Stat 992: Lecture 07
Isotropic kernels on manifolds.

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1. **Partial solution 1.** For given two arbitrary mean zero Gaussian fields, is there mapping that makes them independent? Let $e = (e_1(t), e_2(s))'$ be a vector field. Let A be a constant matrix. Consider transformation Ae and its covariance $\mathbb{E}[Ae(Ae)'] = A\mathbb{E}[ee']A'$. Note that $\mathbb{E}[ee']$ is symmetric and its diagonal terms are positive so it is a symmetric positive definite matrix so we have a singular value decomposition of the form $\mathbb{E}[ee'] = QDiag(\lambda_1, \lambda_2)Q'$ where Q is an orthogonal matrix. Simply let $A = Q'$ and it should make the component of Ae uncorrelated for all t and s. But they are still not independent.

   Partial solution 2. Given zero mean Gaussian field $X(t), t = (t_1, \cdots, t_n) \in \mathbb{R}^n$, compute the expectation of the determinant of the Hessian of $X(t)$. Hessian matrix field $H(t)$ is given as $H(t) = \left(\frac{\partial^2 X(t)}{\partial t_i \partial t_j}\right)$. If we have mean zero Gaussian random variables $Z_1, \cdots, Z_n, \mathbb{E}(Z_1 \cdots Z_n) = 0$ if n odd. Hence the expectation of the determinant of Hessian of a mean zero Gaussian field vanishes. For n even and assuming isotropic covariance $R(t,s) = R(\|t-s\|)$, i.e. stationarity, one can further simplify the expression.

   Solution 3. Let $X(t)$ be a zero mean Gaussian fields in Ω with covariance function R. Find the distribution of $\int_\Omega X(t)\ dt$. Solution by Tulaya Limpiti. Obviously this is a zero mean Gaussian random variable so we only need to find the second moment

$$
\begin{aligned}
& \mathbb{E}\Big[\int_\Omega X(t)\ dt \int_\Omega X(s)\ ds\Big] \\
= & \int_\Omega \int_\Omega \mathbb{E}[X(t)X(s)]\ dt\ ds \\
= & \int_\Omega \int_\Omega R(t,s)\ dt\ ds.
\end{aligned}
$$

   She also provided another solution based on Kanhunen-Loeve expansion and Mercer's theorem - we will study these topics soon.

2. *Regression on manifolds.* To construct kernel based smoothing on manifolds, we need to understand the properties of heal kernel. Read Schoen, R. and Yau S.-T. Lectures on Differential Geometry (Vol I. Conference Proceedings and Lecture notes in Geometry and Topology. International Press. 1994), Diffusion kernels on statistical manifolds by Lafferty, J. and Lebanon, G. Technical Report CMU-CS-04-101, School of Computer Science, CMU, 2004 and J. Diffusion smoothing on brain surface via finite element method by Chung, M.K. and Taylor, J. ISBI 2004.

   Suppose we have differentiable manifolds $M \subset \mathbb{R}^n$. Consider M to be a very smooth surface. For instance, measurement like the brain cortical thickness can be assumed to follow additive model

$$Y(x) = \mu(x) + \epsilon(x) \tag{1}$$

   where $e(x)$ is a mean zero Gaussian random field. As in the case of kernel smoothing in the Euclidean space, we may be tempted to estimate the thickness by

$$\hat{\mu}(x) = K_\sigma * Y(x). \tag{2}$$

However kernel K_σ is isotropic in Euclidean space but anisotropic in arbitrary manifolds and may end up giving larger weights to data that is located far along the surface. To avoid this, we need to use isotropic kernel along the geodesic curves on manifolds.

3. *Geodesic curves.* Let $C \subset M$ be a curve segment connecting p and q and parameterized by $\gamma_c(t)$ with $\gamma_c(0) = p$ and $\gamma_c(1) = q$. In Cartesian coordinates, $\gamma_c(t) = (\gamma_c^1(t), \cdots, \gamma_c^n(t)) \in \mathbb{R}^n$. The length of C is given by

$$\int_0^1 \langle \frac{d\gamma_c}{dt}, \frac{d\gamma_c}{dt} \rangle^{1/2} \, dt$$

where the inner product $\langle \cdot, \cdot \rangle$ is inner product in the tangent space of the manifold. For a straight line in $\mathbb{R}^n$, the inner product is the usual Euclidean distance metric but for a curve in a curved surface, we need to give weights $G = (g_{ij})$ such that for tangent vectors $V = (v^i), W = (w^j)$ belonging tangent space T_p at p

$$\langle V, W \rangle = V'GW = \sum_{i,j} v^i g_{ij} w^j.$$

The weights $G = (g_{ij})$ are the *Riemannian metric tensors* and it is a function p.

The geodesic curve connecting p and q is then defined as the minimizer

$$d(p, q) = \min_C \int_0^1 \langle \frac{d\gamma_c}{dt}, \frac{d\gamma_c}{dt} \rangle^{1/2} \, dt.$$

It is usually given as a solution the an Euler equation and computational technique is available for polygonal surfaces. Now we define isotropic kernel in M as a kernel that only depends on the geodesic distance, i.e.

$$K_\sigma(x, y) = K_\sigma(d(x, y)).$$

There are infinitely many such isotropic kernels in manifolds. One of them is a heat kernel that is identical to Gaussian kernel in the Euclidean space.

Problem 14. On polygonal mesh `gray.obj`, given two vertices p and q, find a geodesic curve connecting them. You are only allowed to travel along edges. This is a simple discrete minimization problem that can be solved by *dynamic programming*. This can be done as a project if no one takes it.

4. *Heat kernel on manifolds.* Constructing a kernel function that is isotropic in M is not easy because there is a difficulty constructing it in an arbitrary manifold. Constructing such kernel is quite easy on a sphere since there exists spherical harmonics that can serve as the basis function expansion of the kernel so we only need to estimate the coefficient of the spherical harmonics. In arbitrary manifold M, a heat kernel K_σ that satisfies an isotropic diffusion equation

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

is a such isotropic kernel. Now Δ is the Laplace-Beltrami operator which generalizes the usual Laplacian via the Riemannian metric tensors. When the manifold M is flat, i.e. Euclidean flat space, the Laplace-Beltrami operator becomes the usual Euclidian Laplacian. Suppose M is parameterized by X such that any point $p \in M$ can be written as $p = X(u^1, u^2)$ for $u^1, u^2 \in \Omega$, the parameter space. Then the Laplace-Beltrami operator Δ corresponding to the surface parameterization X can be written as

$$\Delta K_\sigma = \frac{1}{\det G^{1/2}} \sum_{i,j=1}^{2} \frac{\partial}{\partial u^i} \Big(\det G^{1/2} g^{ij} \frac{\partial K_\sigma}{\partial u^j} \Big).$$

Problem 15. What is the Laplacian on an unit sphere and an ellipsoid $(x/a)^2 + (y/b)^2 + (z/c)^2 = 1$?

Some useful properties of the heat kernel due to Schoen and Yau (1994) are

(a) $K_\sigma(x, y) = K_\sigma(y, x)$

(b) $\lim_{\sigma \to 0} K_\sigma(x, y) = \delta(x - y)$

(c) $K_\sigma(x, y) = \int_M K_s(x, z) K_{t-s}(z, y) \, dz$ for any $0 < s < t$. If we take K_σ as the transition probability in random walk, this is the Chapman-Kolmogorov equation. Read my TR 1081. Probabilistic Connectivity Measure in Diffusion Tensor Imaging via Anisotropic Kernel Smoothing where this is used as a way of setting up iteration in spatially adaptive filter.

Problem 16. What is the heat kernel on a unit sphere ?