Lecture #17 Convolution Theorem, Signal Processing and Discrete Fourier Transforms

I. Convolution Theorem Applications

A. Ex: Green's Function for Poisson Eq

1. $\psi(r) = \frac{1}{4\pi}\int \frac{\rho(\underset{\sim}{r}')}{|\underset{\sim}{r}-\underset{\sim}{r}'|} d^3\underset{\sim}{r}'$ ← Form of a convolution.

2. Use $$\boxed{\int g(\underset{\sim}{r}')f(\underset{\sim}{r}-\underset{\sim}{r}')d^3\underset{\sim}{r}' = \int F(\underset{\sim}{k})G(\underset{\sim}{k})e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}}d^3\underset{\sim}{k}}$$ Convolution Theorem

where $g(\underset{\sim}{r}') = \rho(\underset{\sim}{r}')$ and $f(r) = \frac{1}{r} \Rightarrow f(\underset{\sim}{r}-\underset{\sim}{r}') = \frac{1}{|\underset{\sim}{r}-\underset{\sim}{r}'|}$

3. $F(\underset{\sim}{k}) = [f(\underset{\sim}{r}-\underset{\sim}{r}')]^T = \frac{1}{(2\pi)^{\frac{3}{2}}}\frac{4\pi}{k^2}$ (20.42), $G(\underset{\sim}{k}) = \rho^T(\underset{\sim}{k})$

4. Thus $$\boxed{\psi(\underset{\sim}{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int \frac{\rho^T(\underset{\sim}{k})}{k^2}e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}}d^3\underset{\sim}{k}}$$ May be easier to evaluate

B. Ex: Two-Center Overlap Integral

1. $S_{ab} = \int \phi_a^*(\underset{\sim}{r}-\underset{\sim}{A})\,\phi_b(\underset{\sim}{r}-\underset{\sim}{B})\,d^3\underset{\sim}{r}$
   a. Scalar product of two atomic orbitals: ϕ_a centered at $\underset{\sim}{A}$, ϕ_b at $\underset{\sim}{B}$.

2. Change coordinates to origin at $\underset{\sim}{A}$: $\underset{\sim}{r}' = \underset{\sim}{r}-\underset{\sim}{A}$
   a. Thus $\underset{\sim}{r}-\underset{\sim}{B} = \underset{\sim}{r}' - (\underset{\sim}{B}-\underset{\sim}{A}) \equiv \underset{\sim}{r}' - \underset{\sim}{R}$ where $\underset{\sim}{R} = \underset{\sim}{B}-\underset{\sim}{A}$ is separation!
   b. Yields $S_{ab} = \int \phi_a^*(\underset{\sim}{r}')\,\phi_b(\underset{\sim}{r}'-\underset{\sim}{R})\,d^3\underset{\sim}{r}'$
   $\underset{\sim}{R}-\underset{\sim}{r}'$ would yield standard convolution form!
   c. Use (20.50), $[\phi_b(-[\underset{\sim}{R}-\underset{\sim}{r}'])]^T = \phi_b^T(-\underset{\sim}{k})$

3. Use Conv. Thm, $$\boxed{S_{ab} = \int \phi_a^{*T}(\underset{\sim}{k})\,\phi_b^T(-\underset{\sim}{k})\,e^{-i\underset{\sim}{k}\cdot\underset{\sim}{R}}\,d^3\underset{\sim}{k}}$$

I. B. (Continued)

4. If we assume Slater-type Orbitals (STOs) of the form

a. $\phi = \phi^* = e^{-\zeta r}$ with screening parameter ζ.

b. $\phi^T = \frac{1}{(2\pi)^{3/2}} \frac{8\pi\zeta}{(k^2+\zeta^2)^2}$

5. Thus, $S_{ab} = \frac{(8\pi\zeta)^2}{(2\pi)^3} \int \frac{e^{-i\underline{k}\cdot\underline{R}}}{(k^2+\zeta^2)^4} d^3\underline{k}$

a. Evaluated at single point $\underline{k}$ with spacing $\underline{R}$ in complex exponential.

6. Use spherical wave expansion of $e^{-i\underline{k}\cdot\underline{R}}$: (16.61)

$$e^{i\underline{k}\cdot\underline{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr)\, Y_l^m(\Omega_k)\, Y_l^{m*}(\Omega_r)$$

a. Using similar procedure as lect #6, I.B.1, after integration over all $\int d^3\underline{k}$, only Y_0^0 term survives.

b. Simplifies to $S_{ab} = \frac{(8\pi\zeta)^2}{(2\pi)^3} \int_0^\infty \frac{j_0(kR)}{(k^2+\zeta^2)^4} 4\pi k^2 dk$

7. This integral can be expressed in terms of modified spherical Bessel function $k_2(\zeta R)$ [see (20.82) in text], yielding

$$\boxed{S_{ab} = \frac{\pi R^3}{3} k_2(\zeta R) = \frac{\pi e^{-\zeta R}}{3\zeta^3} (\zeta^2 R^2 + 3\zeta R + 3)}$$

C. Multiple Convolutions

1. Consider convolution of $f(x)$ with $[g*h](x)$

$$[f*(g*h)](x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, f(y)\, g(z-y)\, h(x-z)$$

2. Convolution Theorem $\boxed{[f*g*h]^T(\omega) = F(\omega)\, G(\omega)\, H(\omega)}$

a. Functions $f, g, \& h$ can be convolved in any order → same result

I. C. (Continued)

3. $$\boxed{\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\, f(y) g(z-y) h(x-z) = (2\pi)^{\frac{1}{2}} \int_{-\infty}^{\infty} F(\omega) G(\omega) H(\omega) e^{-i\omega x} d\omega}$$

4. Ex: <u>Interaction of Two Charge distributions</u>

a. $$V = \int d^3\underline{r}' \int d^3\underline{r}'' \frac{\rho_1(\underline{r}')\rho_2(\underline{r}'')}{|\underline{r}''-\underline{r}'|}$$ ← Double convolution with $\underline{r}=0$ and sign change in argument of ρ_2.

b. Taking $f(\underline{r}) = \frac{1}{r}$, $g(\underline{r}) = \rho_1(\underline{r})$, $h(\underline{r}) = \rho_2(\underline{r})$, we obtain

$$V = 4\pi \int \frac{d^3\underline{k}}{k^2} \rho_1^T(\underline{k}) \rho_2^T(-\underline{k})$$ ← Single 3D integral
<u>NOTE:</u> $e^{i\underline{k}\cdot\underline{r}} = 1$ $(\underline{r}=0)$

D. <u>Transform of a Product</u>

1. Fourier transform of a product ⇒ Convolution of Fourier Transforms

$$\boxed{[f(x) g(x)]^T = (F * G)(\omega)}$$

2. This arises when Fourier transforming a <u>nonlinear equation</u>.
   a. Nonlinear term yields a convolution.
   b. In practice, in numerical simulations, equations are transformed from Fourier space back to physical space to evaluate nonlinear terms.

II. <u>Signal Processing</u>

A. <u>Concepts</u>

1. Consider a time series $f(t)$
   a. Each frequency ω contributes $F(\omega) e^{i\omega t}$, so

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

II A. (Continued)

2. What do negative frequencies mean?

a. Mathematical consequence of the using two functions (sin & cos) to define the signal. → Needed to get phases correct.

3. Alternate definitions

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

a. Normalization & sign of exponent changed from previous definition.

B. Transfer Function

1. For a single frequency signal $f_\omega(t)$, consider a device which can change its amplitude & phase (but not ω) to yield $g_\omega(t)$.

$$f_\omega(t) \rightarrow \boxed{\text{Device}} \rightarrow g_\omega(t)$$

$\phi(\omega)$

2. Linear Response:

a. Output $g_\omega(t)$ is at same frequency ω as input $f_\omega(t)$

b. Output scales linearly with input

c. Result is independent of other frequencies

$$g_\omega(t) = \phi(\omega) f_\omega(t)$$

→ Transfer Function: Characteristic of device.

3. For full spectrum of ω,

$$\boxed{g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \phi(\omega)F(\omega)e^{i\omega t}\,d\omega}$$

4. Let $\Phi(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\phi(\omega)e^{i\omega t}\,d\omega$

a. By Conv. Thm, we may obtain $g(t) = \int_{-\infty}^{\infty} f(t')\,\Phi(t-t')\,dt'$

II. B. (Continued) Howes 5

5. Causality: $g(t) = \int_{-\infty}^{\infty} f(t') \Phi(t-t') dt'$

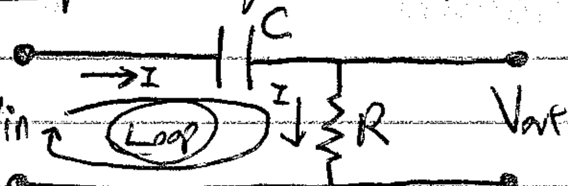
a. Since the effect at time t on $g(t)$ must only depend on times $t' < t$ due to causality, $\Phi(t-t') = 0 \quad t' > t$

6. Thus, $\boxed{g(t) = \int_{-\infty}^{t} f(t') \Phi(t-t') dt'}$

7. Reality of $\Phi(t)$: a. Since $g(t)$ must be real, given a real input $f(t)$, the $\Phi(t)$ must also be real!

$\boxed{\text{Causality and Reality are important properties of transfer function } \Phi(t)}$

8. Example: High-Pass Filter a. Linear response at frequency ω



i. Input: $V_{in}^{(\omega)} e^{i\omega t}$

ii. Output: $V_{out}^{(\omega)} e^{i\omega t}$

iii. Current: $I^{(\omega)} e^{i\omega t}$

$\boxed{V_{out}(\omega) = \phi(\omega) V_{in}(\omega)}$ coefficients may be complex.

b. Electrical Circuit Analysis: Kirchoff's Law: Potential around closed loop $= 0$.

$$V_{in} e^{i\omega t} = \int^{t} dt \frac{I}{C} e^{i\omega t} dt + R I e^{i\omega t}$$

c. Differentiate with respect to time to eliminate integral.

$$V_{in} \frac{d}{dt} e^{i\omega t} = \frac{I}{C} e^{i\omega t} + R I \frac{d}{dt} e^{i\omega t}$$

$$i\omega V_{in} \cancel{e^{i\omega t}} = \frac{I}{C} \cancel{e^{i\omega t}} + i\omega R I \cancel{e^{i\omega t}}$$

d. Solve for Current: $I = \dfrac{i\omega C V_{in}}{1 + i\omega RC}$

strictly function of real constant RC

e. $V_{out} = IR$, so $\boxed{\phi(\omega) = \dfrac{V_{out}(\omega)}{V_{in}(\omega)} = \dfrac{i\omega RC}{1 + i\omega RC}}$

$\lim_{\omega \to \infty} \phi(\omega) = 1$

$\lim_{\omega \to 0} \phi(\omega) = 0$

II. (Continued)

Howes 6

C. Restrictions on $\phi(\omega)$

Forward transform using convention in this section!

1. $\phi(\omega) = \int_0^\infty \Phi(t) e^{-i\omega t} dt$ Recall $\Phi(t) = 0$ for $t<0$.

2. Separate Re & Im: $\phi(\omega) = U(\omega) + iV(\omega)$

   a. We ~~separate real~~ & imaginary since $\Phi(t)$ is real:

$$U(\omega) = \int_0^\infty \Phi(t) \cos\omega t \, dt \quad \leftarrow \text{Cosine transform}$$

$$V(\omega) = -\int_0^\infty \Phi(t) \sin\omega t \, dt \quad \leftarrow \text{Sine transform}$$

3. Inverse Cosine & Sine Transforms yield

   a. $$\Phi(t) = \frac{2}{\pi}\int_0^\infty U(\omega) \cos\omega t \, d\omega$$
   $$= -\frac{2}{\pi}\int_0^\infty V(\omega) \sin\omega t \, d\omega$$ for $t>0$

   b. Thus, $\boxed{\int_0^\infty U(\omega) \cos\omega t \, d\omega = -\int_0^\infty V(\omega)\sin\omega t \, d\omega}$, $t>0$

> Requirements for Causality & Reality lead to an interdependence of real & imaginary parts of transfer function $\phi(\omega)$

III. Discrete Fourier Transforms

A. Motivation

1. Using a Fourier space representation for numerical simulation, we must use Fourier transforms on a discrete set of points.
2. Thus, we need to explore properties of Discrete Fourier Transforms.

B. Orthogonality

1. Need to explore orthogonality for a discrete set of points.
   $\Rightarrow$ Sin, Cos, $e^{i\omega t}$ are orthogonal on discrete set of uniformly spaced points!

III. B. (Continued)

2. Choose $\boxed{x_k = \frac{2\pi k}{N}, \quad k = 0, 1, 2, \ldots, N-1}$

3. Define $\phi_p(x_k) = e^{i p x_k}$ defined only on points x_k!

4. Scalar Product: Discrete version is sum of products

$$\boxed{\langle \phi_p | \phi_q \rangle \equiv \sum_{k=0}^{N-1} \phi_p^*(x_k)\, \phi_q(x_k)}$$

5. Substituting for $\phi_p(x_k)$, etc.

a. $\langle \phi_p | \phi_q \rangle = \sum_{k=0}^{N-1} e^{\frac{i 2\pi k (q-p)}{N}} = \sum_{k=0}^{N-1} r^k$ where $r = e^{\frac{i 2\pi (q-p)}{N}}$

b. Finite Geometric Series: $\langle \phi_p | \phi_q \rangle = \sum_{k=0}^{N-1} r^k = \frac{1-r^N}{1-r}$

c. But, since p and q are integer values, $q-p$ is an integer, and $r^N = \left[e^{\frac{i 2\pi (q-p)}{N}} \right]^N = e^{i 2\pi (q-p)} = 1$ for any integer $(q-p) \neq 0$

d. If $q - p = nN$, then $r = 1$, So $\langle \phi_p | \phi_q \rangle = \sum_{k=0}^{N-1} 1^N = N$.

any integer multiple of N.

e. But, since ϕ_p is defined on N points, only N functions can be linearly independent. $\Rightarrow$ Restricts $0 \leq p, q \leq N-1$.

f. Final Result: $\boxed{\langle \phi_p | \phi_q \rangle = N \delta_{pq} \quad \text{for } 0 \leq p, q, N-1}$

Orthogonality Condition on discrete set of points.

C. Discrete Transforms: 1. Forward: $g_p = N^{-\frac{1}{2}} \sum_{k=0}^{N-1} e^{i 2\pi k p / N} f_k$

2. Inverse: $f_k = N^{-\frac{1}{2}} \sum_{k=0}^{N-1} e^{-i 2\pi k p / N} g_p$

III. C. (Continued)

2. <u>Physical space:</u> $f_k \equiv f(x_k)$

<u>Fourier Space:</u> $g_p \equiv g(\omega_p)$ where $\omega_p \equiv \frac{2\pi p}{N}$, $0 \le p \le N-1$

possible frequencies.

3. <u>Verify:</u>

$$f_k = N^{-\frac{1}{2}} \sum_{k=0}^{N-1} e^{-i2\pi kp/N} \left[N^{-\frac{1}{2}} \sum_{j=0}^{N-1} e^{i2\pi jp/N} f_j \right] = N^{-1} \sum_{k} \sum_{j} \underbrace{\left\{ e^{i2\pi(j-k)p/N} \right\}}_{=\delta_{jk}} f_j$$

$$= N^{-1} \sum_{k=0}^{N-1} \delta_{jk} f_j = \frac{N}{N} f_k = f_k \checkmark$$

4. <u>Properties:</u> Similar to continuous Fourier Transform

a. Ex: Translation $[f_{k-j}]^T_p = e^{i2\pi jp/N} g_p$ Translation by j discrete steps.

5. <u>Discrete Convolution Theorem:</u> $\boxed{[f*g]^T_p = F_p G_p}$

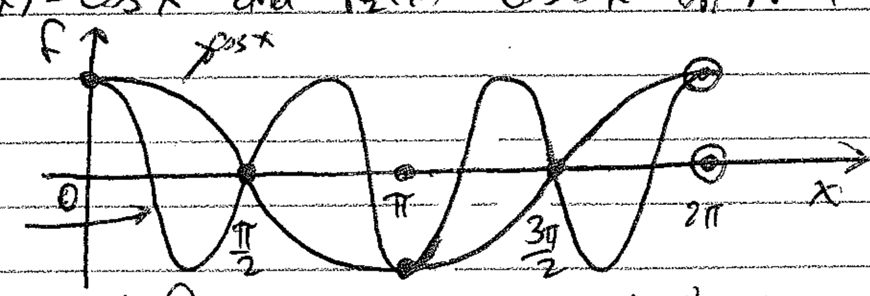
6. <u>Transformation Matrix:</u> <u>Unitary $N \times N$ matrix!</u>

7. <u>Aliasing:</u>

a. On a discrete set of points, higher frequency modes can be mistaken for modes at a lower (resolved frequency).

b. Consider $f_1(x) = \cos x$ and $f_2(x) = \cos 3x$ on $N=4$ points.

c. $x_k = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$



d. Both $f_1(x) = \cos x$ and $f_2(x) = \cos 3x$ have exactly the same values at all x_k! ⇒ Cannot be distinguished on $N=4$ points.

e. Any contribution from $f_2(x) = \cos 3x$ will be mistakenly interpreted as due to $f_1(x) = \cos x$ ⇒ Power is aliased into resolved frequency range!

8. <u>Fast Fourier Transforms:</u> Cooley & Tukey, Math. Comput. 19, 297 (1965)

a. Efficient routine reduces cost from N^2 to $\frac{N}{2}\log_2 N$. For $N=1024$, saves a factor of ~ 200!