10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #34: Fourier Transforms and Fast Fourier Transforms (FFT).

Fourier Analysis / Transforms

$$f(x) = \sum_m c_m \phi_m(x)$$

Basis Set Methods $$\frac{\partial^2}{\partial x^2}\phi_m = \lambda_m \phi_m$$

$$\phi_m = \sin(mx)$$

$$\phi_m = \cos(mx)$$

$$\phi_m = e^{imx}$$

Convolution Integral

$$g * h \equiv \int_{-\infty}^{\infty} g(\tau) h(t-\tau) d\tau$$

$$\hat{F}(g * h) = \hat{F}(g)\hat{F}(h)$$

Correlation (g,h) $\equiv \int_{-\infty}^{\infty} g(t+\tau) h(\tau) d\tau$

$\hat{F}(\text{Correlation}(g,h)) = \hat{F}(g)\left[\hat{F}(h)\right]^*$ ← complex conjugate

Quantum Mechanics

$\Psi(x) = e^{ikx}$ ← state of definite momentum $p_x = \hbar k$

$\Psi(\phi) = e^{im\Phi}$ ← definite angular momentum $J_\Phi = \hbar m$

Spectroscopy

$v = {}^{\Delta E}/_{h}$

pulsed NMR: time domain measurement of I(v)

FTIR:

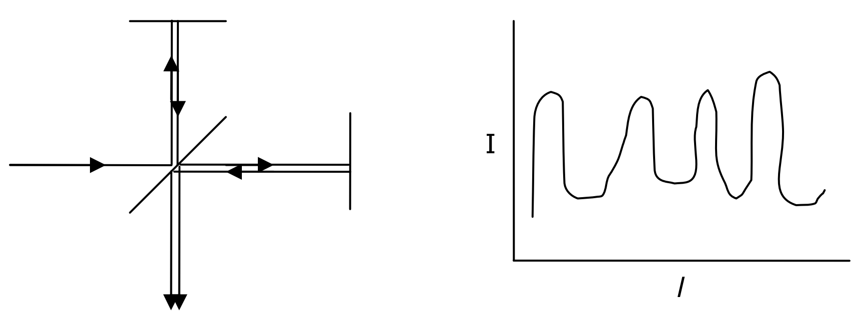

Figure 1. Diagram showing the path of light in an FTIR.

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These methods are powerful, but require a computer to interpret the results

Scattering Experiments

X-ray stattering

neutron scattering

light scattering

Fourier Series

if f(t) = f(t+2P) % P = half-period

$$f(t) = \frac{1}{2}a_o + \sum_{m=1}^{M}\left[a_m \cos\left(\frac{m\pi t}{P}\right) + b_m \sin\left(\frac{m\pi t}{P}\right)\right]$$

$$a_n = \frac{1}{P}\int_0^{2P} f(t)\cos\left(\frac{n\pi t}{P}\right)dt \qquad b_n = \frac{1}{P}\int_0^{2P} f(t)\sin\left(\frac{n\pi t}{P}\right)dt \qquad O(M^2) \text{ effort}$$

Euler's Formula

$e^{i\theta} = \cos(\theta) + i\sin(\theta)$

$$f(t) = \sum_{m=-\infty}^{\infty} c_m e^{\frac{im\pi t}{P}} \qquad c_n = \frac{1}{2P}\int_{-P}^{P} f(t)e^{\frac{in\pi t}{P}}dt$$

If you do not know P, compute Fourier Transform instead of Fourier Series

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\int_{\infty}^{\infty} f(t)e^{-i\omega t}dt$$

Plot $|F(\omega)|^2$ vs. ω, where F(ω) is power density

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{\infty}^{\infty} F(\omega)e^{i\omega t}d\omega$$

(Inverse Fourier Transform)

Discrete Fourier Transform

$f(t_k)$ $t_k = 0 \ldots T$

$f((k-1)\Delta t)$ k = 1 … N evenly spaced time points

$$F_n = \sum_{k=1}^{N} f\big((k-1)\Delta t\big)e^{-i2\pi(n-1)(k-1)/N}$$

$$F_n \approx F\left(\frac{(n-1)2\pi}{T}\right)$$

$$f(t) \approx \frac{1}{N}\sum_{n=1}^{N} F_n e^{i2\pi(n-1)t/T} \qquad O(N^2) \text{ effort}$$

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Fast Fourier Transform (FFT)

$N = 2^k$

$$F_n = \sum_{k\ \text{even}}^{N} f((k-1)\Delta t)e^{i2\pi(n-1)(k-1)/N} + \sum_{k\ \text{odd}}^{N} f((k-1)\Delta t)e^{i2\pi(n-1)(k-1)/N}$$

$$F_n = e^{i2\pi(n-1)/N}\sum_{l=1}^{N/2} f((2l-1)\Delta t)e^{i2\pi(n-1)(l-1)/(N/2)} + \sum_{l=1}^{N/2} f((2l-2)\Delta t)e^{i2\pi(n-1)(l-1)/(N/2)}$$

$$F_n^N = e^{i2\pi(n-1)/N}F_{n\ \text{offset}}^{(N/2)} + F_{\text{n}}^{(N/2)}$$

Can do this iteratively. One can split each F_n^M into even and odd series.

$O(N\log_2 N)$ effort. This is much less than $O(N^2)$. That is why this transform is called Fast.

MatLAB: fft and ifft

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