Math 118 Handout #3 2010.03.04

Poisson Summation Formula

Theorem 1. If f is a nice smooth function and $\hat{f}$ is its Fourier Transform

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

then $$\sqrt{2\pi} \sum_{-\infty}^{\infty} f(2\pi n) = \sum_{-\infty}^{\infty} \hat{f}(n) \cancel{e^{2\pi i n x/T}},$$

and more generally, for any $T > 0$ and $x \in \mathbb{R}$

$$\sum_{-\infty}^{\infty} f(x+kT) = \frac{\sqrt{2\pi}}{T} \sum_{-\infty}^{\infty} \hat{f}\left(\frac{2\pi n}{T}\right) e^{2\pi i n x/T}.$$

Proof. Build the periodization of f by

$$f^{o}(x) = \sum_{-\infty}^{\infty} f(x+kT) = f^{o}(x+T)$$

and expand f^{o} in a T-periodic complex Fourier series

$$f^{o}(x) = \sum_{-\infty}^{\infty} \frac{1}{T} \int_0^T f^{o}(y) e^{-2\pi i n y/T} dy \, e^{2\pi i n x/T}$$

where

$$\frac{1}{T}\int_0^T \sum_{-\infty}^{\infty} f(y+kT) e^{-2\pi i n y/T} dy =$$

$$= \frac{1}{T}\sum_{-\infty}^{\infty} \int_{kT}^{(k+1)T} f(x)\, e^{-2\pi i n x/T}\, dx$$

$$= \frac{1}{T} \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i n x/T}\, dx$$

$$= \frac{1}{T}\hat{f}(2\pi n/T)\sqrt{2\pi}\,.$$

Setting $T = 2\pi$ and $x = 0$ gives

$$f^{\circ}(0) = \sum_{-\infty}^{\infty} f(2\pi k)$$

$$= \sum_{-\infty}^{\infty} \frac{1}{2\pi}\sqrt{2\pi}\,\hat{f}(n)\,. \quad \blacksquare$$

<u>Example 1</u>: This formula implies the Fourier inversion formula. The RHS is a Riemann sum with spacing $2\pi/T$ for the integral

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \hat{f}(k)\, e^{ikx} \qquad \left(k = \frac{2\pi}{T} n\right)$$

while the left-hand side is $f(x)$ plus

$$\sum_{k\neq 0} f(x+kT) \le \sum_{k\neq 0} \frac{1}{(kT)^2} \le \frac{C}{T^2}$$

if $|f(x)| \le \frac{1}{|x|^2}$ for $|x| \ge 1$ and $T \to \infty$.

Example 2: let $f(x) = \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t}$

so

$$\hat{f}(k) = e^{-k^2 t}.$$

Then the PSF says (with $T = 2\pi$)

$$\boxed{\sum_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi t}} e^{-(x-2\pi k)^2/4t} = \sum_{-\infty}^{\infty} e^{-k^2 t} e^{ikx} / \sqrt{2\pi}}$$

This reduces to "Jacobi's Θ-function identity" for $x = 0$. It solves the heat equation

$$u_t = u_{xx} \qquad -\pi < x < \pi, \quad t \geq 0$$

in two different ways: Fourier series expansion on the right-hand side, and the "method of images" on the left-hand side. The latter consists of solving the problem on $-\infty < x < \infty$ and then periodizing the solution. It has many other uses.

<u>Example 3</u>: Let $f(x) = e^{-|x|t}$ where t is a parameter. Then

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}}\left(\int_0^\infty e^{-tx} e^{-ikx}\,dx + \int_{-\infty}^0 e^{tx} e^{-ikx}\,dx\right)$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{e^{-(t+ik)x}}{-(t+ik)}\Big|_0^\infty + \frac{e^{(t-ik)x}}{t-ik}\Big|_{-\infty}^0\right)$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{t+ik} + \frac{1}{t-ik}\right)$$

$$= \sqrt{\frac{2}{\pi}}\,\frac{t}{t^2+k^2}.$$

Hence $\sqrt{2\pi}\sum_{-\infty}^{\infty} e^{-|2\pi k|t} = \sum_{-\infty}^{\infty}\sqrt{\frac{2}{\pi}}\,\frac{t}{t^2+k^2}$

or

$$\boxed{\sum_{-\infty}^{\infty}\frac{1}{t^2+k^2}} = \frac{\pi}{t}\left(1+2\sum_{1}^{\infty} e^{-2\pi t k}\right) \quad (t>0)$$

$$= \frac{\pi}{t}\left(1+2e^{-2\pi t}\frac{1}{1-e^{-2\pi t}}\right)$$

$$= \boxed{\frac{\pi}{t}\left(\frac{1+e^{-2\pi t}}{1-e^{-2\pi t}}\right)}.$$

Note that as $t \to 0$, $\sum_{1}^{\infty}\frac{1}{k^2} = \frac{\pi^2}{6}$ after some algebra.

Ewald summation:

Recall the useful formula

$$(*) \qquad \frac{1}{x} = \int_0^\infty e^{-tx}\,dt \qquad x>0$$

which we used to evaluate $\int_{-\infty}^{\infty} \frac{\sin x}{x}\,dx$, and let's consider the solutions of

$$-u'' = f \qquad -\pi \leq x < \pi$$

for periodic data f and solution u. Clearly u has a Fourier series expansion

$$u(x) = \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} \hat{u}(k) e^{ikx}$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{\substack{-\infty \\ k\neq 0}}^{\infty} \frac{1}{k^2} \hat{f}(k) e^{ikx}$$

where the $k=0$ term is excluded to enforce a mean-zero condition on u. Employing $(*)$ gives

$$u(x) = \frac{1}{\sqrt{2\pi}} \sum_{k\neq 0} \int_0^\infty e^{-tk^2} \hat{f}(k) e^{ikx}\,dt$$

and recognizing the heat kernel suggests that the solution $u(x)$

can be found by solving the heat equation

$$v_t = v_{xx}, \qquad v(x,0) = f(x)$$

So

$$\int_0^\infty v_t \, dt = v(\infty) - v(0) = \int_0^\infty v_{xx} \, dt$$

and

$$-\int_0^\infty v_{xx} \, dt = f.$$

Hence $u(x) = +\int_0^\infty v(x,t)\,dt$ is a solution.

Since

$$\frac{1}{k^2} = \int_0^\infty e^{-tk^2} \, dt,$$

we have

$$u(x) = \int_0^\infty \left(\frac{1}{\sqrt{2\pi}} \sum_{k \neq 0} e^{-k^2 t} e^{ikx} \right) \hat{f}(k) \, dt$$

$$= \int_0^\infty \frac{1}{\sqrt{2\pi}} \sum_{k \neq 0} e^{-k^2 t} \, dt \, e^{ikx} \hat{f}(k)$$

$$+ \int_0^\infty \int_{-\pi}^{\pi} \left(-\frac{1}{\sqrt{2\pi}} + \sum_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi t}} e^{-(x-y-2\pi k)^2/4t} \right) f(y) \, dy \, dt$$

by the convolution theorem $\widehat{f * g} = \hat{f}\hat{g}$, and Example 3 above. If f has mean 0

$$\int_{-\pi}^{\pi} f(y) \, dy = 0$$

then the constant term integrates to 0 and

$$u(x) = \int_{-\pi}^{\pi} g(x-y) f(y)\,dy \quad \text{where}$$

$$g(x) = \frac{1}{\sqrt{2\pi}} \sum_{k \neq 0} \frac{e^{-k^2\delta}}{k^2} e^{ikx}$$

$$+ \sum_{-\infty}^{\infty} \int_0^{\delta} \frac{1}{\sqrt{4\pi t}} e^{-(x-2\pi k)^2/4t}\,dt$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k \neq 0} \frac{e^{-k^2\delta}}{k^2} e^{ikx}$$

$$+ \frac{1}{\sqrt{4\pi}} \sum_{-\infty}^{\infty} \int_{(x-2\pi k)^2/4\delta}^{\infty} e^{-s} s^{-3/2}\,ds\, |x-2\pi k|$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k \neq 0} \frac{e^{-k^2\delta}}{k^2} e^{ikx}$$

$$+ \frac{1}{\sqrt{4\pi}} \sum_{-\infty}^{\infty} |x-2\pi k|\, \Gamma\left(-\tfrac{1}{2}, \frac{(x-2\pi k)^2}{4\delta}\right)$$

where the incomplete Γ function is

$$\Gamma(\alpha, x) = \int_x^{\infty} e^{-s} s^{\alpha-1}\,ds.$$

It decays like a Gaussian as $k \to \infty$ but looks like $|x|^{-1/2}$ as $x \to 0$.

$\boxed{\text{Exercise H3.1}}$ Suppose you can only afford to evaluate 11 terms of either side of the PSF

$$\sum_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi t}} e^{-(x-2\pi k)^2/4t}$$
$$= \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} e^{-k^2 t} e^{ikx}.$$

Find δ such that the error in the right-hand side (truncated after 11 terms) is ~~too~~ smaller than 10^{-14} for $t \geq \delta$, and $|x| \leq \pi$. Show that the error in the left hand side (truncated after 11 terms) is smaller than 10^{-14} for $t \leq \delta$ and $|x| \leq \pi$.

$\boxed{\text{H3.2}}$ Use the Poisson summation formula to prove the Euler-Maclaurin summation formulas

$$\sum_{n=0}^{\infty} f(n) = \frac{1}{2} f(0) + \int_0^{\infty} f(x)\,dx$$
$$- \frac{1}{12} f'(0) + \frac{1}{720} f'''(0) - \cdots$$

for an <u>even</u> function f.