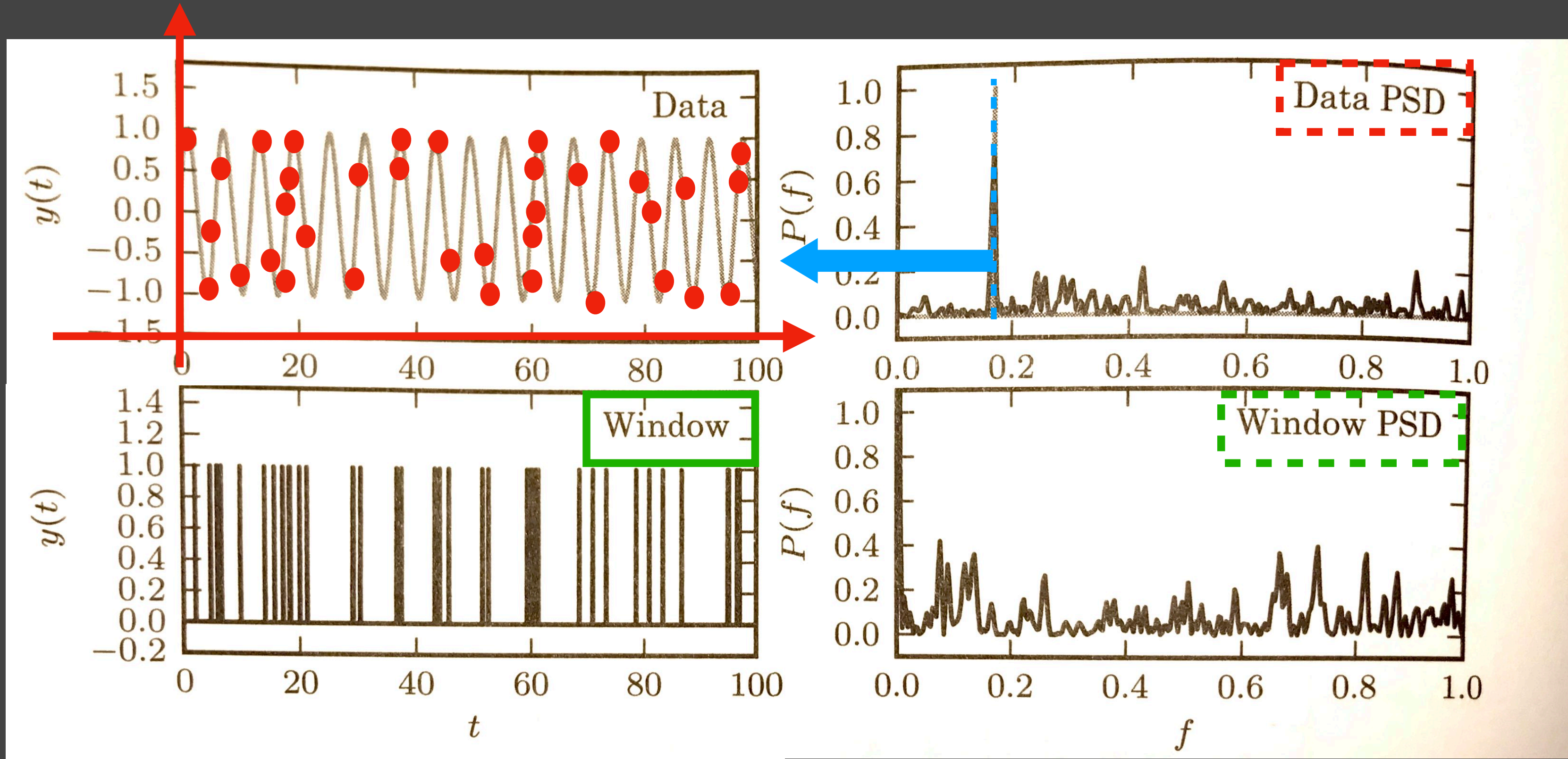


Functional approximation of square wave using 25 harmonics



Functional approximation of square wave using 125 harmonics

Can Fourier transform be used for unevenly sampled signal analysis?



$$y^{\mathrm{D}}(t) = \Sigma_{\mathrm{any}\ j}\, \delta(t - t_j) \times y(t)$$

Piecewise multiplication

Fourier transform (FT)

$$\mathrm{FT}(y^{\mathrm{D}}) = \mathrm{FT}(W) \circledast \mathrm{FT}(y)$$

Convolution

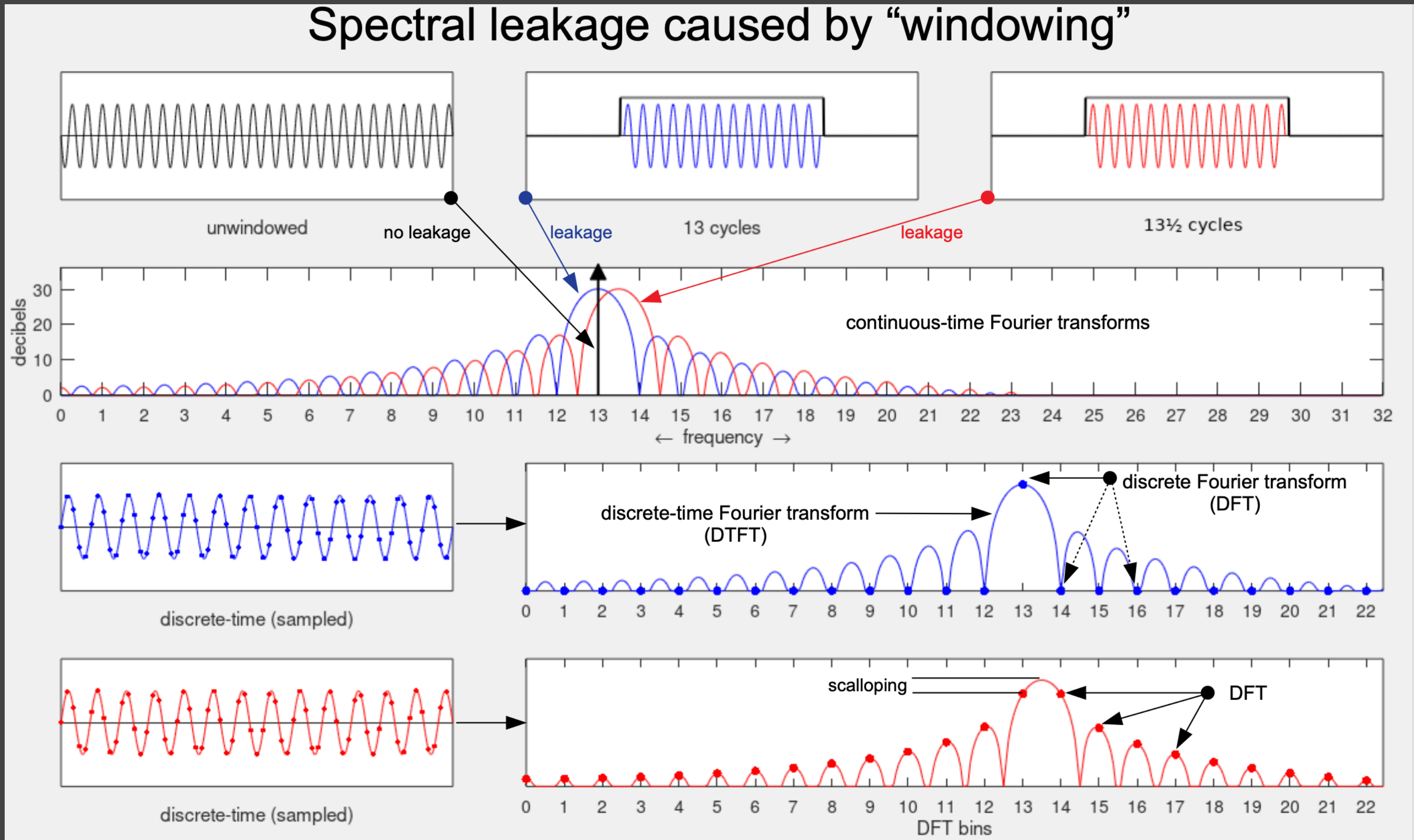
1. Constructing a finer and evenly-spaced grid to re-sample the signal
2. Adopt a window function where 1 is assigned to the sampled places and 0 for elsewhere.
3. Adopt DFT for both window function and signal using the finer grid.

There are two important features of signal analysis through ***DFT***, i.e., *sampling* and *windowing*.

For a ***true*** periodic signal, *sampling* frequency will cause ***aliasing*** if the signal is not sampled with sufficiently high resolution (Whittaker-Shannon sampling theorem).

While *windowing* is related to *spectral leakage* for finite-sized non-periodic signals.

DFT adds another layer of complication due to discretization!



As an example, we will window a sinusoidal signal in two ways (blue and red). In both cases, they will cause spectral leakage, which is evident in the 2nd row, where both blue and red curves show power leakage beyond f = 13. When the sinusoid is sampled with discrete-time Fourier transform (DTFT) (see 3rd and 4th rows), in the blue case (in which a top-hat window is applied to maintain the natural periodicity), the DFT power spectrum does NOT reveal the spectral leakage. While in the red case (where the top-hat window does NOT maintain the natural periodicity), the DFT exhibits the power leakage.

Fast Fourier Transform (FFT)

FFT: an ingenious algorithm to calculate DFT quickly!

- Gives cost of $\mathcal{O}(N \log_2 N)$
- Result is identical to DFT
- (A good reference: Numerical Recipes)

FFT Application I - Periodic signal search

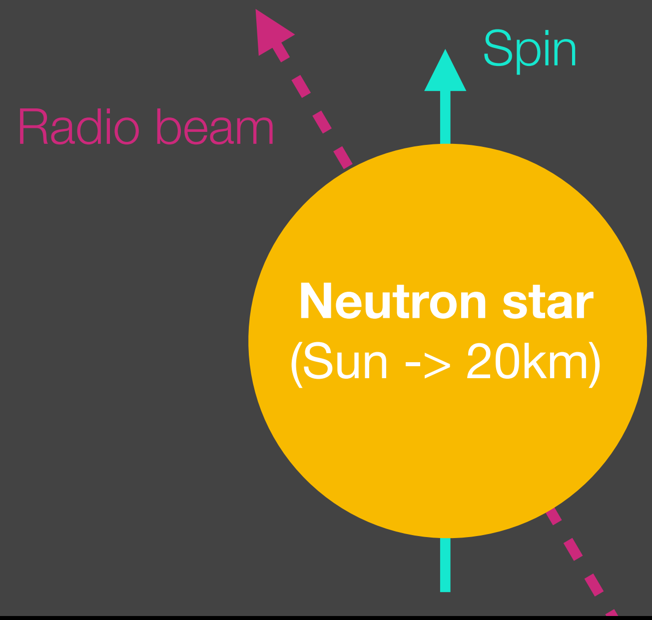
FFT Application II - Convolution calculation

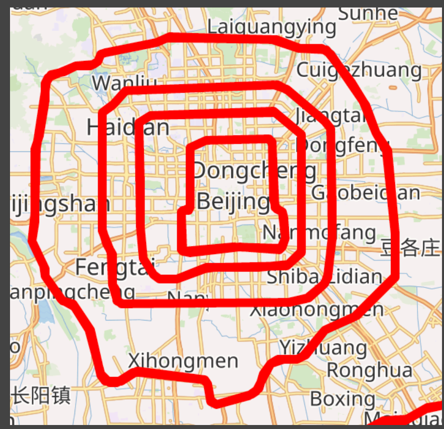
FFT Application III - Correlation calculation

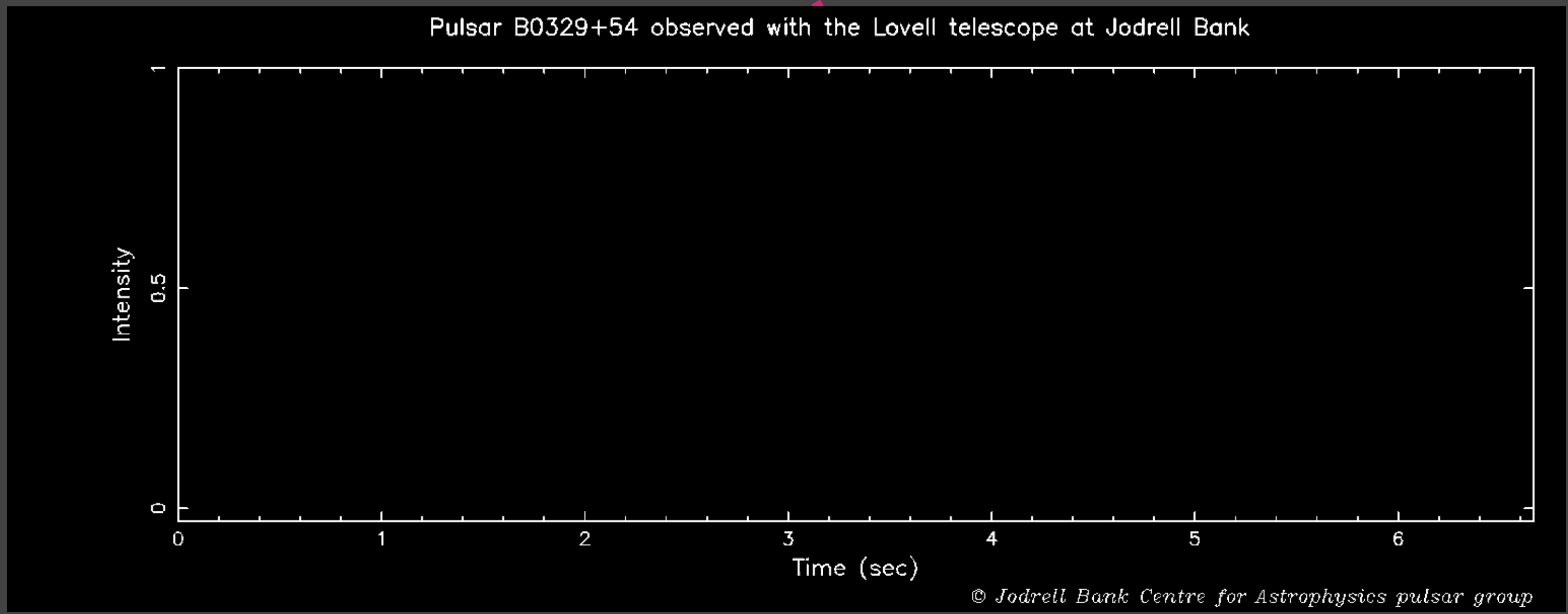
Application I - search periodic signal

Pulsar Searches

as an beautiful and interesting example …



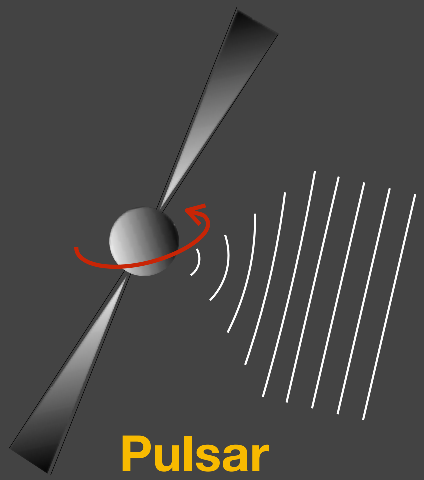




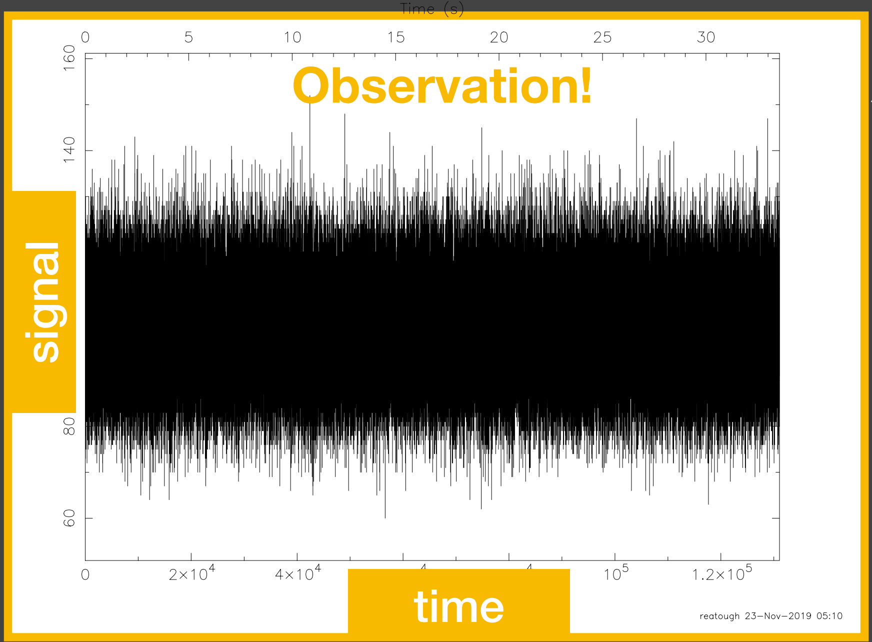
http://www.jb.man.ac.uk/pulsar/Education/Sounds/

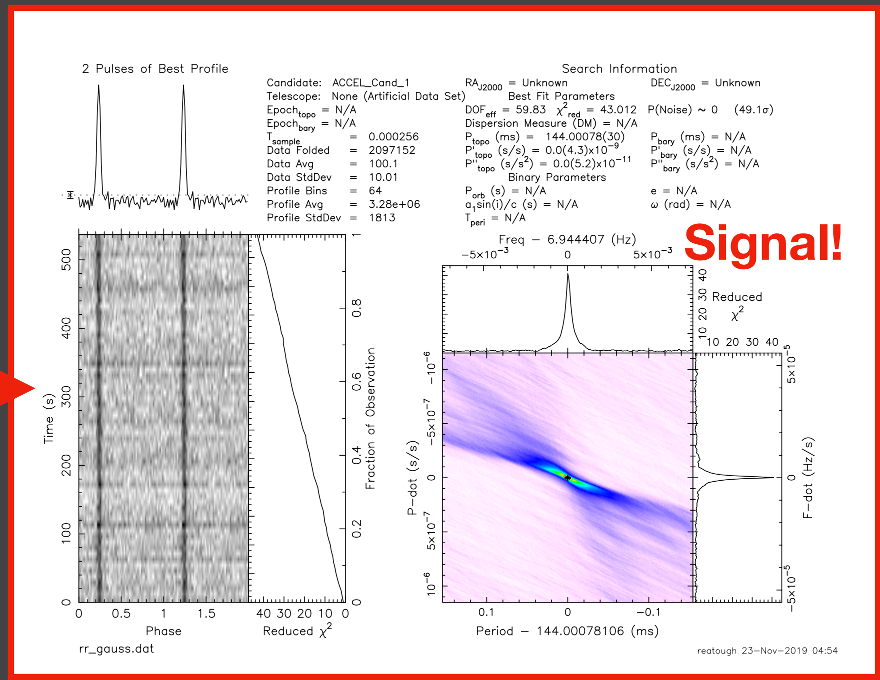
Periodic signal

Pulsar Searches



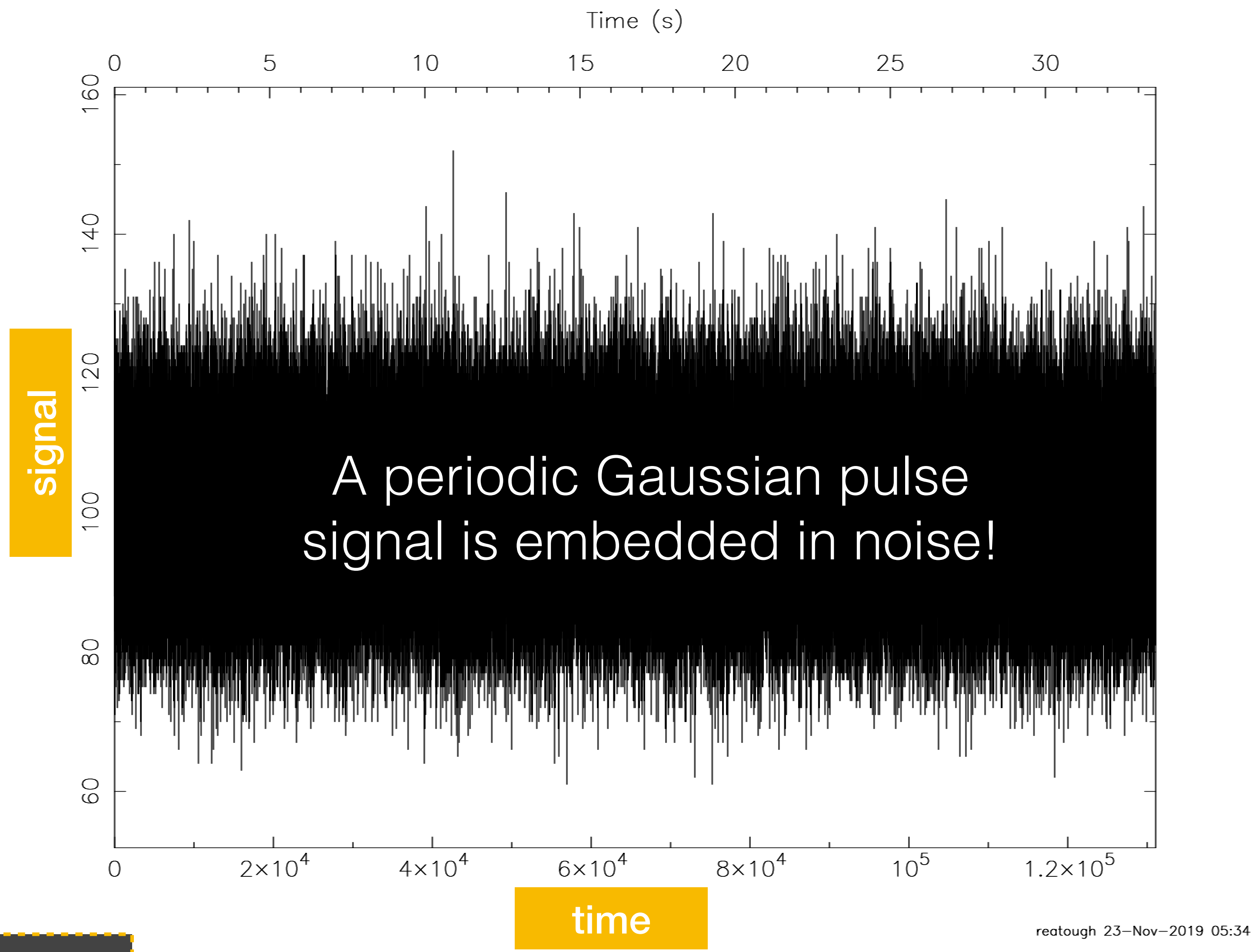
FAST Aerial View (Credit: NAOC)





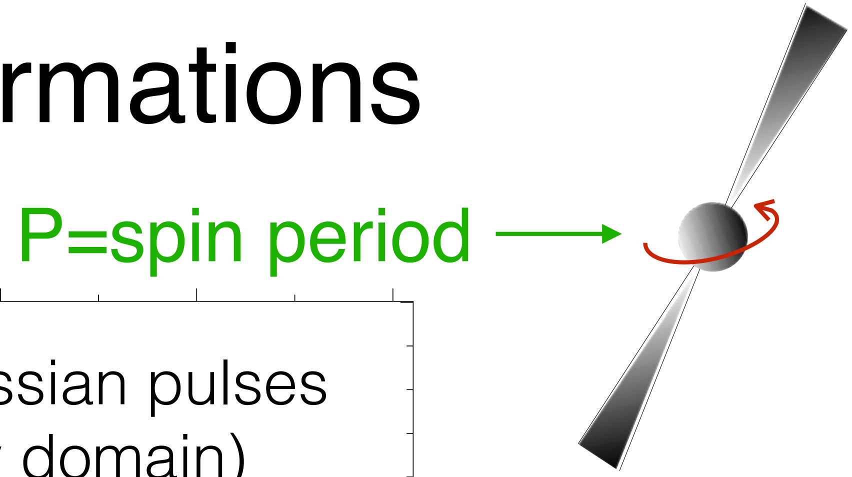
Figures created with PRESTO:
https://www.cv.nrao.edu/~sransom/presto/

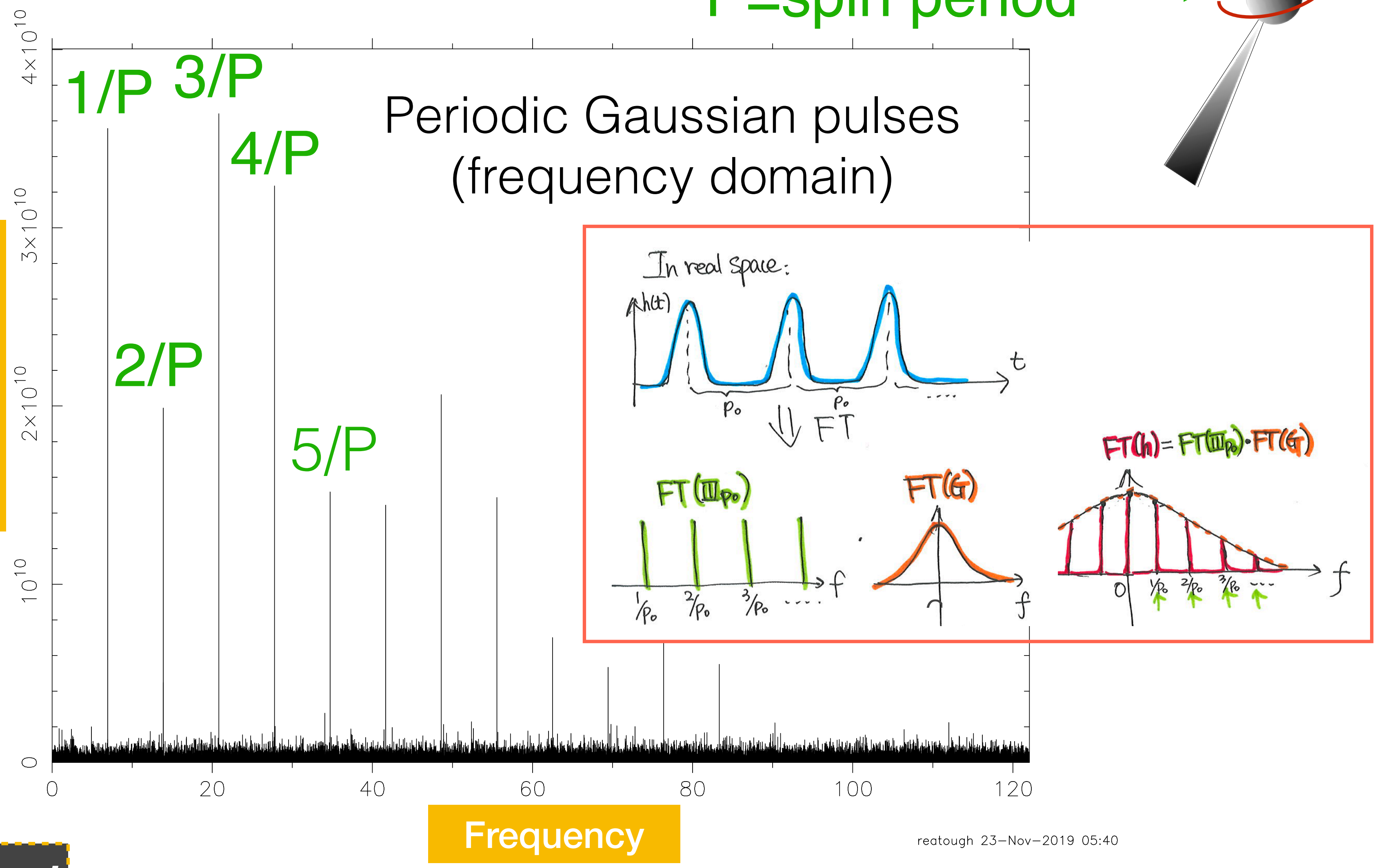
Pulsar Search
Fourier Transformations



Periodic signal

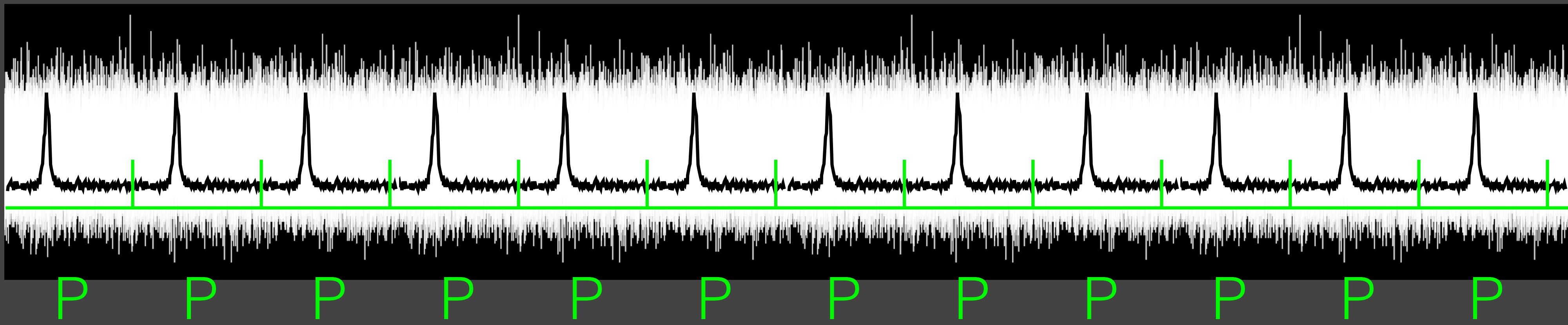
Pulsar Search
Fourier Transformations

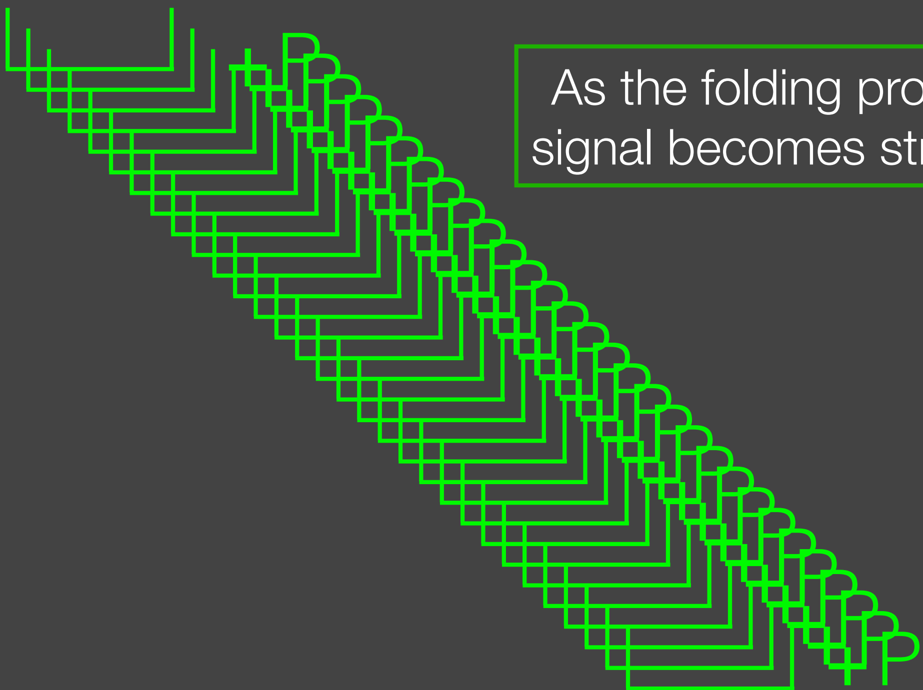




Periodic signal

After FT and find period candidates, apply pulsar “folding”

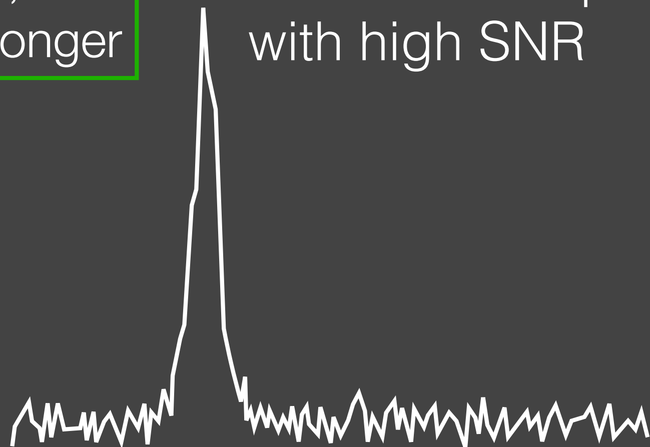




As the folding process happens, the signal becomes stronger and stronger

=

Pulsar folded profile with high SNR



Pulse phase

Periodic signal

Application II - Convolution calculation for gravitational potential

FFT Application I - Periodic signal search

FFT Application II - Convolution calculation

FFT Application III - Correlation calculation

Application of FFT

Particle-Mesh Code

To calculate gravity field of a matter distribution realized through **particles**.

- Basic idea:

Poisson's equation $\nabla^2\phi = 4\pi G\rho$ can be solved with convolution, integral in real space:

$$\phi(\vec{x}) = \int d^3\vec{x}'\left(-\frac{G\rho(\vec{x}')}{|\vec{x}-\vec{x}'|}\right) = \int g(\vec{x}-\vec{x}')\rho(\vec{x}')\,d^3\vec{x}'$$

where $g(\vec{x})$ is the Green's function, $g(\vec{x}) = -\frac{G}{|\vec{x}|}$ ← gravitational Constant.

i.e. $\phi = g \circledast \rho$ (convolution)

The above convolution in real space has a computational cost $O(N^2)$.

According to Convolution Theorem:

$$FT(g \circledast \rho) = FT(g) \times FT(\rho)$$

↓ Straight algeberatic multiplication!

MESH

Hence $\phi = FT^{-1}(FT(g) \times FT(\rho))$

The above operation through FFT has a computation cost $O(N\log_2 N)$.

Gravitational Potential via FFT

Let's see how this is done:

① Construct the density field ρ (from particle N-bodies to Mesh)

② Calculate Potential via Fourier Transforms

③ Compute the force field — either Fourier differentiation / or Finite differencing

④ Intepolate forces back from mesh to particles (inverse of step ①)

* The force field of particles become the basis of updating the system's dynamical status through e.g. leap-frog method...

1. Using particle positions at time t_i to calculate gravitational potential and thus acceleration for each particle.
2. Using particle accelerations at time t_i to update particle velocities given time step Δt.
3. Using particle velocities to update particle positions at time t_{i+1} given time step Δt.
4. Back to step 1.

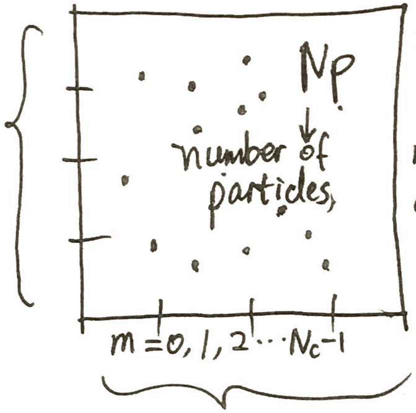
Gravitational Potential via FFT

Step 1:

Step 1: Density (mass/charge) assignment

③

Each particle i with mass of M_i has a "shape": $S(\vec{x})$ with $\int S(\vec{x})\, d\vec{x}^3 = 1$. Kernel of particle



Particle i, $i = 0, 1, 2 \cdots N_p - 1$, mass of M_i, at position $\vec{x}_i$.

To each mesh cell, we assign the fraction of a particle's mass that falls into this cell:

$$W_{\vec{m}}(\vec{x}_i) = \int d\vec{x}^3 \pi\left(\frac{\vec{x} - \vec{x}_{\vec{m}}}{\Delta}\right) s(\vec{x} - \vec{x}_i)$$

Where $\vec{x}_i$ is the position of particle that lives in mesh $\vec{x}_{\vec{m}}$.

In ech dimension: $x_m = (m + 1/2)\Delta$,

where $m = 0, 1, 2 \ldots N_c - 1$ and

$$\pi(x) = \begin{cases} 1 & \text{for } |x| < \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

MESH properties:

L: length of grid

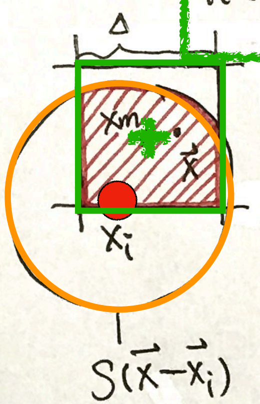
N_c: number of grid cells per dimension

$\Delta = \frac{L}{N_c}$

cell index: $\vec{m} = (m_1, m_2, \ldots)$

Total number of grid cells: $N_{grid} = N_c^d$

d: dimension, 1, 2, 3 ...



e.g. 3D total density assigned to cell at location $\vec{x}_{\vec{m}}$ is then given by $\rho_{\vec{m}} = \frac{1}{\Delta^3} \Sigma_i M_i W_{\vec{m}}(\vec{x}_i)$,

over all particles that contribute to cell $\vec{m}$.

Step 1:

Commonly used kernel assignment scheme

$$W_{\vec{m}} = W_{m_1} W_{m_2} W_{m_3}$$

Total fractional contribution from a given particle

- NGP - assignment (Near-Grid-Point):

  In each dimension, $S(x) = \delta(x)$, $W_m(x_i) = \int_{x_m - \Delta/2}^{x_m + \Delta/2} \pi\left(\frac{x - x_m}{\Delta}\right)\delta(x - x_i)\,\mathrm{d}x = \pi\left(\frac{x_i - x_m}{\Delta}\right)$

  This is equal to assign the whole particle to the cell that it belongs!

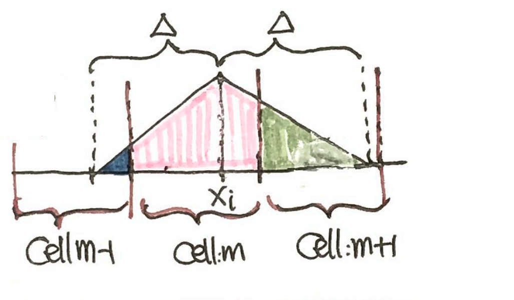
- CIC - assignment (Cloud-In-Cell):

  In each dimension, $S(x) = \frac{1}{\Delta}\pi\left(\frac{x}{\Delta}\right)$, i.e., the particle is a homogeneous cube, with size Δ each dimension. This is equal to assign the particle to the two neighbor cells that it covers!

- TSC - assignment (Triangle-Shaped-Cloud):

  In each dimension with a span of 2Δ, and:

$$S(x) = \frac{1}{\Delta x}\begin{cases} 1 - |x|/\Delta x, & |x| < \Delta x \\ 0, & \text{otherwise} \end{cases}$$



Gravitational Potential via FFT

Step 1:

Commonly used kernel assignment scheme

$$W_{\vec{m}} = W_{m_1} W_{m_2} W_{m_3}$$

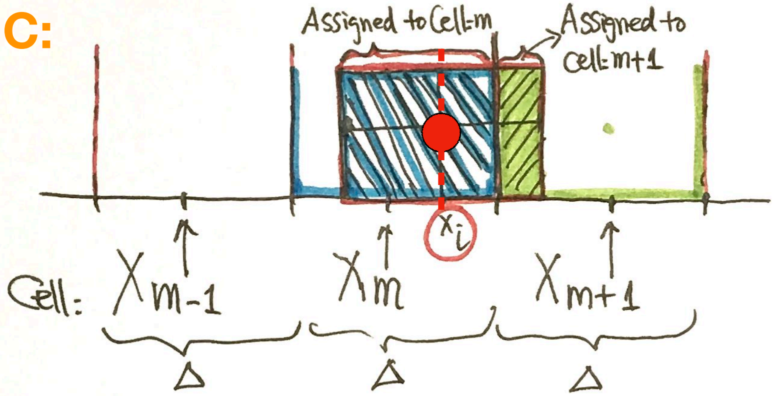
Total fractional contribution from each particle

- CIC - assignment (Cloud-In-Cell):

  In each dimension, $S(x) = \frac{1}{\Delta}\pi\left(\frac{x}{\Delta}\right)$, i.e., the particle is a homogeneous cube, with size Δ each dimension. This is equal to assign the particle to the two neighbor cells that it covers!

CIC:

4



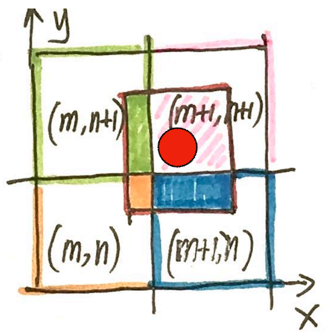
Particle position X_i

$$m_f = \frac{X_i}{\Delta} - \frac{1}{2}, \quad \leftarrow \text{floating point index}$$

$$m_p = (int)(m_f)$$

$$m^* \equiv m_f - m_p, \quad \begin{cases} W_m(X_i) = 1 - m^* \\ W_{m+1}(X_i) = m^* \end{cases}$$

e.g., In 2D:



$$n_f = \frac{y_i}{\Delta} - \frac{1}{2}, \quad n_p = (int)(n_f)$$

$$n^* = n_f - n_p \quad \begin{cases} W_{m,n} = (1-m^*)(1-n^*) \\ W_{m+1,n} = m^*(1-n^*) \\ W_{m,n+1} = (1-m^*)n^* \\ W_{m+1,n+1} = m^* n^* \end{cases}$$

e.g. In 2D:
$$W_{m,n} = W_m W_n$$

Step 1:

SMOOTHED PARTICLE HYDRODYNAMICS

J. J. Monaghan

• SPH-assignment : Smooth Particle hydrodynamics

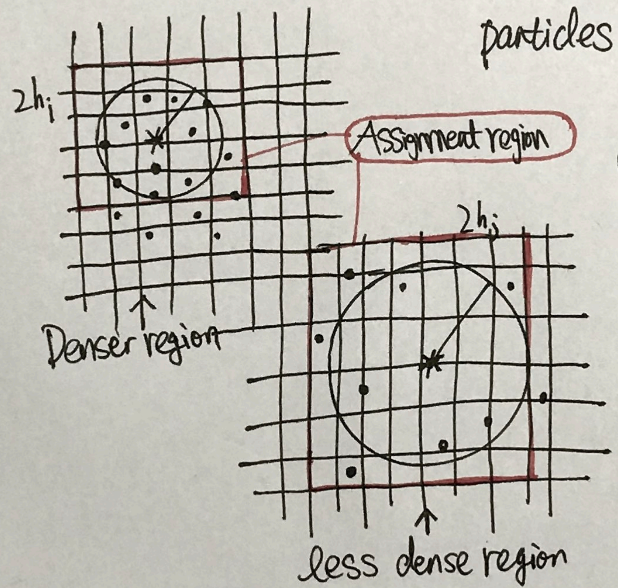
A 3D kernel

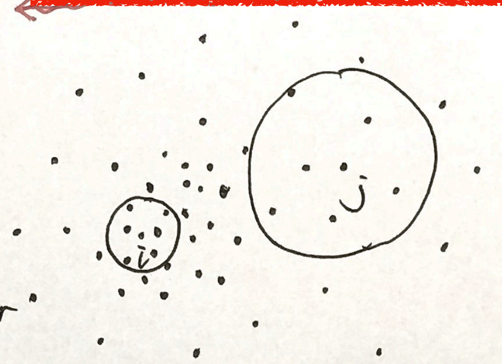
$$S(r, h_i) = \frac{1}{\pi h^3} \begin{cases} 1-6q^2+6q^3 & 0 \leq q \leq \frac{1}{2} \\ 2(1-q)^3 & \frac{1}{2} \leq q \leq 1 \\ 0 & q > 1 \end{cases}$$

different for each particle i.

(3D)

Where $q = r/2h$. Here h_i is the radius, which enclose, e.g. $n = 32, 64 \ldots$ neighbour particles around particle i.





Particles in dense regions natually have smaller h, while those in less dense regions natually have larger h.

① $r = |\vec{X}_m - \vec{X}_i|$

② Renormalization!

$\Rightarrow$

$$\rho_{\vec{m}} = \frac{1}{\Delta^3} \sum_{i \in \text{all particles}} M_i W_{\vec{m}}(\vec{X}_i) \Rightarrow \text{density assigned to cell } m.$$

Renormalization

$$W_{\vec{m}}(\vec{X}_i) = \frac{S(\vec{X}_{\vec{m}} - \vec{X}_i)}{\sum_{m' \in \text{Assignment region}} S(\vec{X}_{\vec{m}'} - \vec{X}_i)}$$

In principle, $W_{\vec{m}}(\vec{x}_i) \approx S(r \equiv |\vec{x}_{\vec{m}} - \vec{x}_i|, h_i)\Delta^3$, but due to discretization, re-normalization is needed when only a few cells are within the region of $r \leqslant 2h$.

Gravitational Potential via FFT

Step 1:

5

What's the difference between these scheme?

→ Smoothness, continuity, noise and differentiability of ρ_m.

* NGP: force jumps discontinuously when particle cross cell boundary.
* CIC: force is piecewise continuous and linear, but 1st derivative jumps.
* TSC: also 1st derivative continuous, but higher-order derivative jumps.

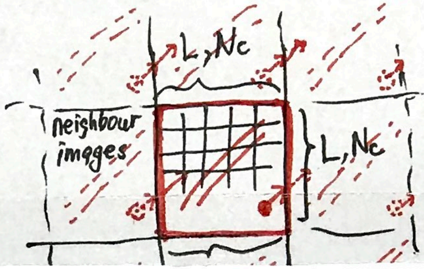
Step 2:

Step 2: Solve for potential ϕ:

in real-space: $\phi(\vec{x}) = \int g(\vec{x}-\vec{x}')\rho(\vec{x}')d\vec{x}'$, $g(x) = -\frac{G}{|\vec{x}|}$

in Fourier space: $\hat{\phi}_{\vec{k}} = \hat{g}_{\vec{k}} \cdot \hat{\rho}_{\vec{k}}$ (~ denote Fourier Transform)

Let's assume periodic boundary condition:
i.e: replicate the system (by DFT)
in each dimension to cover all space.



Periodicity

N_c cell per dimension

$\Delta = \frac{L}{N_c}$ resolution.

Gravitational Potential via FFT

Step 2:

Poisson Equation: $\nabla^2\phi = 4\pi G\rho$

$$\begin{cases} \hat{\phi}_{\vec{k}} = \sum_{\vec{m}} \phi_{\vec{m}} \exp\left(-i\frac{2\pi}{N_c}\vec{k}\cdot\vec{m}\right) \\ \phi_{\vec{m}} = \frac{1}{N_c^3}\sum_{\vec{k}} \hat{\phi}_{\vec{k}} \exp\left(i\frac{2\pi}{N_c}\vec{k}\cdot\vec{m}\right) \end{cases} \qquad \begin{cases} \hat{\rho}_{\vec{k}} = \sum_{\vec{m}} \rho_{\vec{m}} \exp\left(-i\frac{2\pi}{N_c}\vec{k}\cdot\vec{m}\right) \\ \rho_{\vec{m}} = \frac{1}{N_c^3}\sum_{\vec{k}} \hat{\rho}_{\vec{k}} \exp\left(i\frac{2\pi}{N_c}\vec{k}\cdot\vec{m}\right) \end{cases}$$

Real space, cell index

$\vec{m} = (m_1, m_2, m_3)$. $m = 0, 1, 2 \cdots N_c - 1$.

$\vec{k} = (k_1, k_2, k_3)$ $k = 0, \pm 1, \pm 2 \cdots \pm N_c/2$

Frequency space index.

Let's put in Fourier series:

$$\nabla^2\left(\sum_k \hat{\phi}_k \exp\left(i\frac{2\pi}{N_c}km\right)\right) = 4\pi G \sum_k \hat{\rho}_k \exp\left(i\frac{2\pi}{N_c}km\right)$$

$$\xrightarrow{\text{Fourier differentiation:}} \sum_{\vec{k}} -k^2 \hat{\phi}_{\vec{k}} \exp\left(i\frac{2\pi}{N_c}\vec{k}\vec{m}\right) = \sum_{\vec{k}} 4\pi G \hat{\rho}_{\vec{k}} \exp\left(i\frac{2\pi}{N_c}\vec{k}\vec{m}\right)$$

$$\Rightarrow -k^2 \hat{\phi}_{\vec{k}} = 4\pi G \hat{\rho}_{\vec{k}}$$

FFT on Mesh

Analytical Form

Now define $\hat{g}_{\vec{k}} \equiv -\frac{4\pi G}{k^2}$, then $\hat{\phi}_{\vec{k}} = \hat{\rho}_{\vec{k}} \times \hat{g}_{\vec{k}}$

This this the Fourier Transform of the Green's function!

k here is angular frequency, $k = 2\pi/\lambda_k$.

Then potential (on mesh) is given by:

$$\phi_{\vec{m}} = FT^{-1}(\hat{\phi}_{\vec{k}})$$

mesh index

Frequency index

Under periodic boundary condition, $\tilde{g}_k = -4\pi G/k^2$ can be used for pairwise multiplication directly. We will see for isolated boundary condition, the Green's function shall be tabulated onto another mesh for FFT for convolution.

Gravitational Potential via FFT

Step 3:

Step 3: Calculate Force/acceleration:

$$\vec{a} = -\nabla\phi$$

① Via finite differencing:

x, y, z index

$$a_x(m_1, m_2, m_3) = -\frac{\phi(m_1+1, m_2, m_3) - \phi(m_1-1, m_2, m_3)}{2\Delta}$$

Trancation error is $O(\Delta^2)$.

or: 4-point differenting:

$$a_x(m_1, m_2, m_3) = -\frac{1}{2\Delta}\Big[\frac{4}{3}\big(\phi(m_1+1, m_2, m_3) - \phi(m_1-1, m_2, m_3)\big) - \frac{1}{6}\big(\phi(m_1+2, m_2, m_3) - \phi(m_1-2, m_2, m_3)\big)\Big]$$

Trancation error is $O(\Delta^4)$.

② Via Fourier differencing: $\hat{\vec{a}}_{\vec{k}} = -i\vec{k}\,\hat{\phi}_{\vec{k}}$, $\vec{a}_{\vec{m}} = FT^{-1}(\hat{\vec{a}}_{\vec{k}})$.

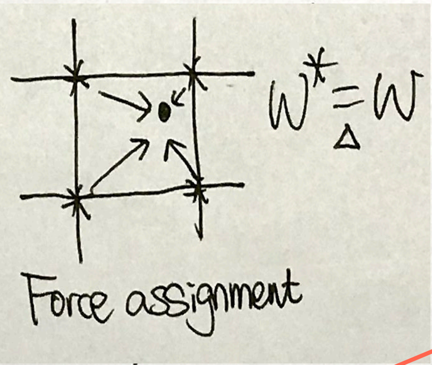
Advantage: Perfectly accurate without truncation error!

Disadvantage: Time consuming as one has to practice it for 3 times for X, Y, Z!

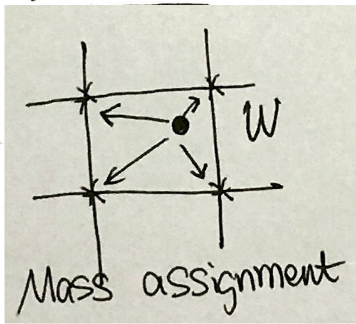
Step 4:

Step 4 : Interpolate the forces back to particle positions:

Recall: mass/charge assignment: $\rho_{\vec{m}} = \frac{1}{\Delta^3} \sum_i M_i W_{\vec{m}}(\vec{x}_i)$



For the force interpolation, we need to use the same assignment function, must!



$$\vec{F}(\vec{x}_i) = M_i \sum_{\vec{m}} \vec{a}_{\vec{m}} W^*(\vec{x}_i - \vec{x}_{\vec{m}})$$

Sum over all cells that participate the mass/charge assignment in Step 1.

Back assign acceleration in each dimension separately!

- Why do we want the same kernel?

Because:
① we want the self-force to vanish!
② we want antisymmetry force between mutual particles so that we have momentum conservation.

Let's prove that:

the field $\vec a(\vec x)$ at mesh point $\vec m$, $\vec a_{\vec m}$, is simply a linear response to the masses at all mesh points $\vec m'$, i.e.,:

$$\vec a_{\vec m} = \sum_{\vec m'} \vec d(\vec m, \vec m') \rho_{\vec m'} \Delta^3 \quad \text{, where } \vec d(\vec m, \vec m') = \frac{(\vec m - \vec m')G}{|\vec m - \vec m'|^3 \Delta^2}$$

Equivalent force kernel,

NOTE: $\vec d(\vec m, \vec m') = -\vec d(\vec m', \vec m)$.

• Self-force $F_{self}(\vec x_i)$:

$$\vec F_{self}(\vec x_i) = M_i \sum_{\vec m} \vec a_{\vec m} W^*(\vec x_i - \vec x_{\vec m})$$

$$= M_i \sum_{\vec m} \Big[\sum_{\vec m'} \vec d(\vec m, \vec m') \rho_{\vec m'} \Delta^3 \Big] W^*(\vec x_i - \vec x_{\vec m})$$

$$= M_i^2 \sum_{\vec m} \sum_{\vec m'} \vec d(\vec m, \vec m') W(\vec x_{\vec m'} - \vec x_i) W^*(\vec x_i - \vec x_{\vec m})$$

Recall:

$$\rho_{\vec m'} = \frac{1}{\Delta^3} \sum_i M_i W(\vec x_{\vec m'} - \vec x_i)$$

but let's now only consider this one particle to be involved/assigned. This will not lose generality. $\Rightarrow$

$$\rho_{\vec m'} = \frac{1}{\Delta^3} M_i W(\vec x_{\vec m'} - \vec x_i)$$

rename $\vec m$ as $\vec m'$, and rename $\vec m'$ as $\vec m$ also

$$= M_i^2 \sum_{\vec m'} \sum_{\vec m} \vec d(\vec m', \vec m) W(\vec x_{\vec m} - \vec x_i) W^*(\vec x_i - \vec x_{\vec m'})$$

$\vec d(\vec m, \vec m') = -\vec d(\vec m', \vec m)$

$$= M_i^2 \sum_{\vec m'} \sum_{\vec m} -\vec d(\vec m, \vec m') W(\vec x_{\vec m} - \vec x_i) W^*(\vec x_i - \vec x_{\vec m'})$$

swap $\sum_{\vec m'} \sum_{\vec m}$ order

$$= M_i^2 \sum_{\vec m} \sum_{\vec m'} -\vec d(\vec m, \vec m') W(\vec x_{\vec m} - \vec x_i) W^*(\vec x_i - \vec x_{\vec m'})$$

Work it out yourself!

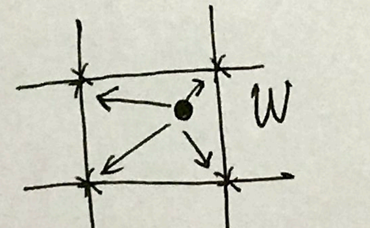
$$\Rightarrow 2\vec{F}_{self}(\vec{x}_i) = M_i^2 \sum_{\vec{m}} \sum_{\vec{m}'} \vec{d}(\vec{m},\vec{m}') \left[W(\vec{x}_{\vec{m}'} - \vec{x}_i) W^*(\vec{x}_i - \vec{x}_{\vec{m}}) - W(\vec{x}_{\vec{m}} - \vec{x}_i) W^*(\vec{x}_i - \vec{x}_{\vec{m}'}) \right]$$

In all kernels above, $W(-\vec{x}) = W(\vec{x})$

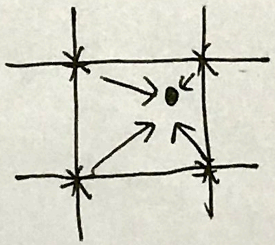
To make $\vec{F}_{self} = 0$ (vanish), then:

$$W(\vec{x}_{\vec{m}'} - \vec{x}_i) W^*(\vec{x}_i - \vec{x}_{\vec{m}}) = W(\vec{x}_{\vec{m}} - \vec{x}_i) W^*(\vec{x}_i - \vec{x}_{\vec{m}'})$$

which request the force assignment funtion W^* must have the same functional form as the mass assignment function W.



Mass assignment



$$W^* \triangleq W$$

Force assignment

Work it out yourself!

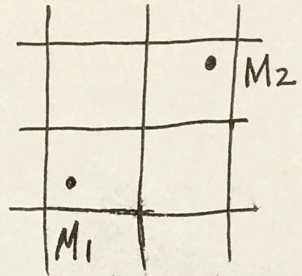
- $\boxed{\text{Force Antisymmetry:}}$

$$\vec{F}_{12} = M_1 \sum_{\vec{m}} \vec{a}_{\vec{m}} W^*(\vec{x}_1 - \vec{x}_{\vec{m}})$$

$$= \cancel{M_1} M_1 M_2 \sum_{\vec{m}} \sum_{\vec{m}'} \vec{d}(\vec{m}, \vec{m}') W(\vec{x}_{\vec{m}'} - \vec{x}_2) W^*(\vec{x}_1 - \vec{x}_{\vec{m}})$$

$$\vec{F}_{21} = M_2 \sum_{\vec{m}} \vec{a}_{\vec{m}} W^*(\vec{x}_2 - \vec{x}_{\vec{m}})$$

$$= M_2 M_1 \sum_{\vec{m}} \sum_{\vec{m}'} \vec{d}(\vec{m}, \vec{m}') W(\vec{x}_{\vec{m}'} - \vec{x}_1) W^*(\vec{x}_2 - \vec{x}_{\vec{m}})$$



$$\vec{a}_{\vec{m}} = \sum_{\vec{m}'} \vec{d}(\vec{m}, \vec{m}') \rho_{\vec{m}'} \Delta^3$$

For M1: $\rho_{\vec{m}'} = \frac{M_2}{\Delta^3} W(\vec{x}_{\vec{m}'} - \vec{x}_2)$

For M2: $\rho_{\vec{m}'} = \frac{M_1}{\Delta^3} W(\vec{x}_{\vec{m}'} - \vec{x}_1)$

$$\underline{\underline{\text{Rename } \vec{m} \rightleftarrows \vec{m}'}} \; M_2 M_1 \sum_{\vec{m}'} \sum_{\vec{m}} \vec{d}(\vec{m}', \vec{m}) W(\vec{x}_{\vec{m}} - \vec{x}_1) W^*(\vec{x}_2 - \vec{x}_{\vec{m}'})$$

$$\underline{\underline{\vec{d}(\vec{m}',\vec{m}) = -\vec{d}(\vec{m},\vec{m}')}} \; M_2 M_1 \sum_{\vec{m}'} \sum_{\vec{m}} -\vec{d}(\vec{m}, \vec{m}') W(\vec{x}_{\vec{m}} - \vec{x}_1) W^*(\vec{x}_2 - \vec{x}_{\vec{m}'})$$

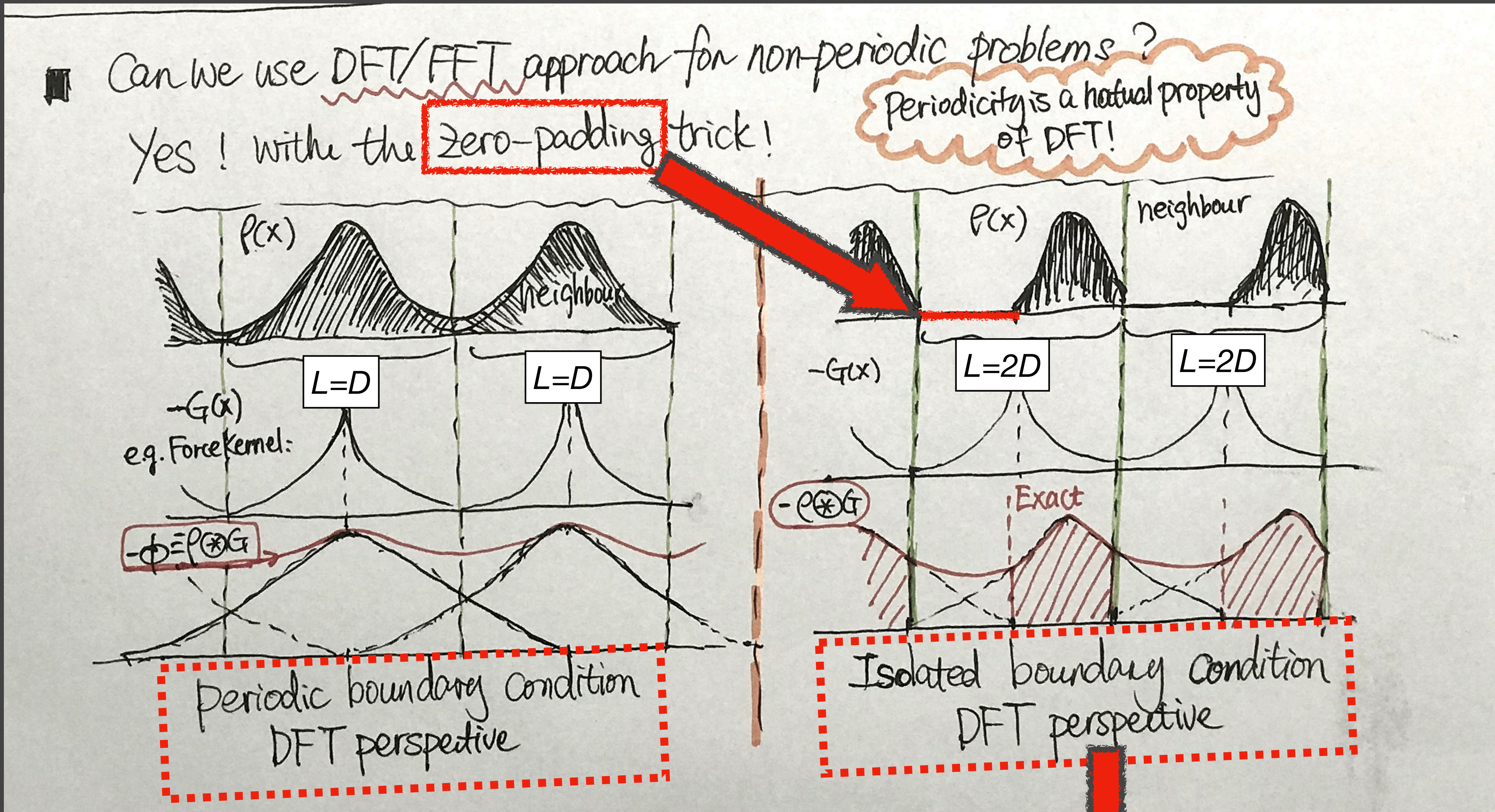
$$\underline{\underline{\text{Swap } \sum_{\vec{m}'} \sum_{\vec{m}} \text{ order}}} \; M_1 M_2 \sum_{\vec{m}} \sum_{\vec{m}'} -\vec{d}(\vec{m}, \vec{m}') W^*(\vec{x}_{\vec{m}'} - \vec{x}_2) W(\vec{x}_1 - \vec{x}_{\vec{m}})$$

To have $\vec{F}_{12} = \vec{F}_{21}$, $W(\vec{x}_{\vec{m}'} - \vec{x}_2) W^*(\vec{x}_1 - \vec{x}_{\vec{m}}) = W^*(\vec{x}_{\vec{m}'} - \vec{x}_2) W(\vec{x}_1 - \vec{x}_{\vec{m}})$

which again request the force assignment kernel W^* must have the same functional form as the mass assignment kernel W.

Isolated boundary condition - Detailed implementation

But this is not true for galaxies on scales D of 100 kpc!

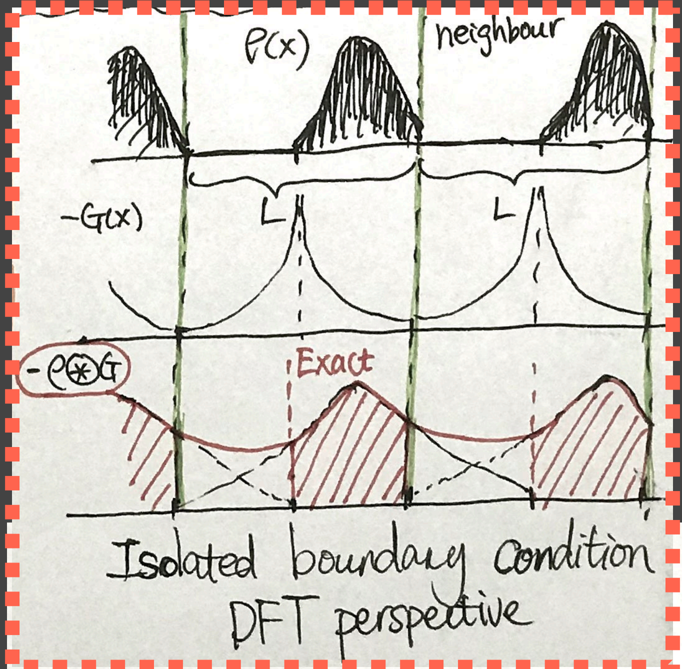


Cosmological simulations take periodic boundary condition assuming structures are periodic on scales D over 100 Mpc

Eliminating "aliasing" in the region of interest by inflating the box side-length by a factor of 2, and padding half of it with zero!

Gravitational Potential via FFT

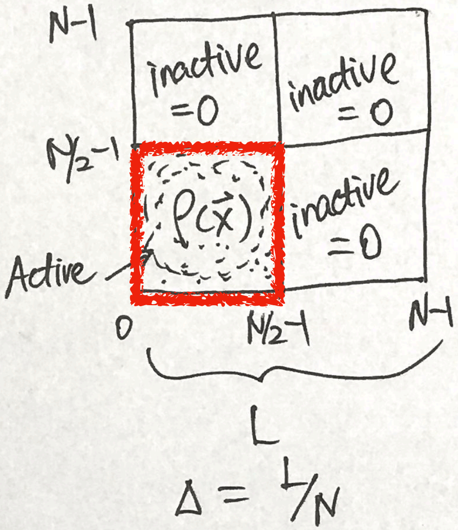
Isolated boundary condition
- Detailed implementation



Setup: as an example, we take a 2d matter density distribution $\rho(x)$ that spans a length of D (per dimension). I will adopt a mesh with side-length $L = 2D$. The mesh has N cells per dimension.

(9)

① Source distribution lives only in one quater of the mesh, others set to zero!



② Green's function is firstly calculated in active mesh; as the response for a charge at origin (0,0)

For example, point potential $\phi(r) = \frac{G}{r+\varepsilon}$

ϵ: softening length

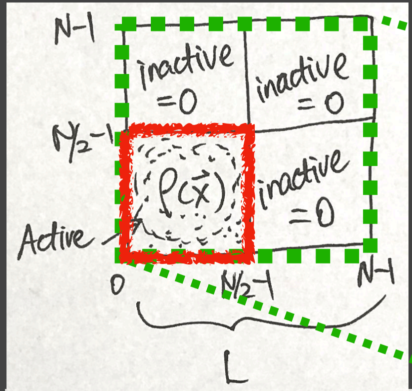
then $\underbrace{g_{ij}}_{\text{Green's function}} = \frac{1}{\sqrt{i^2+j^2}\cdot\Delta+\varepsilon}$, where i,j are cell index $i,j \in [0, N/2]$

For the rest of the mesh:

$$g_{N-i,j} = g_{i,N-j} = g_{N-i,N-j} = g_{ij}.$$

Gravitational Potential via FFT

Isolated boundary condition
- Detailed implementation



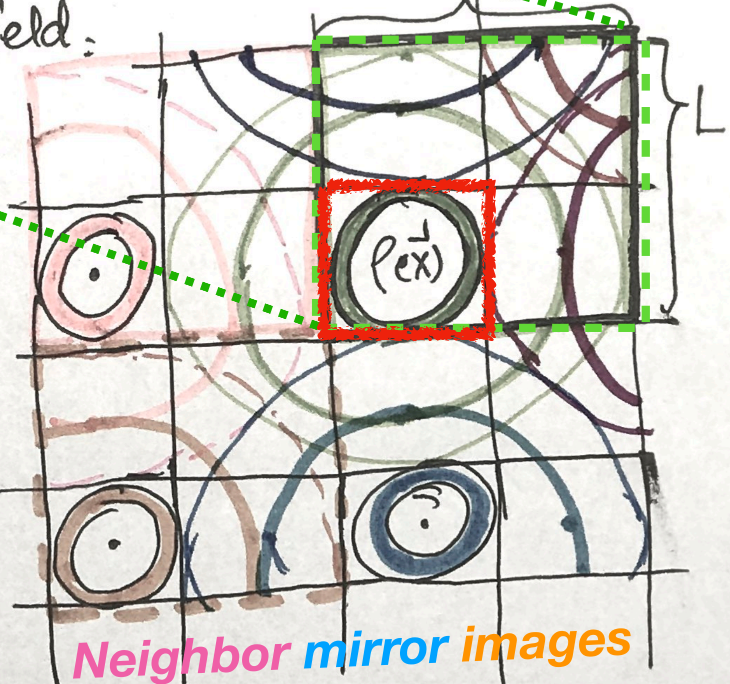
③ Convolution of g with zero-padded source field:

⇒ In the selected active quadrant, we get correct non-periodic potential,

⇒ All other inactive quadrants, results need to be disgarded.

⇒ Fourier transform of density field (in the active quadrant) will occupy all space in frequency domain, therefore nothing can be thrown away at FFT stage in frequency space!

⇒ However, doubling the mesh size for zero-padding while keeping the same spatial resolution, increases memory and CPU dramatically!



Gravitational Potential via FFT

1. 首先计算引力势加速度，如果是direct summation, 对于N个particle, 计算代价是N^2。如果采用FFT的方法，N为格点，计算代价是N log_2 N. 远远降低。这是针对力的计算本身。

2. 那么实现FFT时候就是要基于格点，也就是我们要把particle assign到格点上，这个本身确实是要运算代价的。比如SPH比CIC昂贵很多，在宇宙学模拟中这些过程都是通过并行的计算来实现的。但是作为rules of thumb，有哪些方法可以降低计算成本？其中之一是使用look-up-tabble，针对这种给定kernel的问题，每个particle assignment的kernel都形同不改变。所以look-up-table特别适合：可以使用比如 (linear or log) 空间里100-200个点来首先采样一个kernel，把它存到表格里。接下来每个particle的assignment，针对particle and cell distance，只需要做一次线性插值，直接从表格里读取kernel指给的weight. 但是注意，当2h内的格点数低于一定数量，就要记得renormalization.

3. 关于Green function的kernel，ppt里特定给了大家具体的assignment方法，其中首先包括需要指定一个softening length。可以看到，如果没有这个softening, 我们指定在i=0, j=0的格林函数就是发散的值，对应着当两个质点无限接近的引力效应。我们需要意识到，使用FFT的计算真的是计算smooth gravitational field。也就是说，我们选择的算法，要求我们避免近距离的引力散射，这是需要引入softening的原因。我们可以简单使用1个cell size来做这个平滑，把引力的散射效应在1个cell size之内做平滑。显然这个规定很人为，而实际上 softening length的选取是有讲究的，也是由所模拟的物理决定的。

4. 其次，在ppt上明确写出的assignment的算法中，大家留心可以看到i=0, j=0的那个格点正好是Green function的中心（虽然是被smooth的）。我们会发现，整个网格其实只有这一点采样到了Green function的中心。但是，如果我们稍微挪动网格，使得Green function的中心刚好落在2个格子的中间（即不被任何一个格点采样到），我们会发现，正是因为没有真正采样到Green’s function中心期待的power，实际结果总会在不同程度上偏离理论值（这正是前面讲到的DFT windowing不合适导致power leakage问题的一个具体例子）。 ppt里给出的方法是真正采样到Green function中心并且符合周期条件要求的正确方式。

Fast Fourier Transform

Write your own cosmic evolution simulation code!

Application III - Calculation of two point correlation function

FFT Application I - Periodic signal search

FFT Application II - Convolution calculation

FFT Application III - Correlation calculation (1)

Correlation function

$$h(x) = (f \boxtimes g)(x) \equiv \int_{\infty}^{\infty} f^*(x')g(x+x')\,\mathrm{d}x'$$

1. Correlation functions allow us to study clustering features.
2. In particular, it is extensively use to study density structures, from primordial perturbation, to today's cosmic structures!
3. Providing insight to the physics process and hierarchy of clustering and structure formation (Elmegreen & Efremov 1996; Efremov & Elmegreen 1998)

Correlation theorem:

then $H(\xi) = F^*(\xi) \cdot G(\xi)$

Correlation function $\xi(\mathbf{x})$

The average probability of finding a point in a volume element $\mathrm{d}V$ is proportional to the *mean* density of the background assuming random homogeneous distribution, i.e., $\mathrm{d}P \propto \bar{\rho}$, $\bar{\rho} \equiv \langle \rho(\mathbf{x}) \rangle$, where operation $\langle\ \rangle$ is taking average over the entire data region. How about the probability of finding a pair of points?

The average probability of finding a pair of points in two volume elements $\mathrm{d}V_1$ and $\mathrm{d}V_2$, separated by a distance vector $\mathbf{x} = \mathbf{x_2} - \mathbf{x_1}$, is proportional to the *mean* density pair at the two positions, i.e., $\mathrm{d}P_{12}(\mathbf{x}) \propto \langle \rho_1 \rho_2 \rangle \mathrm{d}V_1 \mathrm{d}V_2$.

In order to make comparisons of clustering at different scales within the same field, we can normalize it in the following way:

we seek for *the average relative probability, w.r.t random mean field*, of finding a pair of points in two volume elements $\mathrm{d}V_1$ and $\mathrm{d}V_2$, separated by distance vector $\mathbf{x}$.

It is given by: $\mathrm{d}P_{12}(\mathbf{x}) = \langle \rho_1 \rho_2 \rangle / \bar{\rho}^2 \mathrm{d}V_1 \mathrm{d}V_2 = \langle (\delta_1 + 1)(\delta_2 + 1) \rangle \mathrm{d}V_1 \mathrm{d}V_2$,

where $\delta_i(\mathbf{x}) \equiv \rho_i / \bar{\rho} - 1$ is the local over-density evaluated at a given position $\mathbf{x_i}$,

Specifically, $\langle \delta \rangle = 0$.

Correlation function $\xi(\mathbf{x})$

$$\mathrm{d}P_{12}((\mathbf{x})) = \langle(\delta_1 + 1)(\delta_2 + 1)\rangle \mathrm{d}V_1 \mathrm{d}V_2$$

$$= (1 + \langle\delta_1\delta_2\rangle + \cancel{\langle\delta_1\rangle} + \cancel{\langle\delta_2\rangle})\, \mathrm{d}V_1 \mathrm{d}V_2 = (1 + \langle\delta_1\delta_2\rangle)\, \mathrm{d}V_1 \mathrm{d}V_2$$

$$\xi(\mathbf{x}) \equiv \langle\delta_1\delta_2\rangle = \langle\delta(\mathbf{x}')\delta(\mathbf{x}' + \mathbf{x})\rangle = \frac{1}{V}\int \delta(\mathbf{x}')\delta(\mathbf{x}' + \mathbf{x})\, \mathrm{d}^3x'$$

is the volume-averaged two-point auto-correlation function of the *real* over-density distribution $\delta(\mathbf{x})$, describing *the strength of clustering as a function of scale.*

In particular, $\xi(0) = \langle\, |\delta(\mathbf{x})|^2 \rangle$ gives the variance of the density perturbation.

As a result, $\mathrm{d}P_{12}(\mathbf{x}) = < \rho_1\rho_2 > /\bar{\rho}^2 \mathrm{d}V_1 \mathrm{d}V_2 = \left[1 + \xi(\mathbf{x})\right] \mathrm{d}V_1 \mathrm{d}V_2$, indicating that the auto-correlation function $\xi(\mathbf{x})$ describes *the excess or deficit probability of finding a pair (with a given separation) compared to uniform/random distribution.*

- If $\xi(\mathbf{x}) > 0$, then the clustering strength at this scale is higher than that of the random field.
- If $\xi(\mathbf{x}) = 0$, then the clustering strength at this scale is the same as that of the random field.
- If $\xi(\mathbf{x}) < 0$, then the clustering strength at this scale is lower than that of the random field.

Let's consider the Fourier space correspondence of these quantities.

Correlation function $\xi(\mathbf{x})$ and Power spectrum $P(\mathbf{k})$

Note: $\delta(\mathbf{k}) = \int_V \delta(\mathbf{x}) \, \exp(-i\mathbf{k}\cdot\mathbf{x}) \, \mathrm{d}\mathbf{x}$, and $\delta_k = \frac{1}{V}\int_V \delta(\mathbf{x}) \, \exp(-i\mathbf{k}\cdot\mathbf{x}) \, \mathrm{d}\mathbf{x}$,

where $\delta(\mathbf{x})$ is the over-density, not delta function.

Recall the correlation theorem: $H(k) = F^*(k)\cdot G(k)$ for $h(x) = \int_\infty^\infty f^*(x')g(x+x')\,\mathrm{d}x'$.

In the case of auto-correlation where $g(x) = f(x)$, then $H(k) = |F(k)|^2$.

Now we make $f(\mathbf{x}) = \delta(\mathbf{x})$, and $h(\mathbf{x}) = \int \delta(\mathbf{x}')\delta(\mathbf{x}'+\mathbf{x})\,\mathrm{d}^3x' = V\langle\delta(\mathbf{x}')\delta(\mathbf{x}'+\mathbf{x})\rangle = V\xi(\mathbf{x})$

then the Fourier transform $F(\mathbf{k}) = \delta(\mathbf{k}) = V\delta_{\mathbf{k}}$, $H(\mathbf{k}) = V\,\mathrm{FT}[\xi(\mathbf{x})] = |\delta(\mathbf{k})|^2 = V^2|\delta_{\mathbf{k}}|^2$.

Let us define power spectrum $P(\mathbf{k}) \equiv |\delta(\mathbf{k})|^2/V = |\delta_{\mathbf{k}}|^2 V$, i.e.,

$$\mathrm{FT}[\xi(\mathbf{x})] = P(\mathbf{k}) = \int \xi(\mathbf{x}) \, \exp(-i\mathbf{k}\cdot\mathbf{x})\,\mathrm{d}^3x$$

$$\xi(\mathbf{x}) = \frac{1}{(2\pi)^3}\int P(\mathbf{k}) \, \exp(i\mathbf{k}\cdot\mathbf{x})\,\mathrm{d}^3k$$

Power spectrum $\longleftrightarrow$ Autocorrelation
(in one domain) (in the other domain)

With the help of FFT, two-point correlation functions and the power spectrum can be connected can be calculated through Fourier transform! ***Theoretically*** *the two provide equal amount of information.*

Correlation function $\xi(\mathbf{x})$ and Power spectrum $P(\mathbf{k})$

The Fourier transform of $V\xi(\overrightarrow{x}) = \int \delta(\overrightarrow{x'})\delta(\overrightarrow{x'} + \overrightarrow{x})\,\mathrm{d}\overrightarrow{x'}$ is given by:

$$
\begin{aligned}
V\int \xi(\mathbf{x})\,\exp(-i\mathbf{k}\cdot\mathbf{x})\mathrm{d}\mathbf{x} &= \int\!\!\int \delta(\mathbf{x}+\mathbf{x}')\delta(\mathbf{x}')\,\exp(-i\mathbf{k}\cdot\mathbf{x})\mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x} \\
&= \int \delta(\mathbf{x}+\mathbf{x}')\,\exp[-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{x}')]\,\mathrm{d}(\mathbf{x}+\mathbf{x}') \int \delta(\mathbf{x}')\,\exp(i\mathbf{k}\cdot\mathbf{x}')\mathrm{d}\mathbf{x}' \\
&= \tilde{\delta}(\mathbf{k})\cdot\delta^*(\mathbf{k}) = |\tilde{\delta}(\mathbf{k})|^2 \equiv VP(\mathbf{k})
\end{aligned}
$$

— proof, work this out yourself!

In the case of isotropy (i.e., independent of direction), $\xi(\mathbf{x})$ becomes 1d correlation function $\xi(r)$, where r is the separation of any two positions. And $P(\mathbf{k})$ becomes 1d power spectrum $P(k)$, where $k = |\mathbf{k}| = \sqrt{k_\mathrm{x}^2 + k_\mathrm{y}^2 + k_\mathrm{z}^2}$.

$$
P(k) = \int_0^\infty \xi(r)\frac{\sin kr}{kr}4\pi r^2\,\mathrm{d}r, \qquad \xi(r) = \frac{1}{(2\pi)^3}\int_0^\infty P(k)\frac{\sin kr}{kr}4\pi k^2\,\mathrm{d}k
$$

In particular, $\xi(0) = \frac{1}{(2\pi)^3}\int_0^\infty P(k)4\pi k^2\,\mathrm{d}k = \frac{1}{2\pi^2}\int_{-\infty}^\infty k^3P(k)\,\mathrm{d}\ln k = \int_{-\infty}^\infty \mathscr{P}(k)\,\mathrm{d}\ln k$,

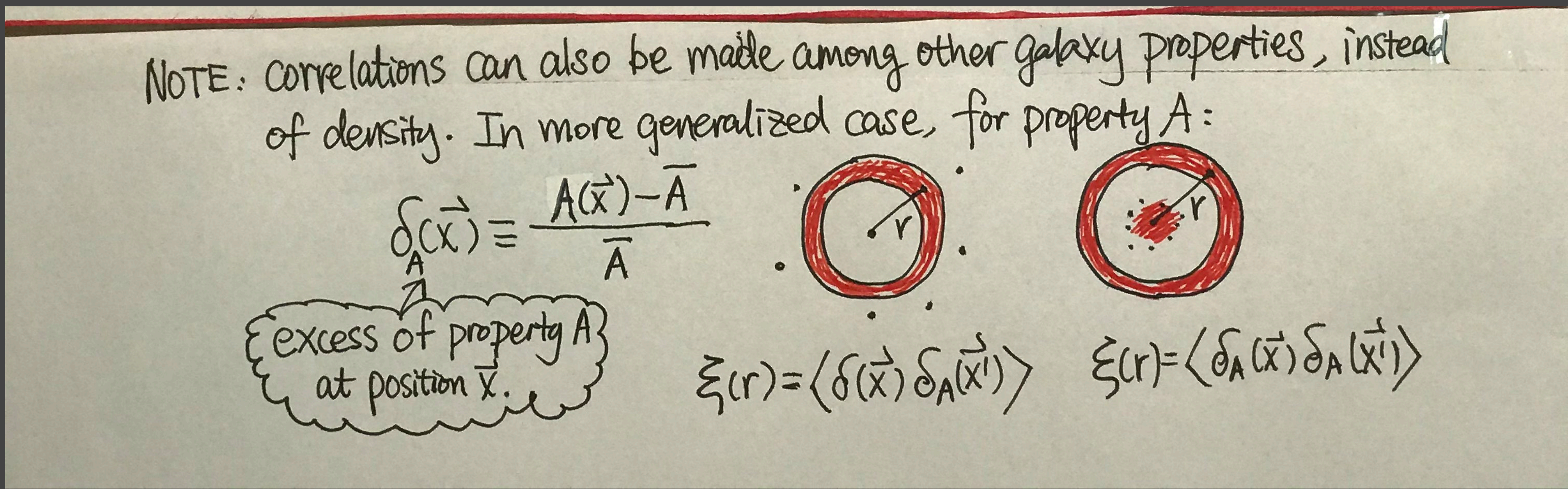
where $\mathscr{P}(k) \equiv \frac{k^3}{2\pi^2}P(k)$ is the (dimensionless) power spectrum per $\ln k$ interval,

while $P(k)$ is the power per d^3k internal and with dimension of V.

Two-point correlation function of the over-density field and the power spectrum introduced here, are important concepts in the field of cosmological density perturbation and structure evolution.

Two-point auto-correlation function does not have to be only of the over-density field of a given point distribution. It can be for any properties, for example, galaxy mass, color, even formation time etc.

Two-point correlation functions do not have to be in form of auto-correlation.



NOTE: correlations can also be made among other galaxy properties, instead of density. In more generalized case, for property A:

$$\delta_A(\vec{x}) \equiv \frac{A(\vec{x})-\bar{A}}{\bar{A}}$$

excess of property A at position $\vec{x}$.

$$\xi(r)=\langle \delta(\vec{x})\,\delta_A(\vec{x}')\rangle \qquad \xi(r)=\langle \delta_A(\vec{x})\,\delta_A(\vec{x}')\rangle$$

The calculation of two-point correlation function does not have to be necessarily through inverse Fourier transform, we can also calculate this statistical quantity using pair and cell estimation (next lecture).

Correlation function - at higher order

Just like two-point correlation function, we can also define three-point correlation function as:

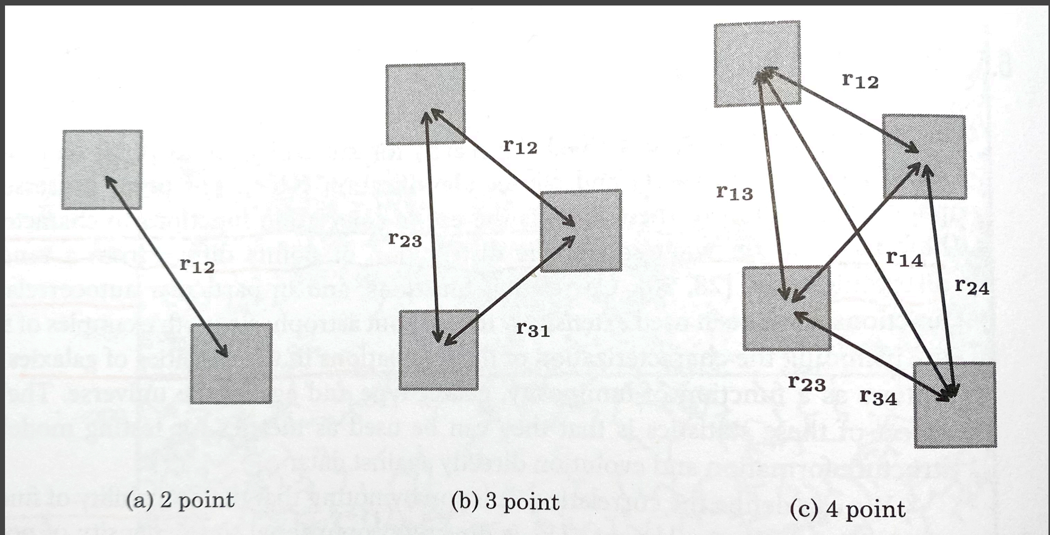
$$\mathrm{d}P_{123}(r) = \langle \rho_1 \rho_2 \rho_3 \rangle / \bar{\rho}^3 \mathrm{d}V_1 \mathrm{d}V_2 \mathrm{d}V_3 = \left[1 + \xi(r_{12}) + \xi(r_{23}) + \xi(r_{13}) + \boxed{\zeta(r_{12}, r_{23}, r_{13})}\right] \mathrm{d}V_1 \mathrm{d}V_2 \mathrm{d}V_3$$

where ζ is the connected three-point correlation function.

The corresponding spectrum in the Fourier domain is called the “bispectrum” $B(k_1, k_2, k_3)$.

Also, four-point correlation function corresponds to trispectrum in the Fourier domain.

For a field generated through a Gaussian random process, two-point correlation function or the power spectrum provides a full statistical description to the field. Any non-Gaussianity and/or asymmetry in the underlying mechanism that generates the field can only be reflected by higher-order statistics, e.g., three- or four-point correlation functions (or equivalently, bispectrum and trispectrum in the Fourier domain).



Note: higher-order correlation functions depends on the configuration of the triplets (3-point) and quadruplets (4-point). For example, the commonly used configuration including equilateral triangle configuration.