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*Image Processing Basics*
*(FFT, Convolution, Filtration)*

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Fourier Series. Periodic function \( f(x) \), period \( a \) so that
\[
f(x + na) = f(x) \quad , \quad \text{integral } n.
\]

Expand in trigonometric functions in form:
\[
f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos \left( \frac{2\pi nx}{a} \right) + \sum_{n=1}^{\infty} b_n \sin \left( \frac{2\pi nx}{a} \right)
\]  \( (1) \)

Arguments of trig. functions scaled so that there are integral numbers of wavelengths of each trig. fn. in each period \( a \) of \( f(x) \).

Given a particular \( f(x) \) coefficient, \( a_n \), \( b_n \) (Fourier coefficients) can be worked out using orthogonality relations.

\[
\int_0^a \cos \left( \frac{m\cdot2\pi x}{a} \right) \cos \left( \frac{n\cdot2\pi x}{a} \right) \, dx = \frac{a}{2}, \quad m = n \quad \text{or} \quad \sin \sin
\]  \( (2) \)
Multiply each side of (1) by \( \cos \left( \frac{2\pi nx}{a} \right) \) or \( \sin \left( \frac{2\pi nx}{a} \right) \), integrate and use (2) giving

\[
\begin{align*}
\frac{a}{n} &= 2 \int_{a}^{b} f(x) \cos \left( \frac{2\pi nx}{a} \right) \, dx \\
\frac{b}{n} &= 2 \int_{a}^{b} f(x) \sin \left( \frac{2\pi nx}{a} \right) \, dx.
\end{align*}
\]

(3).

Coefficients \( a_n \) and \( b_n \) represent "weights" of corresponding cosine and sine terms in original function \( f(x) \). Term \( \frac{a}{n} \) represents average value of function.

Given coefficients \( a_n \) and \( b_n \), function \( f(x) \) can be regenerated by summing series (1).

(3) represents "Fourier analysis" — breaking \( f(x) \) down into different frequencies.

(1) represents "Fourier synthesis" or "Fourier inversion" — building up \( f(x) \) from different frequency components.
The cos terms represent the symmetric part and the sin terms the antisymmetric part of \( f(x) \).

\[
\begin{align*}
\text{symmetric} & \quad \cos \text{ terms only} \\
\text{cos terms only} & \quad \sin \text{ terms only} \\
\text{Same function displaced } 90^\circ & \quad \text{antisymmetric, sin terms only.}
\end{align*}
\]

Fourier analysis therefore depends on choice of origin.

Complexification:

Useful to introduce complex notation and write:

\[
e^{i \frac{2\pi x}{a}} = \cos\left(h \cdot \frac{2\pi x}{a}\right) + i \sin\left(h \cdot \frac{2\pi x}{a}\right) \quad i^2 = -1
\]

Define new coefficients \( c_h \) by:

\[
c_h = \frac{1}{2}(a_n + ib_n), \quad c_{-h} = \frac{1}{2}(a_n - ib_n) = c_h^* \quad (\text{complex conjugate})
\]
Then (1) can be re-written as:

\[ f(x) = \sum_{h=-\infty}^{\infty} C_h \ e^{-ih \frac{2\pi x}{a}} \]

Where \( C_h = \frac{1}{a} \int_{-a}^{a} f(x) \ e^{ih \frac{2\pi x}{a}} \ dx. \)

Have assumed real valued \( f(x) \) which leads to \( C_h = C_h^* \)

Combining \( \pm h \) terms:

\[ C_h e^{-ih \frac{2\pi x}{a}} + C_h e^{ih \frac{2\pi x}{a}} = a_h \cos h \frac{2\pi x}{a} + b_h \sin h \frac{2\pi x}{a} \]

Which agrees with (1).

Combining terms get:

\[ (b_h^2 + \frac{a_h^2}{\alpha})^{1/2} \cos h \frac{2\pi x}{a} + \alpha h \]

Where \( \alpha h = \tan^{-1} \left( \frac{b_h}{\alpha a_h} \right). \)

Thus combination of two complex conjugate terms \( \pm h \) leads to real valued cosine wave, amplitude \( (a_h^2 + b_h^2)^{1/2} = 2 \left| C_h \right| \) and phase \( \alpha h = \arg(C_h). \)
Fourier spectrum

Given results of Fourier analysis in form of a spectrum eg for square wave

Think of spectrum as defining function $F(X)$ which is non-zero only at points

$X_n = \frac{n\lambda}{a}$ with $F(X_n) = C_n = \frac{1}{2\pi\lambda\Delta t} \sin\left(\frac{2\pi n\Delta t}{a}\right)$

Large we make period $\Delta t$ of function $f(x)$ more clearly spaced become spectral points $X_n$ and in limit as $a \to \infty$

we can imagine that $F$ will become a function of the continuous variable $X$, mapping out the Fourier transform of a single square pulse (non-periodic).
Fig. 3.5. Illustrating the progression from Fourier series to transform.
Fourier transform and inverse:

\[ F(X) = \int_{-\infty}^{\infty} f(x) e^{2\pi i x X} \, dx \]

\[ f(x) = \int_{-\infty}^{\infty} F(X) e^{-2\pi i x X} \, dX \]

Fourier transform ("analysis")

Inverse ("synthesis")

Small letters denote functions, coordinates in real (spatial) space.
Large letters denote functions, coordinates in Fourier (frequency) space.

These formulae are the crystallographic conventions.

N.B. Physics / Maths / Electrical engineering conventions may be different with regard to sign convention and normalization.

With \( 2\pi \) included in exponent as above, the spatial frequency \( X \) is measured in cycles per unit length in real space.
Symmetry

Spectral f(x) into symmetric/antisymmetric parts.

\[ f(x) = f_s(x) + f_A(x) \]

Then

\[ F(X) = \int_{-\infty}^{\infty} \left[ f_s(x) + f_A(x) \right] \left[ \cos 2\pi X x + i \sin 2\pi X x \right] dx \]

\[ = \int_{-\infty}^{\infty} \left[ f_s(x) \cos 2\pi X x + i f_A(x) \sin 2\pi X x \right] dx \]

\[ = \text{real} \quad \text{imaginary} \]

Thus real part of \( F(X) \) comes from cosine transform of symmetric part \( f_s(x) \).

\[ \text{imaginary} \quad \text{sine} \quad \text{antisymmetric} \]

\[ \Rightarrow \text{Transform of symmetric real function is real} \]

\[ \Rightarrow \text{Transform of antisymmetric real function is pure imaginary} \]

Remember symmetry depends on choice of real space origin.

If \( f(x) \) is a (general) real function then

\[ F(-X) = \bar{F}(X) \]

\[ \bar{F}(X) \text{ denotes complex conjugate} \]

This is "Friedel relation" in crystallography.

\[ i.e. \ |F(-x)| = |F(x)| \quad \text{and} \quad \text{as} \ F(X) = -\bar{F}(X) \]
Some examples.

Split function: \( f(x) = \text{rect} \left( \frac{x}{t} \right) = \begin{cases} \frac{1}{2t} & , \quad |x| < t \\ 0 & , \quad |x| > t \end{cases} \quad \text{N.B. unit area.} \)

\[
F(x) = \int_{-\infty}^{\infty} \text{rect} \left( \frac{x}{t} \right) e^{2\pi i x t} \, dx = \frac{1}{2t} \int_{-t}^{t} e^{2\pi i x t} \, dx = \frac{1}{2t} \left[ \frac{e^{2\pi i x t}}{2\pi i} \right]_{x=-t}^{x=t} \\
= \frac{1}{2t} \cdot \frac{1}{2\pi i} \left[ e^{2\pi i t^2} - e^{-2\pi i t^2} \right] = \frac{\sin \pi (2t)x}{\pi (2t)x} \\
= \text{sinc} 2tx \quad \text{where} \quad \text{sinc} x = \frac{\sin \pi x}{\pi x}
\]
Now make slit narrower keeping unit area.

\[ f(x) = \text{rect} \left( \frac{x}{\frac{1}{2}} \right) = \begin{cases} \frac{1}{2} & |x| \leq \frac{1}{2} \\ 0 & |x| > \frac{1}{2} \end{cases} \]

\[ F(X) = \text{sinc} \left( 2 \cdot \frac{1}{2} \cdot X \right) \]

Illustrates "reciprocity" - squashing in one space leads to stretching of other space and vice versa. The sharper square pulse needs more power at high frequencies to build it.

\( S \)-function Limit as \( t \to 0 \) keeping unit area under pulse.

\[ S(x) = 0, \quad x \neq 0 \]

\[ \int_{-\infty}^{\infty} S(x) \, dx = 1 \]

Also \[ S(x) f(x) \, dx = f(0) \] \quad Sampling property.

\[ \int_{-\infty}^{\infty} S(x-a)f(x) \, dx = f(a) \]

Contains all frequencies with equal weight.
Shifted $S$-function $S(x-a)$.

$$f(x) = S(x-a)$$

$$F(x) = \int_{-\infty}^{\infty} S(x-a) e^{2\pi i a x} \, dx = e^{2\pi i a x} = \cos 2\pi a x + i \sin 2\pi a x.$$  

$F(x)$ has unit amplitude but varying phase depending linearly on $a$ and $x$.

---

Part of $S$-functions in phase

$$f(x) = S(x+a) + S(x-a)$$

$$F(x) = e^{-2\pi i a x} + e^{2\pi i a x} = 2 \cos 2\pi a x.$$  

---

"Point sources in phase"  

"Interference with bright fringe at origin"
Pair of $\delta$-functions out of phase

\[ f(x) = -\delta(x+a) + \delta(x-a) \]

"Point sources out of phase"

\[ F(X) = -e^{-2\pi i a} + e^{2\pi i a} = 2i \sin 2\pi X a. \]

"Fringes with dark fringe at origin."

\[ \begin{array}{c}
\text{Lattice} \\
\uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \\
\quad a \quad a \quad a \quad a \quad a \quad a \\
\end{array} \]

Infinite regularly spaced array of $\delta$-functions.

\[ f(x) = \text{comb} \left( \frac{x}{a} \right) = \sum_{n=-\infty}^{\infty} \delta(x-na) \]

Reciprocal lattice - spacing inversely proportional to spacing of real lattice.

\[ F(X) = \text{comb} \left( Xa \right) = \sum_{n=-\infty}^{\infty} \delta(X-\frac{n}{a}) \]
Convolution

Operation of smoothing, smoothing, folding, repeating.

\[ h(x) = \int_{-\infty}^{\infty} f(u) g(x-u) \, du = f \ast g \]
Building a crystal by convolution:

\[
\begin{array}{c}
\text{Lattice } f \\
\text{molecule } g \\
\text{crystal } h = f \ast g
\end{array}
\]

Significance of change of hand in convolution:

As molecule "slides past" 8-junction, successive samples are taken building a molecule the right way found in the lattice.
Convolution theorem:

\[ f (f g) = F \ast G \]

\[ f (f \ast g) = FG. \]

Apply to periodic structure ("crystal").

Crystal = molecule \ast lattice

\[ \rightarrow \text{ crystal transform } = \text{ molecular transform \ast reciprocal lattice} \]

Thus the transform of a crystal represents sampled values of the continuous transform of a single molecule (strictly single unit cell) of Fourier spectrum joined from Fourier series coefficients.
Smoothing or Sweeping (with finite window size e.g.
measuring spectral content with photomultiplier tube)

\[ f(x) \]
\[ g(x) \]
\[ h = f \ast g \]

\[ F(X) \]
\[ G(X) \]
\[ H(X) = F(X) \cdot G(X) \]

- The instantaneous output of the PM tube is the
  convolution of \( f \) and \( g \).
- Noise "smoothed" and "smeared".
- Transforms \( F \) and \( G \) multiply, slightly reducing signal (smearing)
  and almost completely removing noise (smoothing).
Fourier transforms in 2 and 3 dimensions.

\[ F(X, Y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) e^{2\pi i (xX + yY)} \, dx \, dy = \int_{-\infty}^{\infty} f(x) e^{2\pi i x \cdot X} \, dx. \]

\[ f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(X, Y) e^{-2\pi i (xX + yY)} \, dX \, dY = \int_{-\infty}^{\infty} F(X) e^{-2\pi i X \cdot x} \, dX. \]

Similarly:

\[ F(X, Y, Z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z) e^{2\pi i (xX + yY + zZ)} \, dx \, dy \, dz \]

\[ f(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(X, Y, Z) e^{-2\pi i (xX + yY + zZ)} \, dX \, dY \, dZ. \]
In 2-D symmetric pairs of 8-functions (point sources) give rise to sinusoidal fringes running at right angles to line joining 8-functions.

\[ f(x,y) \]

\[ F(x,y) \]

\[ S(x + a \cos \alpha, y + a \sin \alpha) + S(x - a \cos \alpha, y - a \sin \alpha) \]

"Pair of point sources in phase."

\[ e^{-2\pi i (x \cos \alpha + y \sin \alpha)} + e^{2\pi i (x \cos \alpha + y \sin \alpha)} = 2 \cos (2\pi a (x \cos \alpha + y \sin \alpha)) \]

Point sources in anti-phase give sine wave.
Two dimensional spatial frequencies.
Demonstration of importance of phase.
Computing Fourier transforms

In order to manipulate inside computer must represent optical density on micrograph by a discrete set of sampled values.

Do this by scanning negative with a film scanner or densitometer.
(Flat bed or drum type — advantages/disadvantages)

Ease of setting up, speed of scanning

Important: that sample spacing is even and no displacement (backlash) between successive line scans. Also fairly important that output is linearly proportional to O.D. )
Because image is sampled on a lattice, spacing $d$ say, the computed transform will be convoluted with the reciprocal lattice, spacing $1/d$.

\begin{align*}
\text{Continuous object} & \quad \rightarrow \quad \mathcal{F}\{f(x)\} \\
\text{Sampled object} & \quad \rightarrow \quad \mathcal{F}\{f(x), \text{ lat.}\} \ast \text{rec latt}
\end{align*}

Note that periodic transform also sampled (at $1/d$ say), so when transform inverted a periodic object density is recovered, period $1/D$.

\begin{align*}
\mathcal{F}\{f(x), \text{ lat. } d\} & \ast \text{ latt. } D
\end{align*}
Shannon–Nyquist sampling and aliasing.

Hence if object density contains fine details out to a spatial frequency \( \frac{1}{2d} \) (ie spatial period \( 2d \)) then sampling must not be coarser than \( d \), otherwise neighbouring copies of the periodic transform begin to overlap. If the overlap were severe, high frequency terms from one copy of the transform overlap and contaminate low frequencies of the next, ie high frequencies would masquerade as low ones. This is known as aliasing.

\[ < d < \text{coarsely sampled object} \]

\[ > \frac{1}{2d} < \text{high frequency components overlap lower frequency components} \]
Thus the finest spatial period (2d) must be sampled at least twice \( (\text{sample spacing} \leq d) \) to avoid aliasing. This is the Shannon-Nyquist sampling limit.

![Diagram with labelled 2d and d intervals]

Need to see peaks and troughs of highest frequency.

Note a corollary of this. Namely when inverting a sampled transform of an object of size D, transform sampling must be finer than \( \frac{1}{D} \) otherwise periodic copies of the object will overlap. In the limit when sampling equals \( \frac{1}{D} \) have same situation as a Fourier series.
**Discrete Fourier Transform (DFT)**

- **Real space**
  - Sampled at $N$ points.
  - Sample values $f_k$ (real).

- **Complex transform on $N$ points**
  - Complex transform with $F_j = F_j^*$, $F_0$, $F_{N/2}$ real.

Both spaces considered to be repeated periodically.

If real space period $a$, sampling at then $d = \frac{a}{N}$

Transform sampling $\frac{1}{Nd}$\[\exp(2\pi i x X) = \exp(2\pi i \cdot \frac{k a}{N} \cdot \frac{j}{Nd}) = \exp(2\pi i jk/N)\]

Fourier transform becomes \[F_j = \sum_{k=0}^{N-1} \exp\left(i \cdot \frac{2\pi jk}{N}\right) f_k\] \[\text{Continuous orthogonality} \int_0^1 \exp(-i 2\pi mx) \exp(i 2\pi nx) dx = \delta_{mn}\]

Becomes discrete orthogonality \[\sum_j \exp(-i 2\pi mj) \exp(i 2\pi n j) \frac{1}{N} = \delta_{m n}\]

So (1) has inverse \[f_j = \frac{1}{N} \sum_{k=0}^{N-1} \exp(-i \frac{2\pi jk}{N}) F_k\]
Fast Fourier transform (FFT) (Cooley-Tukey 1965)

To evaluate $\mathcal{F}$ in the naive way requires $\sim N^2$ complex multiplications.

Write $\mathcal{F}$ as $F_j = w_{jk} f_k$, $w_{jk} = \exp\left( i \frac{2\pi jk}{N} \right)$

Then if $N$ is compound, $w_{jk}$ can be factored into a product of sparse matrices. In particular, if $N = 2^n$

$$w = w^{(1)} w^{(2)} \ldots w^{(n)}$$

where each $w^{(k)}$ contains only $N$ non-zero elements.

Number of multiplications now $= n N = N \log_2 N$.

E.g. if $N = 1024 = 2^{10}$

$N^2 \approx 10^6$

$N \log_2 N \approx 10^4$ Savery of factor of 100 compared with naive method.
Masking and floating

Before transforming have to select out particle or area
required by drawing box and setting outside to zero.

[Diagram showing a box with labeled areas A and B, and a notation about particle boxed out and demistered area.]

Labeled Sammy of transform by amount of zero padding around boxed-off particle.
After zoom masking there will generally be a large discontinuity at edge of mask, which when transformed produces a large spike in transform.

A line trace across AB might look like:

\[
\begin{array}{c}
\text{small particle contrast} \\
\text{large discontinuity}
\end{array}
\]

Get round this partly by "floating" density inside mask to have zero mean discontinuity. This:

\[
\text{floating}
\]

May still be small discontinuities whose effect on transform can be further reduced by "apodization" - i.e., setting a Gaussian or wine-bell roll-off around edge. This:

\[
\text{apodization}
\]

These precautions are most important when trying to see low resolution terms along axis or equator. Sometimes useful to mask at an angle.
Effect of aperture size in the densitometer.

Densitometer will not make point samples of optical density but will integrate or average OD within sampling aperture. This has two effects. If OD changes rapidly across aperture average density will be underestimated because

\[ OD = \log_{10} \left( \frac{I_0}{I} \right) \]

\[ I_0 \text{ incident light} \]

\[ I \text{ transmitted light} \]

and

\[ < \log_{10} \frac{I_0}{I} > < \log_{10} < \frac{I_0}{I} > \]

true mean OD in aperture

OD measured by densitometer - dominated by parts of low OD within aperture.
Secondly even if "true average" or were measured, high spatial frequencies in object will be weighted down.

Generally, use circular aperture of diameter equal to or slightly larger than sampling interval $d$.

Function transformed is $f(x) \ast \text{circ. lattd} \cdot F(X) \cdot F(\text{circ}) \ast \text{circ. lattd}$

Transform of circle, radius $R$ is $F(\text{circ}) = \frac{\text{Re}^2}{4} \cdot \frac{2 J_1(\pi d R)}{\pi d R}$

First zero at $R = \frac{3.83}{d}$

At halfway point $\frac{d}{2}$, periodic repeat of $F(X)$ every $\frac{d}{2}$, $F(\text{circ})$ falls to $\frac{4}{\pi} J_1 \left( \frac{\pi d}{2} \right) \approx 0.75$.

Thus for a sampling aperture diameter $d$, there is only a slight down weighting of the highest recoverable frequency $\frac{d}{2}$. 

\[ \text{drawings and equations} \]
Phase change with origin shift.

Shift origin \((\Delta x, \Delta y)\).

Equivalent to shifting object \((-\Delta x, -\Delta y)\).

\(f'\) is shifted density or density relative to shifted origin.

In old coordinates:

\[
F'(X,Y) = \iint_{-\infty}^{\infty} f'(x,y) e^{2\pi i (xX + yY)} \, dx \, dy.
\]

\[
= \iint_{-\infty}^{\infty} f(x+\Delta x, y+\Delta y) e^{2\pi i (xX + yY)} \, dx \, dy.
\]

Put \(x' = x + \Delta x\), \(y' = y + \Delta y\).

\[
F'(X,Y) = \iint_{-\infty}^{\infty} f(x',y') e^{2\pi i (X - \Delta x)x + (Y - \Delta y)y} \, dx' \, dy'.
\]

\[
= e^{-2\pi i (\Delta x x + \Delta y y)} F(X,Y).
\]
Hence amplitude unchanged \[ |F'(x,y)| = |F(x,y)| \]

Phase change \[-2\pi (\Delta x \cdot x + \Delta y \cdot y)\] depends linearly on size of origin shift and on spatial frequency.

Note that with positive sign in exponent of Fourier transform, a positive shift of phase origin causes a negative phase change in positive quadrant of transform.

Depends on convention — check any program by explicit test.
Fourier transforming property of a lens. (Simple justification)

Cohherent illumination  Subject  Lens  Focal plane

Let transmittance of subject be \( f(x) \) and resulting amplitude in focal plane be \( g(x) \).
Consider beam scattered through angle \( \alpha \) and draw wavefront \( AB \).
Since phase across \( AC \) is constant, phase across \( AB \) may be written with suitable choice of origin as:

\[
\phi(x) = \frac{2\pi x \sin \alpha}{\lambda}
\]
Lens property is that all rays from AB to I have same optical path length so complex amplitude at I is:

\[ g(x) = \int_{-\infty}^{\infty} f(x) \exp \left( i \frac{2\pi}{\lambda} x \sin \alpha \right) \, dx. \]

Now \( x = f \tan \alpha \) and for small \( \alpha \), \( \tan \alpha \approx \sin \alpha \approx \alpha \)
so that \( g(x) = \int_{-\infty}^{\infty} f(x) \exp \left( i \frac{2\pi}{\lambda} x \frac{f}{x} \right) \, dx. \)

\[ = F \left( \frac{X}{xf} \right). \]

Here \( F(X) \) is the Fourier transform of \( f(x) \). Hence amplitude distribution \( g(X) \) in back focal plane is Fourier transform of transmission but with coordinate scaled by \( xt \) where \( \lambda \) is wavelength of light used and \( f \) is focal length of lens.

These parameters jointly determine magnification of diffraction pattern.

There is an extra phase factor arising in more general treatment.
- Different lens set-ups can be used.

See J.W. Goodman - *Intro. to Fourier Optics*.

(2) Laser \( \lambda = 630 \text{ nm} \), \( f = 150 \text{ cm} \) (Optical cout \( 2f = 1 \text{ mm} \))
Spacing \( d \) in object gives \( \frac{d}{\lambda} \) in transform \( \Rightarrow \frac{d}{\lambda} = \frac{x}{xf} \Rightarrow xd = 2f \)
The projective theorem.

The two-dimensional transform of a plane projection of a three-dimensional density is identical with the central section of the three-dimensional transform normal to the direction of projection.

If

\[ F(x, y, z) = \iiint_{-\infty}^{\infty} f(x, y, z) e^{2\pi i (xX + yY + zZ)} \, dx \, dy \, dz \]

then

\[ F(x, y, 0) = \iint_{-\infty}^{\infty} \left\{ \int_{-\infty}^{\infty} f(x, y, z) \, dz \right\} e^{2\pi i (xX + yY)} \, dx \, dy \]

\[ = \iint_{-\infty}^{\infty} \sigma_z(x, y) e^{2\pi i (xX + yY)} \, dx \, dy \]

where \( \sigma_z(x, y) = \int_{-\infty}^{\infty} f(x, y, z) \, dz \)

is the projection of the density onto a plane normal to the \( z \) axis. Prove for general direction of projection by rotation of axes.

Generalises directly to line sections and projections.
Overall scheme for 3D reconstruction

Directions of view

Transmission image is a projection

Fourier transformation of a projection gives coefficients in a section of "Fourier space"

Reconstruction by Fourier synthesis using all sections

(DeRosier & Klug (1968) Nature 217, 130)
Common lines.

5-fold generates 2 pairs
(\(OA, OA'\))
(\(OB, OB'\))

3-fold generates 1 pair
(\(OA, OA'\))

2-fold generates 1 real line
\(F(OA) = F(OA') = F^*(OA)\)
Friedel.

Hence for general view, icosahedral symmetry generates:

5-folds: \(\frac{12 \times 2}{2} = 12\) pairs.

3-folds: \(\frac{20 \times 1}{2} = 10\) pairs.

2-folds: \(\frac{30 \times 1}{2} = 15\) real lines.
Correlation functions.

Self-correlation function (Pattern function).

\[ C_{uu}(h) = \int f_i^*(x) f_i(x+h) \, dx \]

\[ = \int \frac{\Sigma}{h} F(u)^* e^{2\pi i h x} \sum F(u') e^{-2\pi i h}(x+h) \, dx \]

\[ = \sum \frac{\Sigma}{h} F(u)^* F(u') e^{-2\pi i h u} \int e^{2\pi i (h-h') x} \, dx \]

\[ = \sum \frac{\Sigma}{h} F(u)^2 \, e^{-2\pi i h u} . \]

This function just contains information about "interatomic vectors" in the function \( f_i \), so origin displacement is removed. (Fourier coefficients are intensities - no phases.)
Cross-correlation function (CCF)

\[ C_{12}(u) = \int f_1^*(x) f_2(x+u) \, dx \]

\[ = \int \sum \frac{F_1^*(\omega)}{2\pi} e^{2\pi i \omega x} \sum \frac{F_2(\omega')}{-2\pi i \omega'} e^{-2\pi i \omega' (x+u)} \, dx \]

\[ = \sum \frac{F_1^*(\omega)}{2\pi} F_2(\omega) e^{-2\pi i \omega u} \]

Compute CCF by Fourier transforming both functions \( f_1, f_2 \), multiplying corresponding Fourier coefficients (one complex conjugated) and back transforming to get \( C_{12} \).
Maximizing $C_{12}$ is equivalent to minimizing difference between $f_1$ and $f_2$ since:

$$\int (f_1 - f_2)^2 \, dx = \int (f_1^2 + f_2^2 - 2f_1 f_2) \, dx$$

and $\int (f_1^2 + f_2^2) \, dx$ is constant.

Hence values of function $C_{12}(u)$ will be large when displacement $u$ moves $f_2$ to a position where it agrees well with $f_1$. 
Separate alignment problem into:

1. Rotational alignment (angular CCF) of self-correlation functions of two images (thus relative origin displacements removed).

2. Translational alignment of correctly rotationally aligned images using CCF.

(This is like doing rotation + translation functions in crystallography.)

Rotationally and translationally aligned images can then be averaged.