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Diffusion Smoothing on Brain Surface via Finite Element Method

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Introduction

In order to perform statistical analysis on the brain cortical surface, data are usually diffused to increase the signal-to-noise ratio and Gaussianness [1, 3]. Most of the diffusion equation approaches for polygonal surfaces are based on the finite element method (FEM) without the explicit representation of the Laplace-Beltrami operator. We present two new methods for solving the diffusion equations on the brain manifolds. The first method uses the explicit representation of the Laplace-Beltrami operator from and the diffusion equation is solved via a simple finite difference scheme that speed up computation. The second methods uses the heat kernel on the brain manifolds and the diffusion equations are solved via iterative kernel smoothing.

Laplace-Beltrami Operator

Consider orientable smooth twice-differentiable 2-dimensional surface $\partial\Omega \subset \mathbb{R}^3$. Then we have a parameterization of $\partial\Omega$: $X : D \to \partial\Omega$ for some planar domain $D \subset \mathbb{R}^2$. Let $T_p(\partial\Omega)$ be a tangent space at any $p = X(u) \in \partial\Omega$ such that partial derivatives

$$X_1(u) = \partial_{u^1} X(u), X_2(u) = \partial_{u^2} X(u)$$

form a basis in $T_p(\partial\Omega)$. The inner products $g_{ij} = \langle X_i, X_j \rangle$ are the Riemannian metric tensors. Then the isotropic diffusion equation on $\partial\Omega$ is given by

$$\partial_t F = \Delta F \tag{1}$$

with initial condition $F(p, 0) = f(p)$ and the *Laplace-Beltrami operator*

$$\Delta F = \frac{1}{|g|^{1/2}} \sum_{i,j=1}^{2} \frac{\partial}{\partial u^i}\Big(|g|^{1/2} g^{ij} \frac{\partial F}{\partial u^j}\Big).$$

Since the Laplace-Beltrami operator is *self adjoint* with respect to the $L^2(\partial\Omega)$ norm $\langle F, G\rangle_{\partial\Omega} = \int_{\partial\Omega} F(p)F(p)\, d\mu(p)$, we have

$$\langle G, \Delta F\rangle_{\partial\Omega} = -\int_{\partial\Omega} \langle \nabla F, \nabla G\rangle \, d\mu(p) = \langle F, \Delta G\rangle_{\partial\Omega}. \tag{2}$$

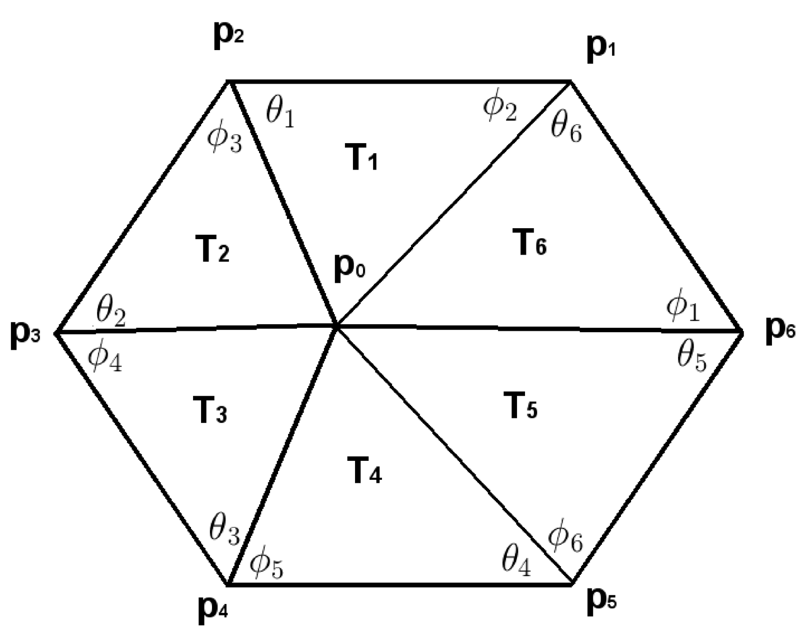

Figure 1: A typical triangular elements.

Finite Element Method

Let N_T be the number of triangles in the triangular mesh S that is the discrete realization of true manifold $\partial\Omega$ (Figure 4). We seek solution F_i to the diffusion equation in each triangle T_i such that the solution $F_i(p, t)$ is continuous across neighboring triangles, i.e. piecewise linear function. The solution F for S is then

$$F(p, t) \doteq \sum_{i=1}^{N_T} F_i(p, t). \tag{3}$$

Let $p_{i_1}, p_{i_2}, p_{i_3}$ be the vertices of element T_i. In T_i, we interpolate F_i linearly by

$$F_i(p, t) = \sum_{j=1}^{3} \xi_{i_j}(p) F(p_{i_j}, t), \tag{4}$$

where nonnegative ξ_{i_k} are given by the *barycentric coordinates* [8]. Let G and $F(x, t)$ be arbitrary piecewise linear functions given by the barycentric coordinate representation with $G_{i_k} = G(p_{i_k})$ and $F_{i_k} = F(p_{i_k}, t)$. Then from (2), the diffusion equation can be written as

$$\langle G, \partial_t F\rangle_{T_i} = -\int_{T_i} \langle \nabla F, \nabla G\rangle \, d\mu(p) \tag{5}$$

The above integral equation can be written in matrix form:

$$[G_i]'[A^i]\frac{d}{dt}[F_i] = -[G_i]'[C^i][F_i]. \tag{6}$$

where $[G_i] = (G_{i_1}, G_{i_2}, G_{i_3})'$, $[F_i] = (F_{i_1}, F_{i_2}, F_{i_3})'$, $[A^i] = (A^i_{kl}), A^i_{kl} = \int_{T_i} \xi_{i_k}\xi_{i_l} \, d\mu(p)$, $[C^i] = (C^i_{kl}), C^i_{kl} = \int_{T_i} \langle \nabla\xi_{i_k}, \nabla\xi_{i_l}\rangle \, d\mu(p)$. Since equation (6) should be true for all $[G_i]$, we have a system of ordinary differential equations (ODE)

$$\frac{d[F_i]}{dt} = -[A^i]^{-1}[C^i][F_i] \text{ for all } i. \tag{7}$$

for each element T_i. Having discretized an element, the next step is to assemble all such elements in m incident triangles around vertex p (Figure 1). Combining m elements,

$$\frac{d[F]}{dt} = -[A]^{-1}[C][F]. \tag{8}$$

where $[F] = [F(p, t), F(p_1, t), \cdots, F(p_m, t)]'$ and $[G] = [G(p), G(p_1), \cdots, G(p_m)]'$. Matrix $[C] = (C_{ij})$ is called the global coefficient matrix and comes from all elements containing vertices i and j. It seems we need to solve a huge system of linear equations iteratively; however the first row of the simultaneous ODE (8) gives the diffusion equation at the vertex $p = p_0$:

$$\frac{dF(p,t)}{dt} = -\sum_{i,k=0}^{m} A^{-1}_{0k} C_{ki} F(p_i, t), \tag{9}$$

where A^{-1}_{0k} is the $0k$-th element of A^{-1}. Comparing this with equation (1), we can see the right-hand side of equation (9) is the discrete estimation of the Laplace-Beltrami operator at vertex p. Simplifying the matrix inversion using the computational algebraic system `MAPLE`, we have the FEM estimation for the Laplace-Beltrami operator given by

$$\widehat{\Delta} F(p) = \sum_{i=1}^{m} w_i\big(F(p_i) - F(p)\big) \tag{10}$$

with the weights $w_i = (\cot\theta_i + \cot\phi_i)/|T|$, where θ_i and ϕ_i are the two angles opposite to the edge $p_i - p$ and $|T| = \sum_{i=1}^{m} |T_i|$ is the sum of the areas of the incident triangles (Figure 1). A similar discrete representation that is based on geometric arguments can be found in [6]. The diffusion equation is then solved by the finite difference scheme:

$$F(p, t_{n+1}) = F(p, t_n) + \delta t \widehat{\Delta} F(p, t_n) \tag{11}$$

with the iteration step size $\delta t = t_{n+1} - t_n$. The convergence condition can be found in [4]. Note that the Laplace-Beltrami operator in the conformal coordinate system (u^1, u^2) can be written as $\Delta = \frac{\partial^2}{\partial(u^1)^2} + \frac{\partial^2}{\partial(u^2)^2}$. So we can define the FWHM of diffusion smoothing locally as the FWHM of the corresponding Gaussian kernel in the conformal coordinate system. Then diffusion smoothing with N iterations and the step size δt would be equivalent to Gaussian kernel smoothing with

$$\text{FWHM} = 4(\ln 2)^{1/2}\sqrt{N\delta t}.$$

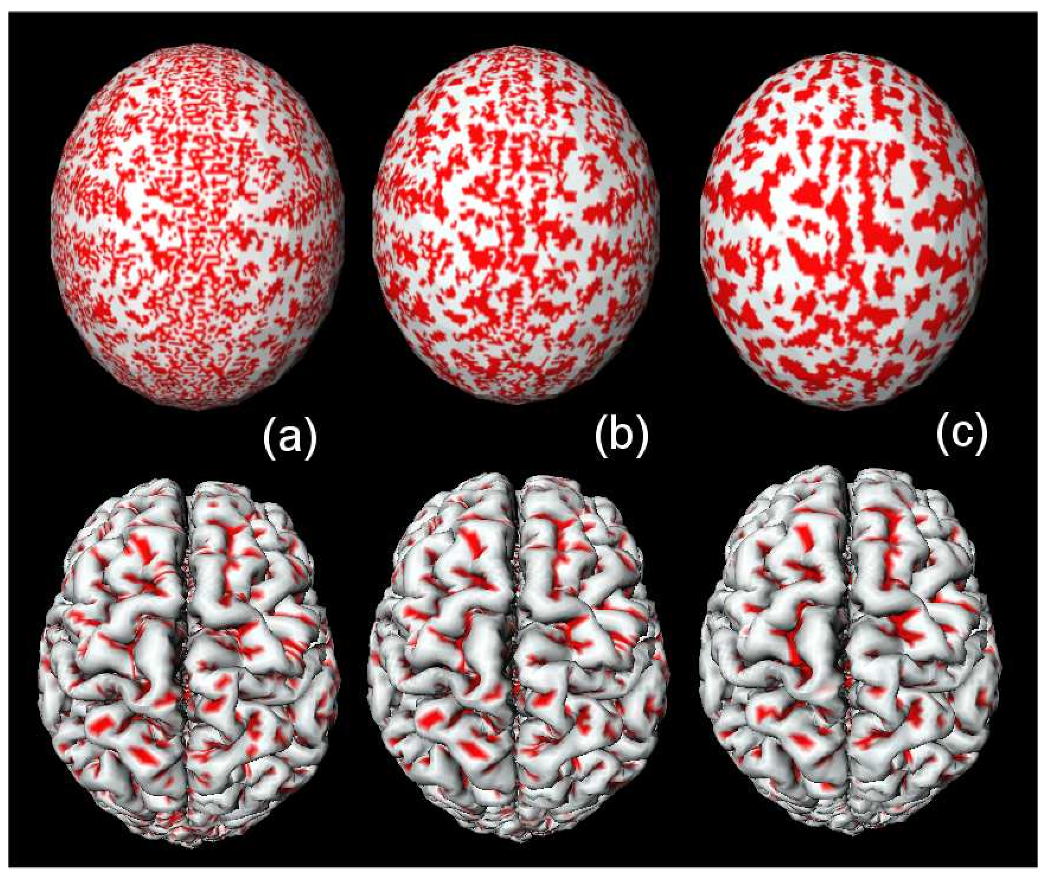

Figure 2: Diffusion smoothing was applied to smooth out the mean curvature and projected onto a sphere to show how the hidden sulcal pattern can be enhanced over time. (a) initial mean curvature. (b) after 20 iterations with $\delta t = 0.2$. (c) after 100 iterations.

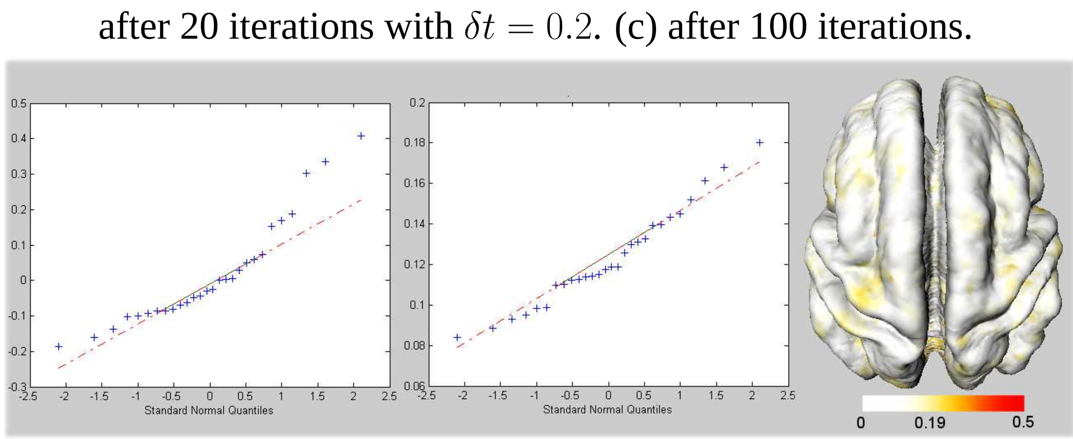

Figure 3: Left, middle: Quantitle-Quantile(QQ) plot of cortical thickness dilatation measurements before and after diffusions smoothing for 28 subjects [3]. The horizontal axis displays the quantiles of Gaussian distribution while the vertical axis displays the quantiles of an empirical distribution. How closely the blue dots lie along the straight red line gives an idea if the underlying empirical distribution follows Gaussian . Right: Lilliefors statistic measures the maximum difference between the empirical and a theoretical Gaussian distributions. Most of cortex shows value less than the cutoff value 0.19 indicating that the data have been smoothed to follow Gaussian after.

Iterated Heat Kernel Smoothing

The drawback of the FEM approach is for larger δt, finite difference scheme (11) may diverge [4]. We have developed a completely different method based on the heat kernel construction that avoids this problem. The solution to diffusion equation (1) when $t = \sigma^2/2$ is given by the convolution

$$F(p, \sigma) = K_\sigma * f(p) = \int_{\partial\Omega} K_\sigma(p, q) f(q)\mu(q)$$

where heat kernel K_σ is given by the *parametrix expansion* [7]:

$$K_\sigma(p, q) = \frac{1}{(2\pi\sigma)^{1/2}} \exp\Big[-\frac{d^2(p,q)}{2\sigma^2}\Big]\big[u_0(p, q) + O(\sigma^2)\big]$$

and $d(p, q)$ is the geodesic distance between x and y and $u_0(p, q) \to 1$ as $p \to q$. Under some regularity condition, K_σ is a probability distribution on $\partial\Omega$. Note that $K_\sigma * (K_\sigma * f)$ is the diffusion of signal f after time σ^2 so that $K_\sigma * (K_\sigma * f) = K_{\sqrt{2}\sigma} * f$. Arguing inductively, we have an iterated kernel smoothing formula

$$K_\sigma^{(m)} * f = \underbrace{K_\sigma * \cdots * K_\sigma}_{m} * f = K_{\sqrt{m}\sigma} * f.$$

So the kernel smoothing with large bandwidth can be performed iteratively with a smaller bandwidth. In practice, we use truncated and normalized kernel

$$\widetilde{K}_\sigma(p, q) = \frac{\exp\big[-\frac{d^2(p,q)}{2\sigma^2}\big]\mathbf{1}_B(p, q)}{\int_B \exp\big[-\frac{d^2(p,q)}{2\sigma^2}\big]\, d\mu(p)d\mu(q)}$$

for some small region $B \subset \partial\Omega$ and indicator function $\mathbf{1}_B$, i.e. $B = T_1 \cup \cdots \cup T_m$. Then our iterated heat kernel smoothing of data f is given by

$$\widetilde{K_\sigma}^{(m)} * f = \underbrace{\widetilde{K_\sigma} * \cdots * \widetilde{K_\sigma}}_{m} * f$$

which is the integral version of the Nadaraya-Watson kernel estimator [2].

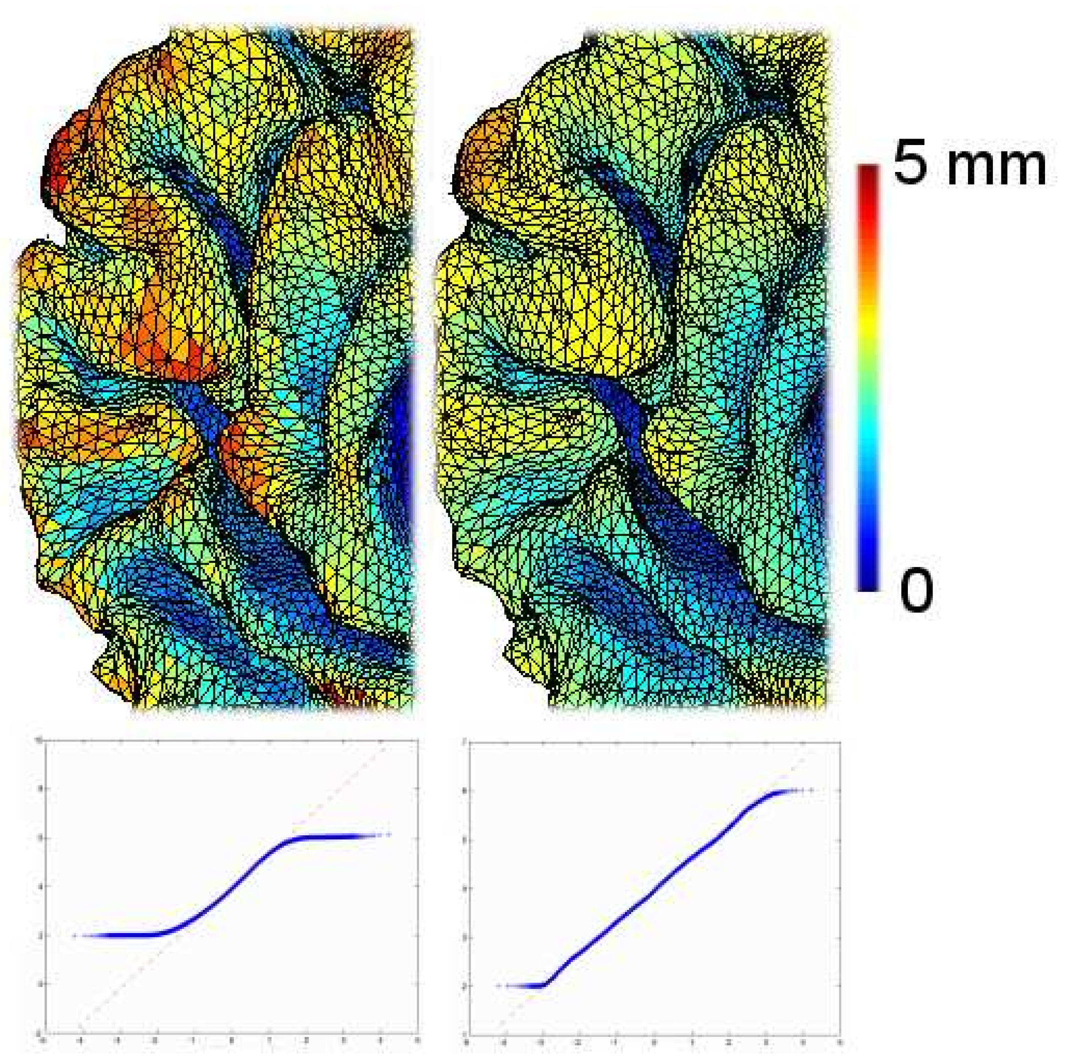

Figure 4: Top: cortical thickness computed at the posterior right hemisphere of the autistic brain and its iterated heat kernel smoothing with $\sigma = 1$ and $m = 100$ iterations. Bottom: QQ-plot of a single subject 108,588 thickness measurements showing increased Gaussianness after smoothing.

Conclusions

Based on the FEM, we discretized a diffusion equation in a triangular mesh patch centered around a vertex and solved a system of linear equation. It turns out that the Laplace-Beltrami operator can be represented as a weighted averaging where the weights are given in terms of the geometry of triangular mesh elements. Then the diffusion equation is solved via the finite difference with a temporal step size that satisfies a convergence criterion. An alternate method is to iteratively convolve with the heat kernel of the Laplace-Beltrami operator with small bandwidth. Our diffusion and much simpler iterated heat kernel smoothing would be highly useful in smoothing fMRI data [1] and anatomical data [3]. Afterwards statistical inference can be based on the random fields theory.

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References

[1] A. Andrade, F. Kherif, J. Mangin, K.J. Worsley, A. Paradis, O. Simon, S. Dehaene, D. Le Bihan, and J-B Poline, "Detection of fMRI activation using cortical surface mapping," *Human Brain Mapping*, **12**:79–93, 2001.

[2] M.K. Chung, "Iterated heat kernel smoothing on manifolds," Department of Statistics, University of Wisconsin-Madison. Technical Report, 2004.

[3] M.K. Chung, K.J. Worsley, S. Robbins, T. Paus, J. Taylor, J. Giedd, J.L. Rapoport, and A.C. Evans, "Deformation-based surface morphometry applied to gray matter deformation," *NeuroImage*, **18**:198–213, 2003.

[4] M.K. Chung, K.J. Worsley, S. Robbins, and A.C. Evans, "Tensor-based brain surface modeling and analysis," in *IEEE Conference on Computer Vision and Pattern Recognition*, 2003, vol. I, pp. 467–473.

[5] A.M. Dale, B. Fischl, M.I. Sereno, "Cortical surface-based analysis I: segmentation and surface reconstruction," *NeuroImage* **9**:179–194, 1999.

[6] M. Meyer, M. Desbrun, P. Schrder, and A. H. Barr, "Discrete differential-geometry operators for triangulated 2-manifolds," in *VisMath*, 2002.

[7] S. Rosenberg *The Laplacian on a Riemannian Manifold*, Cambridge University Press, 1997

[8] M.N.O. Sadiku, *Numerical Techniques in Electromagnetics*, CRC Press, 1992.