Part 2: Fourier transforms

Key to understanding NMR, X-ray crystallography, and all forms of microscopy
Sine waves

\[ y(t) = A \sin(wt + p) \]
\[ y(x) = A \sin(kx + p) \]
To completely specify a sine wave, you need its
(1) direction,
(2) wavelength or frequency,
(3) amplitude, and
(4) phase shift
Adding sine waves

\[ y = \sin(x) \]

\[ y = \sin(2x) \]

\[ y = \sin(3x) \]

\[ y = \sin(x) - 2.3\sin(2x) + 1.8\sin(3x) \]
Taking sine wave sums apart
(a Fourier “decomposition”, or “transform”)
Fourier transforms in music and hearing
Fourier decompositions may not be exact - depends on how many terms you use ("resolution")
The mathematical details

\[ f(x) = \frac{A_0}{2} + \sum_{m=1}^{\infty} A_m \cos \left( \frac{2\pi mx}{\lambda} \right) + \sum_{m=1}^{\infty} B_m \sin \left( \frac{2\pi mx}{\lambda} \right) \]

\[ A_m = \frac{2}{\lambda} \int_{0}^{\lambda} f(x) \cos \left( \frac{2\pi mx}{\lambda} \right) \, dx \]

\[ B_m = \frac{2}{\lambda} \int_{0}^{\lambda} f(x) \sin \left( \frac{2\pi mx}{\lambda} \right) \, dx \]

The balance between sine and cosine terms can be equivalently introduced by giving each sine term a “phase”
One-dimensional sine waves and their sums

Concept check questions:

- What four parameters define a sine wave?
- What is the difference between a temporal and a spatial frequency?
- What in essence is a “Fourier transform”?
- How can the amplitude of each Fourier component of a waveform be found?
Analog versus digital images

“analog”

“digital”
Consider a one-dimensional array:

<table>
<thead>
<tr>
<th>0.3</th>
<th>0.4</th>
<th>1.3</th>
<th>3.4</th>
<th>4.5</th>
<th>4.2</th>
<th>2.8</th>
<th>2.4</th>
<th>1.4</th>
<th>0.1</th>
</tr>
</thead>
</table>

10 numbers

From Fourier transform

<table>
<thead>
<tr>
<th>A₀</th>
<th>P₀</th>
<th>A₁</th>
<th>P₁</th>
<th>A₂</th>
<th>P₂</th>
<th>A₃</th>
<th>P₃</th>
<th>A₄</th>
<th>P₄</th>
<th>A₅</th>
<th>P₅</th>
</tr>
</thead>
</table>

10 numbers + 2
(5 amps & phases + “DC” component)

A₀ = amplitude of “DC” component
A₁ = amplitude of “fundamental” frequency (one wavelength across box)
P₁ = phase of “fundamental” frequency component
A₂ = amplitude of first “harmonic” (two wavelengths across box)
P₂ = phase of first harmonic
A₃ = amplitude of second harmonic
P₃ = phase of second harmonic
   etc.
A₅ = amplitude of “Nyquist” frequency component
One dimensional functions and transforms (spectra)

Hecht, Fig. 11.13
One dimensional functions and transforms (spectra)

Hecht, Fig. 11.13
More complicated functions and their spectra

Hecht, Fig. 11.38
One-dimensional reciprocal space
Concept check questions:

• What is the difference between an “analog” and a “digital” image?
• What is the “fundamental” frequency? A “harmonic”? “Nyquist” frequency?
• What is “reciprocal” space? What are the axes?
• What does a plot of the Fourier transform of a function in reciprocal space tell you?
In microscopy we deal with 2-D images and transforms
Two-dimensional waves and images
Concept check questions:

- What does a two-dimensional sine wave look like?
- What do the “Miller” indices “h” and “k” indicate?
Fourier transform

$N^2$ numbers

$\sim N^2$ numbers
A simple 2-D image and transform (diffraction pattern)

“Real” space: coordinates

“Reciprocal” space: spatial “frequencies”
Another simple 2-D image and transform
More complex 2-D images and transforms
Briegel et al.,
PNAS 2009
“Resolution”

Note here the “power” or intensity of each Fourier component is being plotted, not the phase, and for any real image, the pattern is symmetric.
“low pass” filter

“high pass” filter

“band pass” filter

http://sharp.bu.edu/~slehar/fourier/fourier.html
Two-dimensional transforms and filters
Concept check questions:

• In the Fourier transform of a real image, how much of reciprocal space (positive and negative values of “h” and “k”) is unique?

• If an image “I” is the sum of several component images, what is the relationship of its Fourier transform to the Fourier transforms of the component images?

• What part of a Fourier transform is not displayed in a power spectrum?

• What does the “resolution” of a particular pixel in reciprocal space refer to?

• What is a “low pass” filter? “High pass”? “Band pass”?
In X-ray crystallography, 3-D microscopy, and 3-D NMR we deal with 3-D images and transforms.
What does a 3-D FT look like?

$N^3$ numbers

$\sim N^3$ numbers
Three-dimensional waves and transforms

Concept check questions:

• What does a three-dimensional sine wave look like?

• What does the third “Miller” index “l” represent?
Convolution

\[ g(i) = f \otimes h = \int f(x) h(i-x) \, dx \]
Convolution
\[ g(i,j) = f \otimes h = \iint f(x,y) h(i-x,j-y) \, dx \, dy \]

"Convolution theorem"
Cross-correlation

Hecht, Optics

\[ c(i,j) = \iint f(x,y) h(i+x, j+y) \, dx \, dy \]

\[ c = \mathcal{F}^{-1} \left[ \mathcal{F}[f] \cdot \mathcal{F}[h] \right] \]
Convolution and cross-correlation
Concept check questions:

• What is a “convolution”? 

• What is the “convolution theorem”? 

• What is a “point spread function”? 

• What does convolution have to do with the structure of crystals? 

• What is “cross-correlation”? 

• How might cross-correlations be used in cryo-EM?