Stat 992: Lecture 05
Diffusion equations.

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1. *Laplacian of Gaussian kernel.* To implement iterated kernel smoothing, we need to understand the relationship between kernel smoothing and diffusion equations. Let $H = \sigma I_n$ and represent isotropic kernel in n-dimensional spherical coordinates:

$$K_\sigma(r) = \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\big[-\frac{r^2}{2\sigma^2}\big]$$

where $r = \sum_{i=1}^n x_i^2$. Laplacian Δ in rectangular coordinates is given by $\Delta = \sum_{i=1}^n \frac{\partial^2}{\partial t_i^2}$. In spherical coordinates it can be shown that

$$\Delta K_\sigma = \frac{\partial^2 K_\sigma}{\partial r^2} + \frac{n-1}{r}\frac{\partial K_\sigma}{\partial r}.$$

Note that

$$\frac{\partial K_\sigma}{\partial r} = -\frac{r}{\sigma^2}K_\sigma, \frac{\partial^2 K_\sigma}{\partial r^2} = \big[\frac{r^2}{\sigma^4} - \frac{1}{\sigma^2}\big]K_\sigma.$$

Thus

$$\Delta K_\sigma = \big[\frac{r^2}{\sigma^4} - \frac{n}{\sigma^2}\big]K_\sigma. \quad (1)$$

On the other hand

$$\frac{\partial K_\sigma}{\partial \sigma} = \big[\frac{r^2}{\sigma^3} - \frac{n}{\sigma}\big]K_\sigma \quad (2)$$

From (1) and (2), we have

$$\frac{1}{\sigma}\frac{\partial K_\sigma}{\partial \sigma} = \Delta K_\sigma. \quad (3)$$

This equation is an isotropic diffusion equation but it doesn't look like it. Let $2t = \sigma^2$. Then differential $dt = \sigma d\sigma$ and equation (3) transforms to

$$\frac{\partial K_\sigma}{\partial t} = \Delta K_\sigma.$$

Now apply convolution on both sides and get

$$\frac{\partial K_\sigma * Y(x)}{\partial t} = \Delta\big[K_\sigma * Y(x)\big].$$

Hence $K_\sigma * Y(x)$ is a solution of an isotropic heat equation

$$\frac{\partial f}{\partial t} = \Delta f \quad (4)$$

with initial condition $f(x,0) = Y(x)$ after time $t = \sigma^2/2$. Note that $\lim_{t\to 0} K_\sigma * Y(x) = Y(x)$ so the solution satisfies the initial condition. So if we diffuse observation $Y(x)$ for time duration of $t = \sigma^2/2$. it should be equivalent to kernel smoothing with bandwidth σ. This is a remarkable result that has many important ramifications[1].

Problem 9. Prove the uniqueness of the solution. Look at Greens functions and fundamental solutions. One reference would be Stakgold's Greens Functions and Boundary Value Problems (1979).

Problem 10. Laplacian of image is used to detect edges but since images are discrete, partial derivatives are undefined. So traditionally kernel smoothing is applied before estimating the Laplacian. Implement Laplacian-based edge detector using above kernel smoothing and apply it to `sagittal.data`. Experiment with different filter size σ to see which one detect the best. Can you somehow choose σ automatically?

2. *Iterated Gaussian kernel smoothing.* We will call the solution to (4) as *diffusion smoother*. It is identical to Gaussian kernel smoother so it should inherit all the statistical properties of kernel smoothing estimator and vice versa. When we diffuse observation Y for duration $\delta t = \sigma^2/2$ we get $K_\sigma * Y$. Now we diffuse $K_\sigma * Y$ for additional $\delta t = \sigma^2/2$ and get $K_\sigma * K_\sigma * Y$. The total time it has been diffused is $\sigma^2/2 + \sigma^2/2 = \sigma^2$. Hence it must be equivalent to kernel smoothing with bandwidth $\sqrt{2}\sigma$, i.e.

$$K_\sigma * K_\sigma * Y = K_{\sqrt{2}\sigma} * Y.$$

Let $K_\sigma * K_\sigma = K_\sigma^{(2*)}$. Then $K_\sigma^{(m*)} = K_{\sqrt{m}\sigma}$.

An alternate proof is that noticing that $K_\sigma * K_\sigma$ is the probability density of the sum of two i.i.d. Gaussian random variables with variance σ^2 which gives a Gaussian with variance $2\sigma^2$.

Problem 11. Come up with other methods for proving this. One approach is to compute the convolution directly.

[1] **Project 3.** investigate the statistical properties of diffusion smoother in 1D and higher dimensions. Need to do stochastic simulations.