Towards Understanding More Complex Data

Graph Laplacian on Singular Manifolds

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Manifold Assumption

- Understanding data / spaces
  - Information estimation, data processing (clustering, semi-supervised learning, etc)

- Manifold assumption

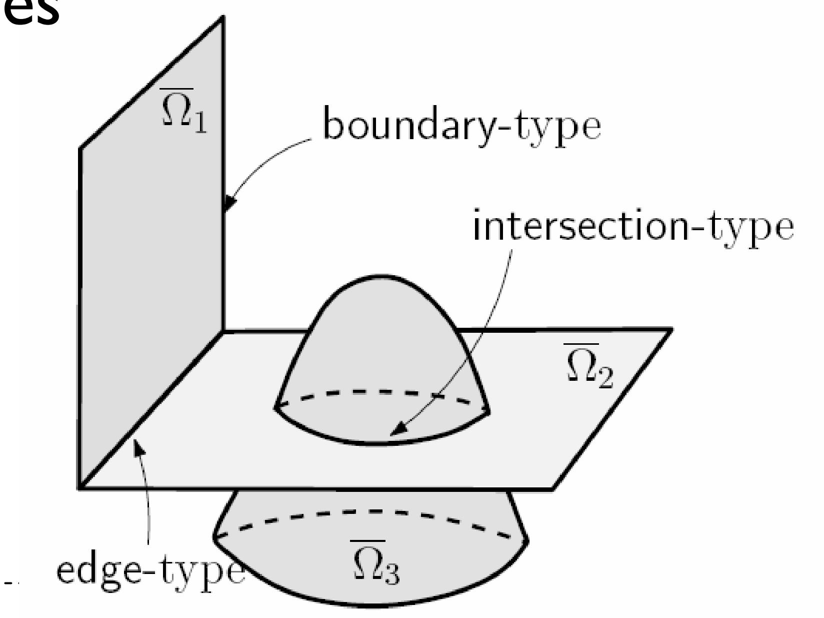
Manifold Assumption:

•Reasonable model for non-linear data

•Provides nice structures and properties that algorithms can leverage

Relax Manifold Assumption

- To model more complex data
  - Aim to relax manifold assumption
  - Still keep some nice properties that manifold assumption can offer
- Allow three types of "singularities"
  - Boundary-type
  - Intersection-type
  - Edge-type



Singularities

- Boundary
  - Configuration space may be constrained / limited

- Intersection-type
  - Two classes of data may contain similar instances

Goal:
Study how singularities may influence learning / information retrieval algorithms and how they can be learned from data.

This Talk

- Aim to study singular manifolds through the lens of Gaussian-weighted graph Laplacian
  - Laplacian-based methods is a widely used class of techniques used for recovering geometric properties of data.
  - There is a fairly good theoretical understanding of properties of Laplacian when data is sampled from a smooth manifold.
- Goal of this talk:
  - Behavior of graph Laplacian for data sampled from a singular manifold
    - when singularities are present

Some Related Work

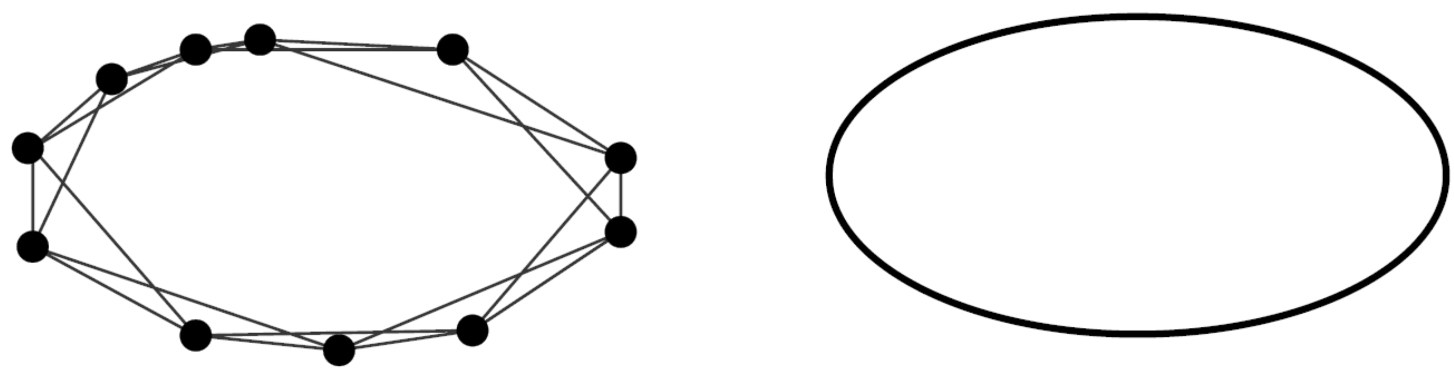
- Sampling theory for compact domains
  - [Chazal, Cohen-Steiner, Lieutier 09], [Chazal,Oudot 08], [Cheng,Dey,Ramos 07], …
- Learning collection of linear sub-spaces
  - [Vidal, Ma, Sastry 05], [Chen, Lerman 09], …
- Learning stratified spaces
  - [Bendich, Cohen-Steiner, Edelsbrunner, Harer, Morozov 07], [Bendich, Wang, Mukherjee 12], …

This Talk

- Introduction
- Graph / Functional Laplacian
- Behavior of Functional Laplacian on / around singularities
  - Boundary-type
  - Edge-type
  - Intersection-type
- Discussion and implications

Extract Manifold

- Data from a hidden smooth manifold
- Construct a graph that describes the manifold
  - Properties of graph reflect those of manifold



What Property?

- Gaussian weighted graph Laplacian
- *n* data points: $P = \{p_1, p_2, \ldots, p_n\}$
- L_P^t: *n x n* matrix

$$\mathsf{L}_P^t[i][j] = \begin{cases} -\frac{1}{n} \cdot \frac{1}{(4\pi t)^{k/2} t} e^{-\frac{\|p_i - p_j\|^2}{4t}}, & \text{if } i \neq j \\ \frac{1}{n} \cdot \frac{1}{(4\pi t)^{k/2} t} \sum_{l \neq i, l \in [1,n]} e^{-\frac{\|p_i - p_l\|^2}{4t}}, & \text{if } i == j \end{cases}$$

- When it performs on a function (*n*-vector) *f*:

Graph Laplacian is a light-weight structure (depending only proximity graph), suitable for high dimensional data analysis.

Laplace-Beltrami Operator

Nice properties of manifold Laplacian

- Reflect manifold geometry
- Eigenfunctions form basis for functions on manifold
- Relation to heat operator
- …

Applications

- Clustering, semi-supervised learning
- Data denoising
- Data representation
- Graphics, mesh smoothing, optimization

Functional Laplacian

- Laplace-Beltrami operator Δ_M is useful
- Gaussian weighted graph Laplacian L_P^t approximates Δ_M
  - For points *P* uniformly randomly sampled from manifold *M*.
  - L_P^t pointwise-converges to Δ_M *[BN05]*
  - Spectral convergence *[BN08]*
- Connection made through functional Laplacian

$$L_t f(x) = \frac{1}{t(4\pi t)^{d/2}} \int_M e^{-\frac{\|y-x\|^2}{4t}} (f(y) - f(x)) d\nu(y)$$

  - can be considered the limit of L_P^t as the size of *P* goes to ∞.

$$\boxed{\mathsf{L}_P^t f(p_i) = \frac{1}{n} \cdot \frac{1}{(4\pi t)^{k/2} t} \sum_{j=1}^{n} e^{-\frac{\|p_i - p_j\|^2}{4t}} (f(p_i) - f(p_j))}$$

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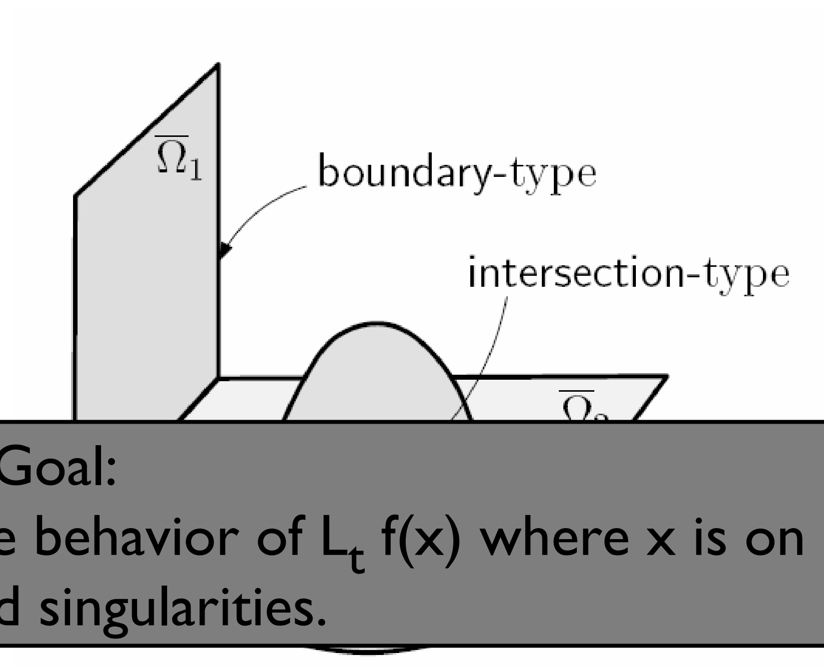
Singular Manifold

- A singular manifold Ω is a collection of smooth manifolds with boundaries $\Omega_1, \Omega_2, \ldots, \Omega_m$
- A point x is
  - Boundary type
    - If $x \in \partial\Omega_i$
  - Intersection type
    - If $x \in \Omega^o{}_i \cap \Omega^o{}_j$
  - Edge type



Goal:
Given a function f, analyze the behavior of $L_t f(x)$ where x is on or around singularities.

Laplacian at a Regular Point

- At a regular point (an interior point of a manifold) *x*

$$\boxed{L_t f(x) = \frac{1}{t(4\pi t)^{d/2}} \int_M e^{-\frac{\|y-x\|^2}{4t}} (f(y) - f(x)) d\nu(y)}$$

- By Taylor expansion:
  - $f(y) \approx f(x) + (y-x)^T \nabla f(x) + (y-x)^T H (y-x)$

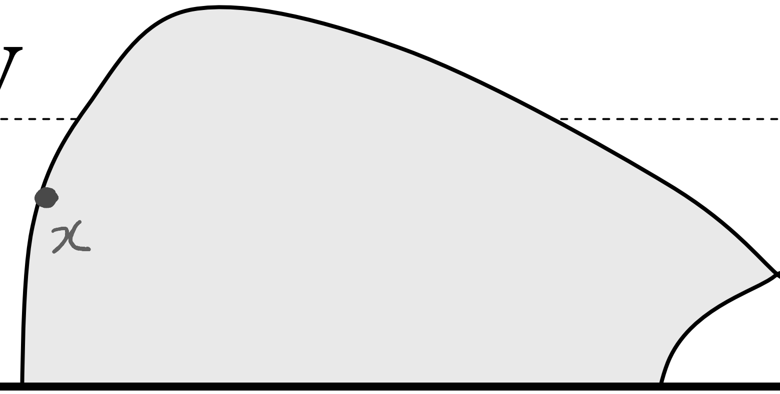
$$\begin{aligned} L_t f(x) &\approx \frac{1}{t} \int_M K_t(x,y)((y-x)^T \nabla f(x) + (y-x)^T H(y-x)) dy \\ &= \frac{1}{t} \int_M K_t(x,y)(y-x)^T H(y-x) dy \end{aligned}$$

= C tr(H)

$$\Rightarrow \quad \boxed{L_t f(x) = C \cdot \Delta f(x) + o(1)}$$

Laplacian at Boundary

- At a boundary point x



$$
\begin{aligned}
L_t f(x) &= \frac{1}{t}\int_M K_t(x,y)(f(y)-f(x))dy \\
&\approx \frac{1}{t}\int_M K_t(x,y)((y-x)^T\nabla f(x) + (y-x)^T H(y-x))dy \\
&= \boxed{\frac{1}{t}\int_M K_t(x,y)(y-x)^T\nabla f(x)dy} \\
&\quad + \frac{1}{t}\int_M K_t(x,y)(y-x)^T H(y-x))dy
\end{aligned}
$$

O(1)

Intuitive Illustration

- First term:

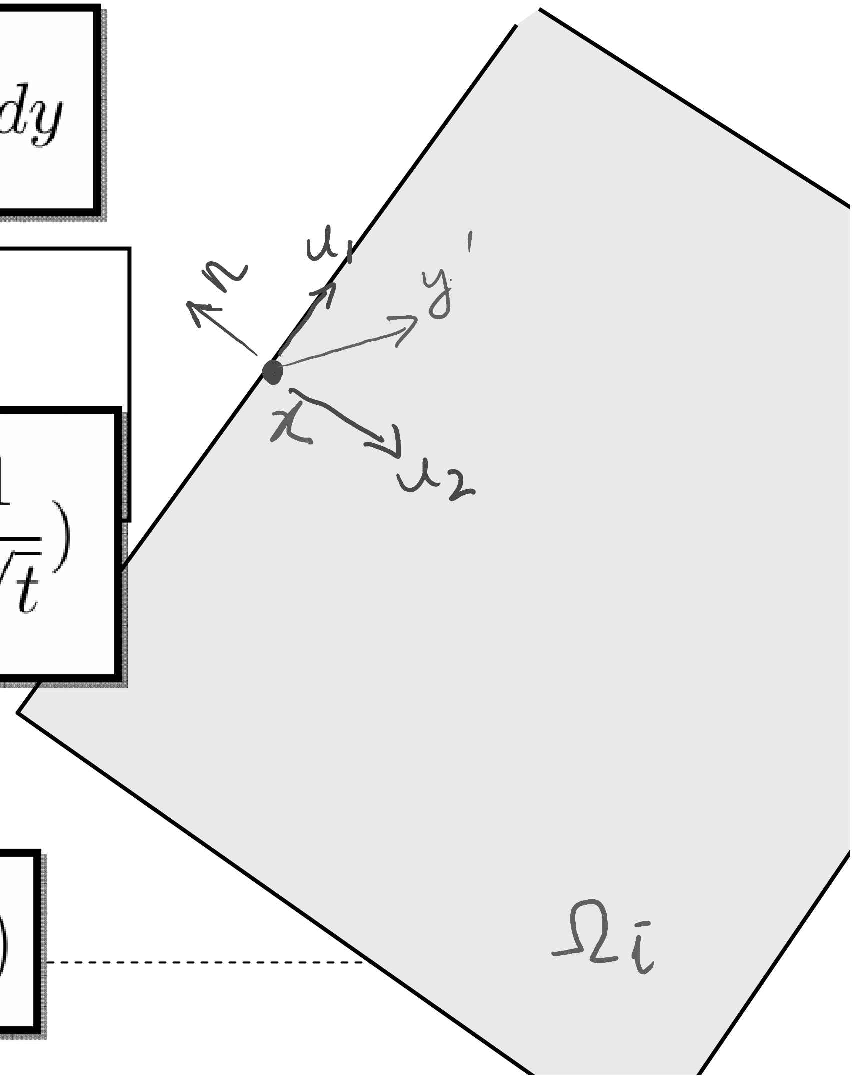
$$\frac{1}{t}\int_M K_t(x,y)(y-x)^T\nabla f(x)dy$$

For a boundary point x

$$L_t f(x) = -\frac{1}{\sqrt{t}}C_1\partial_{\mathbf{n}}f(x) + o(\frac{1}{\sqrt{t}})$$

For a regular point x

$$L_t f(x) = C\cdot\Delta f(x) + o(1)$$



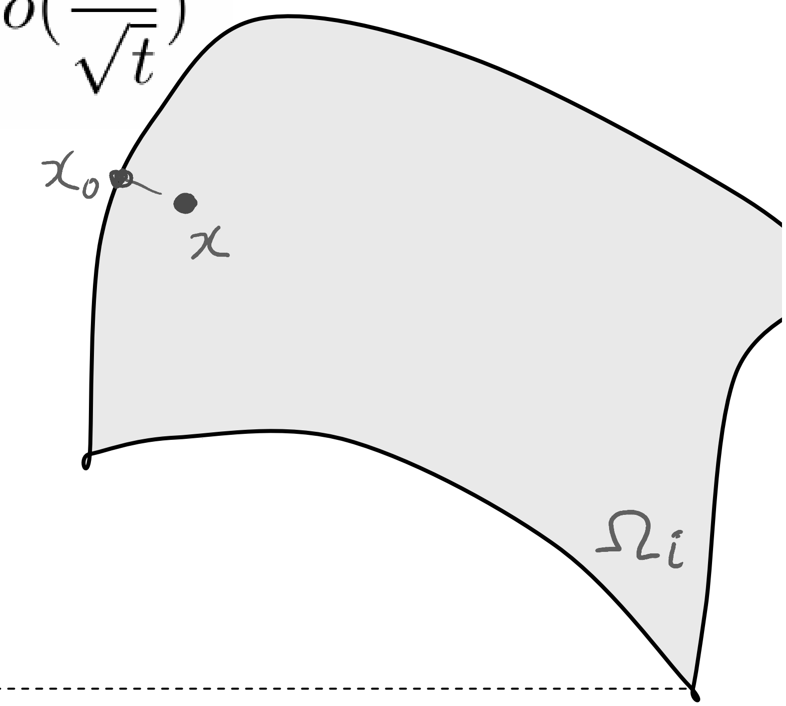
Laplacian Around Boundary

- For a point *x* near boundary
- Let x_0 be nearest neighbor of *x* along the boundary
  - Set $\| x - x_0 \| = r\sqrt{t}$

$$L_t f(x) = -\frac{1}{\sqrt{t}} e^{-r^2} C_1 \partial_{\mathbf{n}} f(x_0) + o(\frac{1}{\sqrt{t}})$$

As x moves away from the boundary, the boundary effect decreases rapidly.

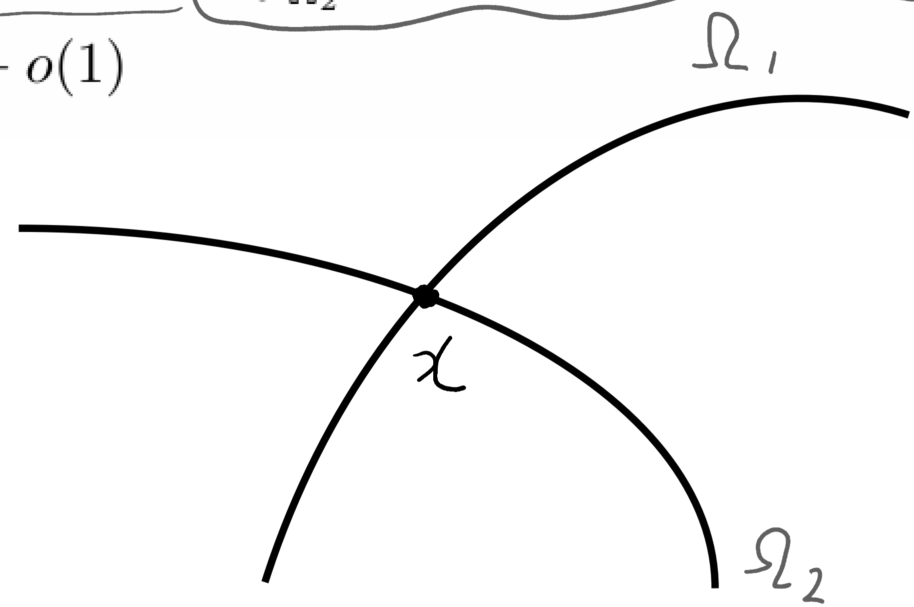
Points roughly within $\sqrt{t}$ distance to boundary have boundary effect.



Laplacian at Intersection Singularity

- For a point *x* on intersection singularity

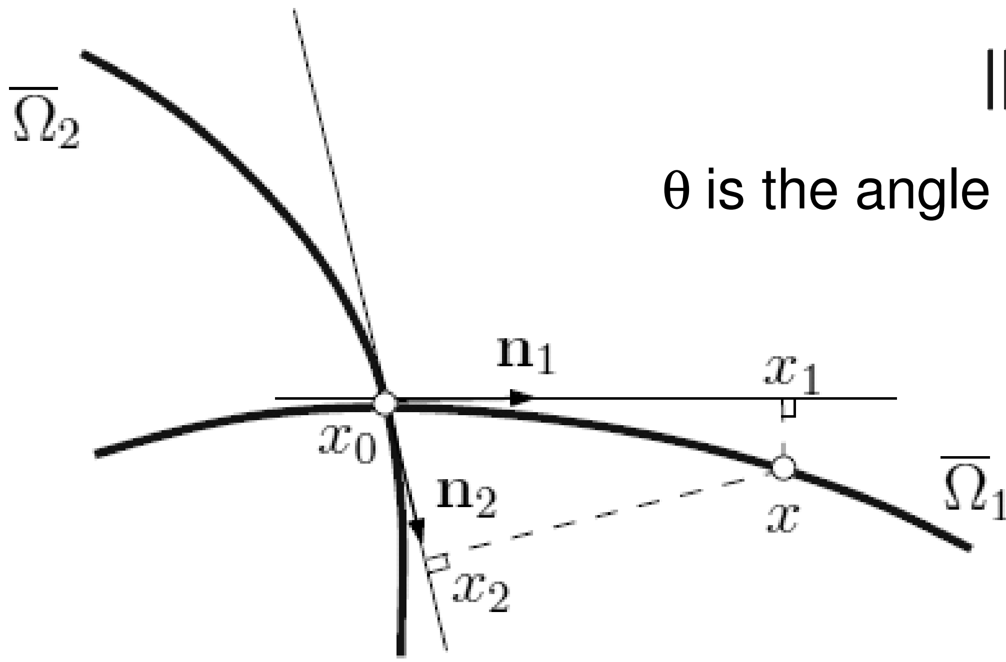
$$
\begin{aligned}
L_t f(x) &= \frac{1}{t}\int_{\Omega_1\cup\Omega_2} K_t(x,y)((f(y)-f(x))dy \\
&= \frac{1}{t}\int_{\Omega_1} K_t(x,y)((f(y)-f(x))dy + \frac{1}{t}\int_{\Omega_2} K_t(x,y)((f(y)-f(x))dy \\
&= C\Delta_{\Omega_1} f(x) + C\Delta_{\Omega_2} f(x) + o(1)
\end{aligned}
$$



Laplacian Around Intersection

- For a point x around intersection singularities

$$L_t f(x) = \boxed{\frac{1}{\sqrt{t}}}\boxed{re^{-r^2 \sin^2 \theta}} C_2(\boxed{\partial_{\mathbf{n}_1} f_1}(x_0) + \cos\theta \cdot \boxed{\partial_{\mathbf{n}_2} f_2}(x_0)) + o(\frac{1}{\sqrt{t}})$$



$\| x - x_0 \| = r\sqrt{t}$

θ is the angle between n_1 and n_2

Laplacian On / Near Edge-Singularities

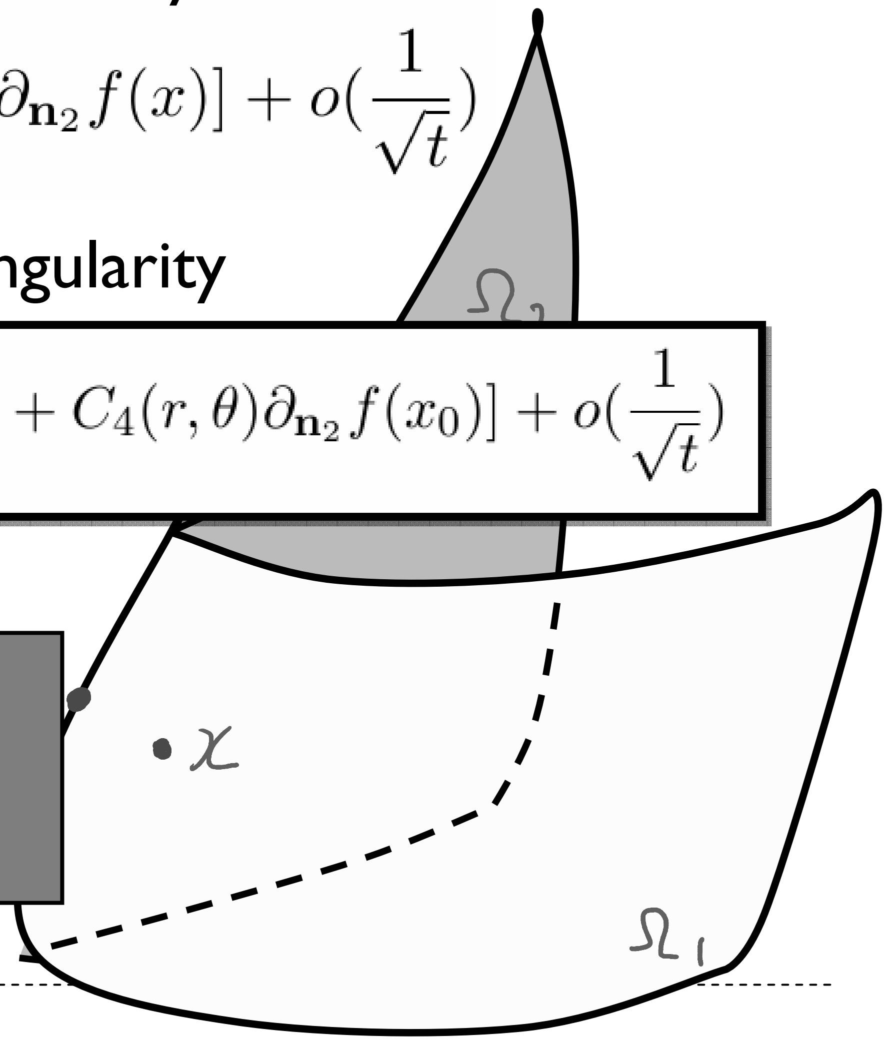
- For a point x on a "glued" boundary of two manifolds

$$L_t f(x) = -\frac{1}{\sqrt{t}} C_1[\partial_{\mathbf{n}_1} f(x) + \partial_{\mathbf{n}_2} f(x)] + o(\frac{1}{\sqrt{t}})$$

- For a point x near an edge singularity

$$\boxed{L_t f(x) = -\frac{1}{\sqrt{t}}[C_3(r,\theta)\partial_{\mathbf{n}_1} f(x_0) + C_4(r,\theta)\partial_{\mathbf{n}_2} f(x_0)] + o(\frac{1}{\sqrt{t}})}$$

Have both boundary effect and effects from points of the other manifold.



This Talk

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- Behavior of Functional Laplacian on / around singularity
  - Boundary-type
  - Edge-type
  - Intersection-type
- Discussion and implications

Key Point I

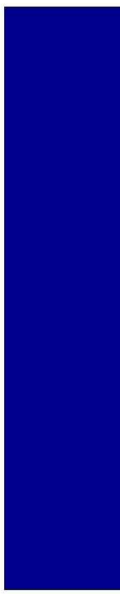
- Graph Laplacian around all three types of singularities
  - Bnd: $L_t f(x) = -\frac{1}{\sqrt{t}} e^{-r^2} C_1 \partial_{\mathbf{n}} f(x_0) + o(\frac{1}{\sqrt{t}})$
  - Intersec: $L_t f(x) = \frac{1}{\sqrt{t}} r e^{-r^2 \sin^2\theta} C_2(\partial_{\mathbf{n}_1} f_1(x_0) + \cos\theta \cdot \partial_{\mathbf{n}_2} f_2(x_0)) + o(\frac{1}{\sqrt{t}})$
  - Edge: $L_t f(x) = -\frac{1}{\sqrt{t}} [C_3(r,\theta)\partial_{\mathbf{n}_1} f(x_0) + C_4(r,\theta)\partial_{\mathbf{n}_2} f(x_0)] + o(\frac{1}{\sqrt{t}})$

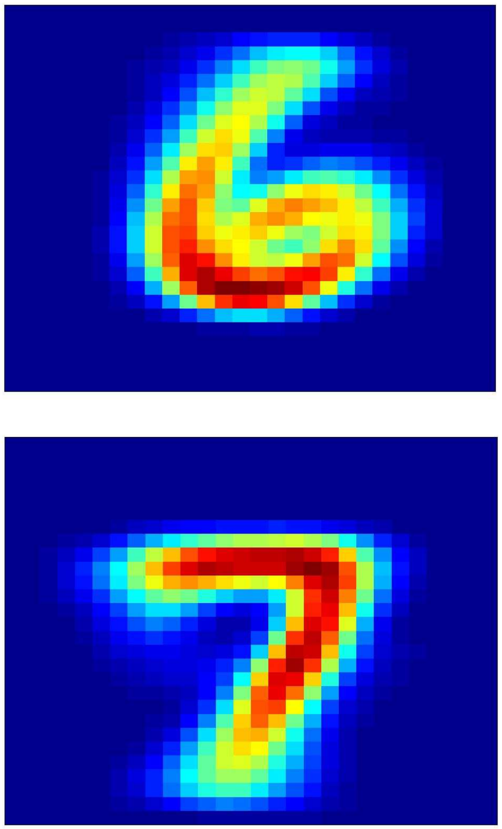
- L_t *f(x)* at points around singularities have significantly different behavior

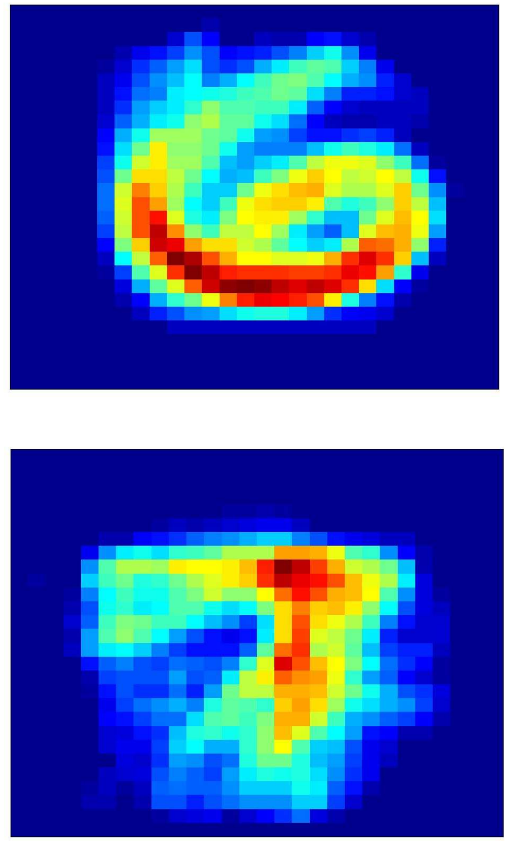
This suggests potentially identifying singularities by finding points with high $L_t f(x)$ values.

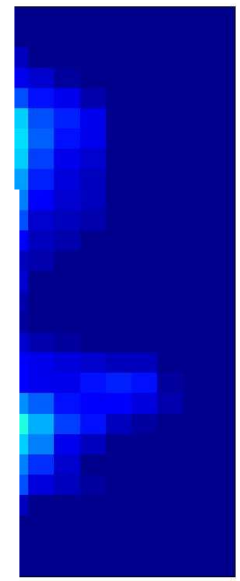
Examples

- MNIST digit images
  - Ea ... ure space
  - Fu







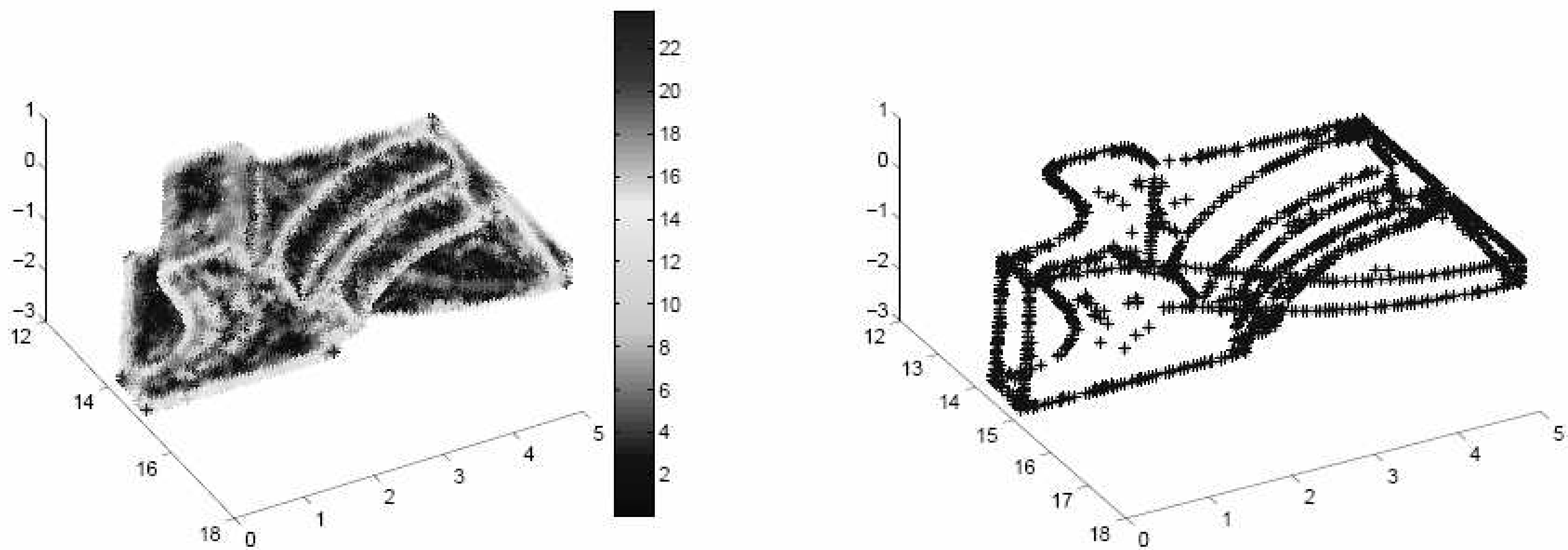


Digit ... average image

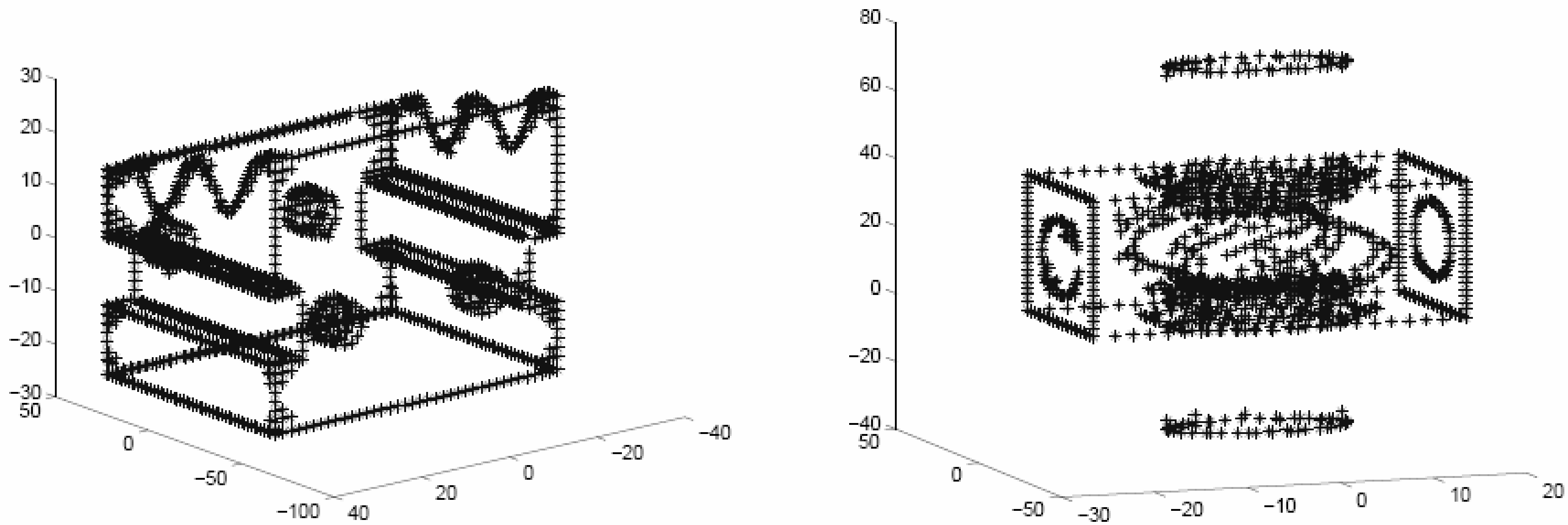
singularity image ... larity image

Examples

- Sharp feature curves identification from point clouds
- Apply L_t to coordinate functions



(a) Norm of V_t on model of fandisk. (b) Points with large norm.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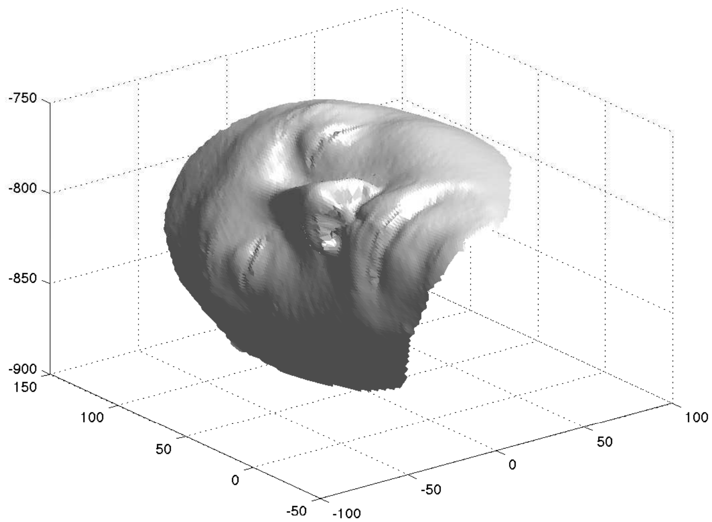
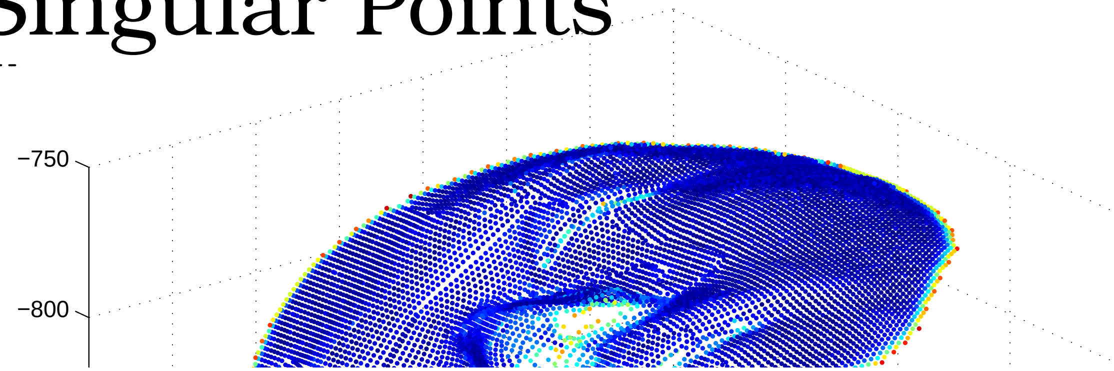
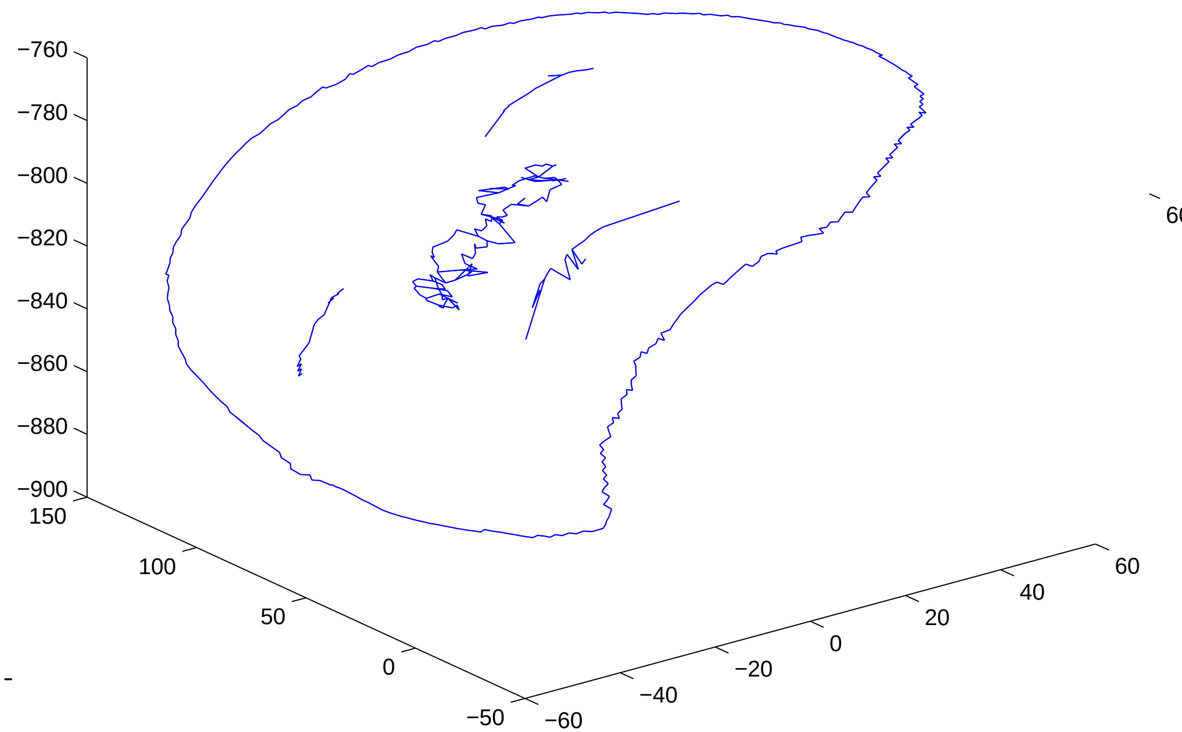
20

(a) (b)

Reeb Graph + Singular Points

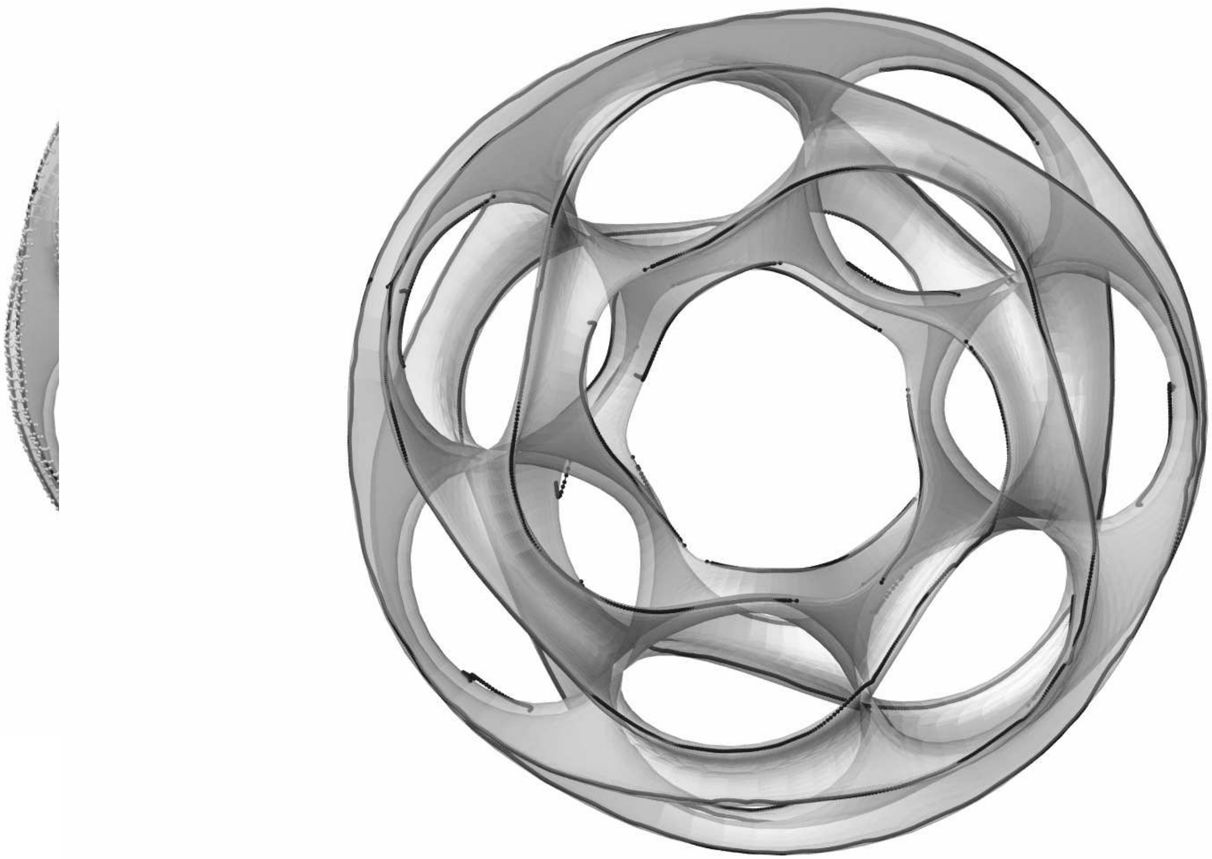






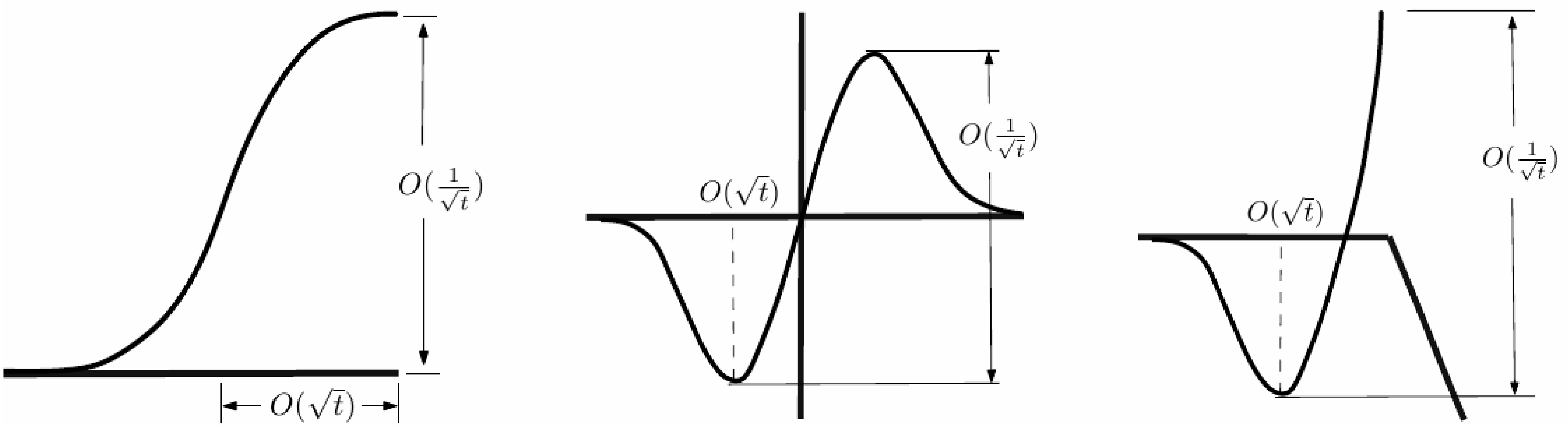
Obtain feature curve

Reeb Graph + Singular Points



Key Point II

- Around different types of singularities, scaling behaviors are different.

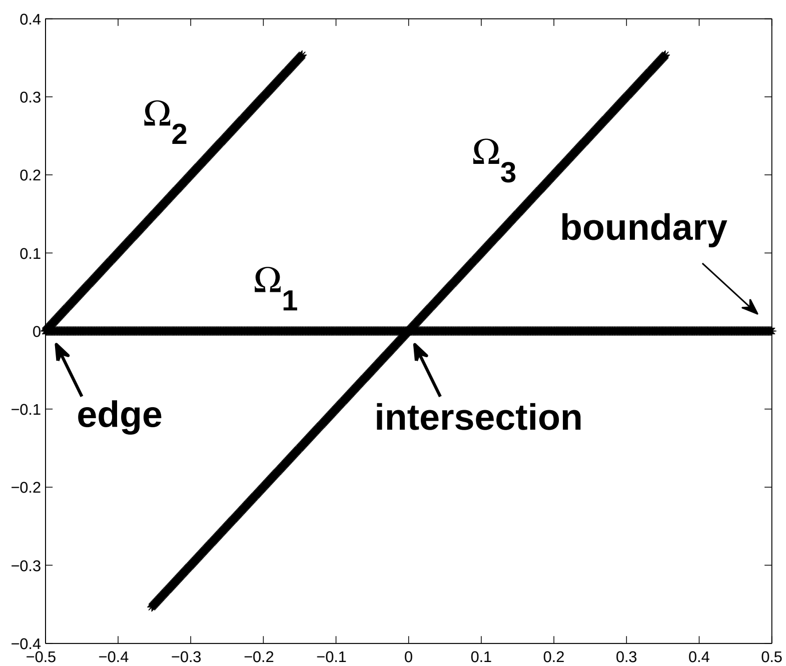


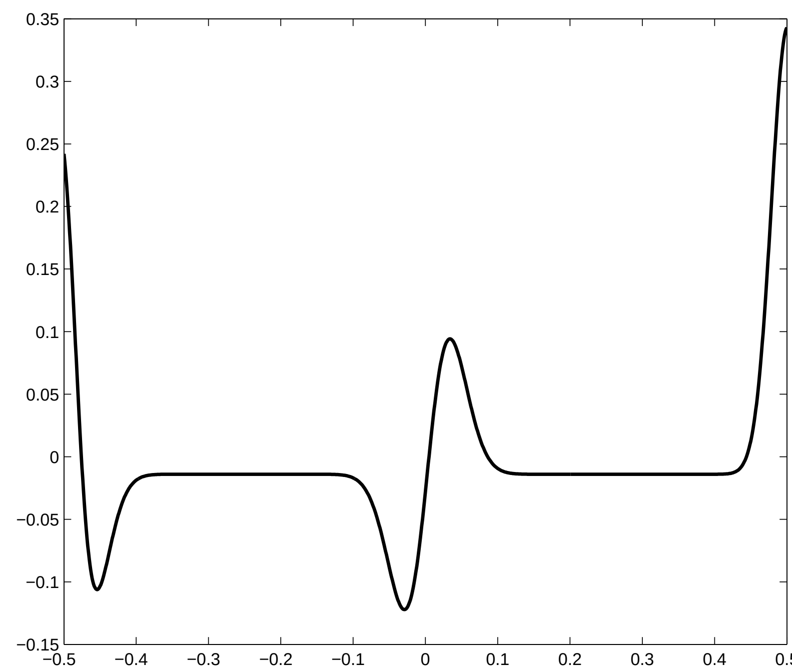
Bour ... lge

These local behaviors can potentially be used to distinguish different type of singularities

$\phi(r) = \ldots \sqrt{t} \ldots \sqrt{t} \ldots \sqrt{t} \ldots {}^{-r^2} + re^{-r^2})$

Examples



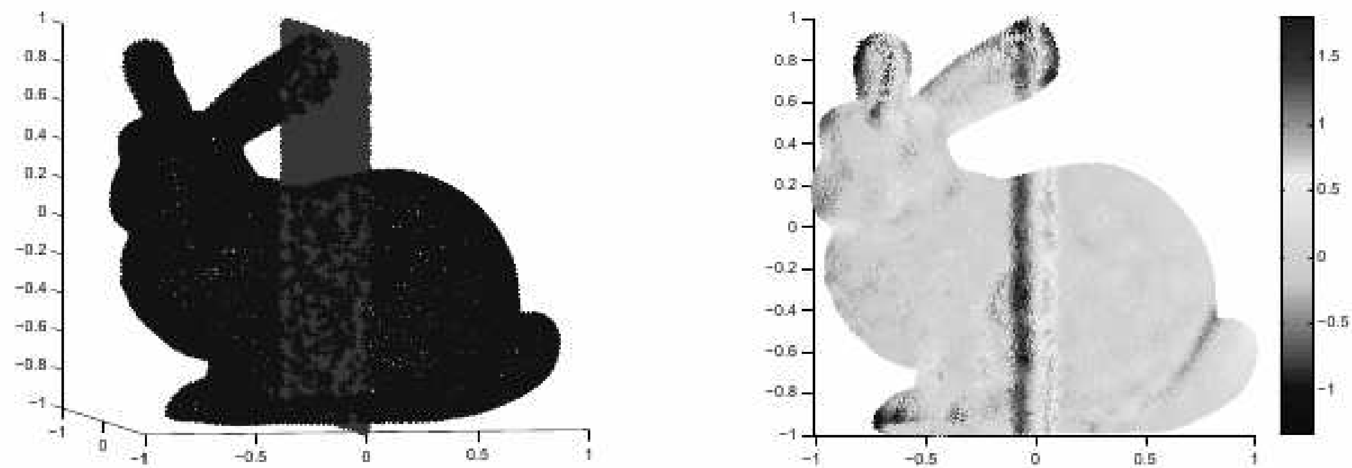


Data Domain

$L_t f$ on Ω_1, where

$$f(x_1, x_2) = (x_1+0.2)^2 + x_2^2$$

Examples



(a) Data set

(b) Values of $L_{n,t}f$ on Bunny when $f = y$.

Disclaimer: No animals were harmed during the making of this slide.

Key Point III

- Can singularity points be simply ignored?
  - After all, these points are of measure zero

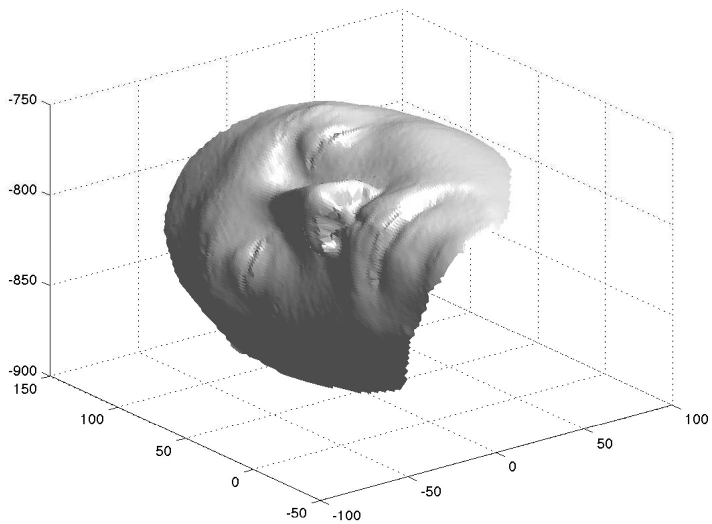
- No. At least not for singularity of codimension-one
  - Roughly, the total effect is $O(\frac{1}{\sqrt{t}}) \cdot O(\sqrt{t}) = O(1)$
  - As t tends to 0, this effect does not vanish

Key Point IV

- Recall for a boundary point x

$$L_t f(x) = -\frac{1}{\sqrt{t}} C_1 \partial_{\mathbf{n}} f(x) + o(\frac{1}{\sqrt{t}})$$

  - It can be used to compute outward-normal at boundary
  - It can also be used to compute the partial derivative of a function along outward-normal at boundary.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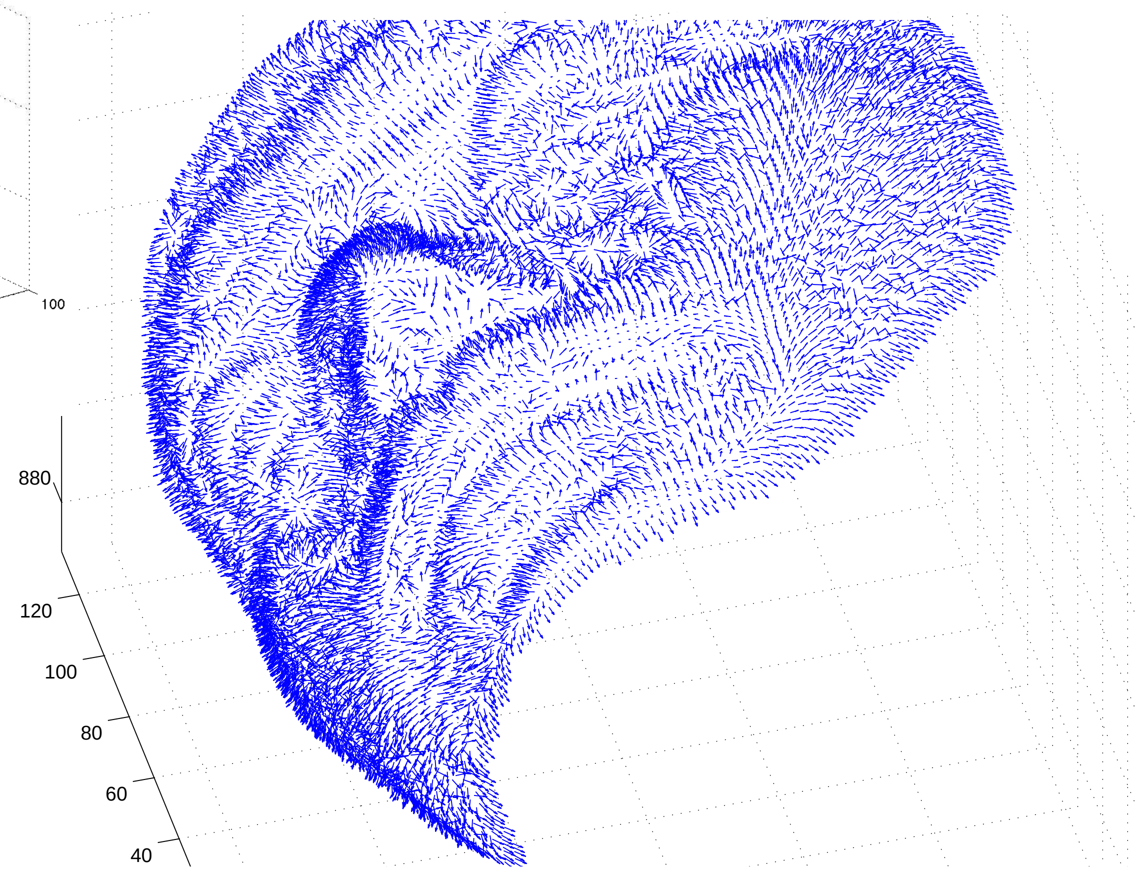

880
120
100
80
60
40

Eigen-functions

- Consider any point x at boundary singularity
- Let ϕ_t be an eigenfunction for L_t .

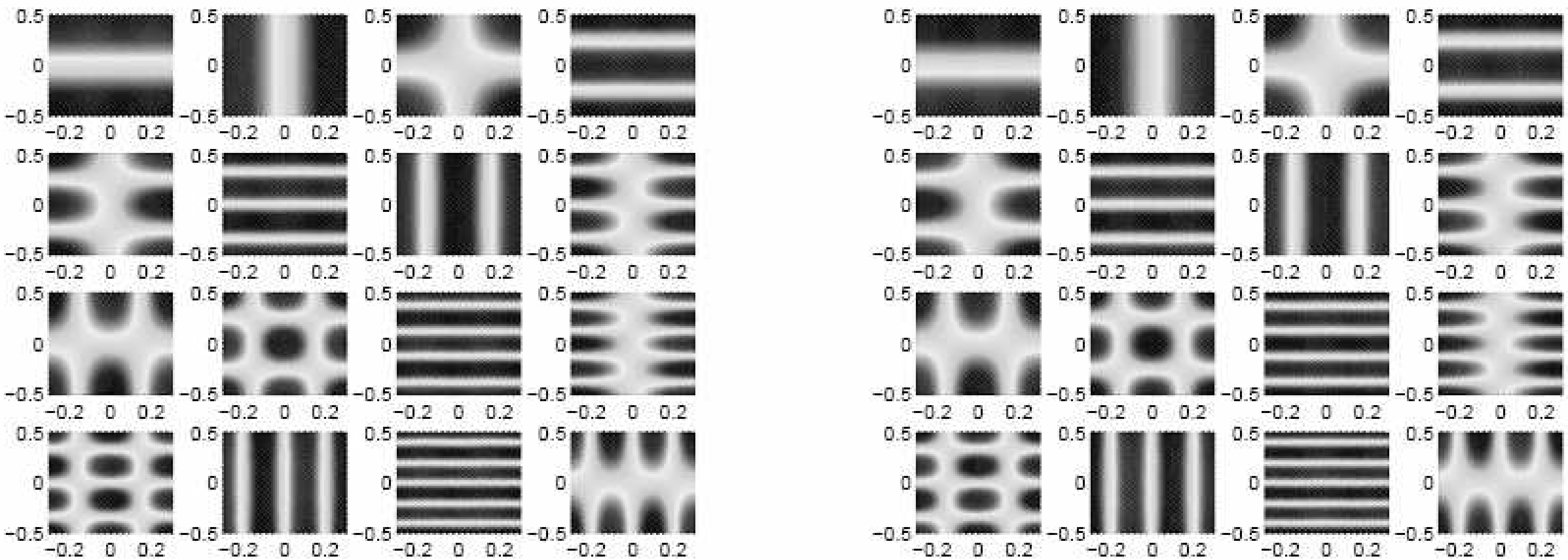
$$-\frac{1}{\sqrt{t}} \cdot C \cdot \partial_{\mathbf{n}} \phi_t(x) \approx L_t \phi_t(x) = \lambda_t \phi_t(x) < \infty$$

- As t tends to 0, if the limit of ϕ_t exists,
  - it takes on Neumann boundary condition
- Initial numerical results seem to confirm this.

Eigen-functions

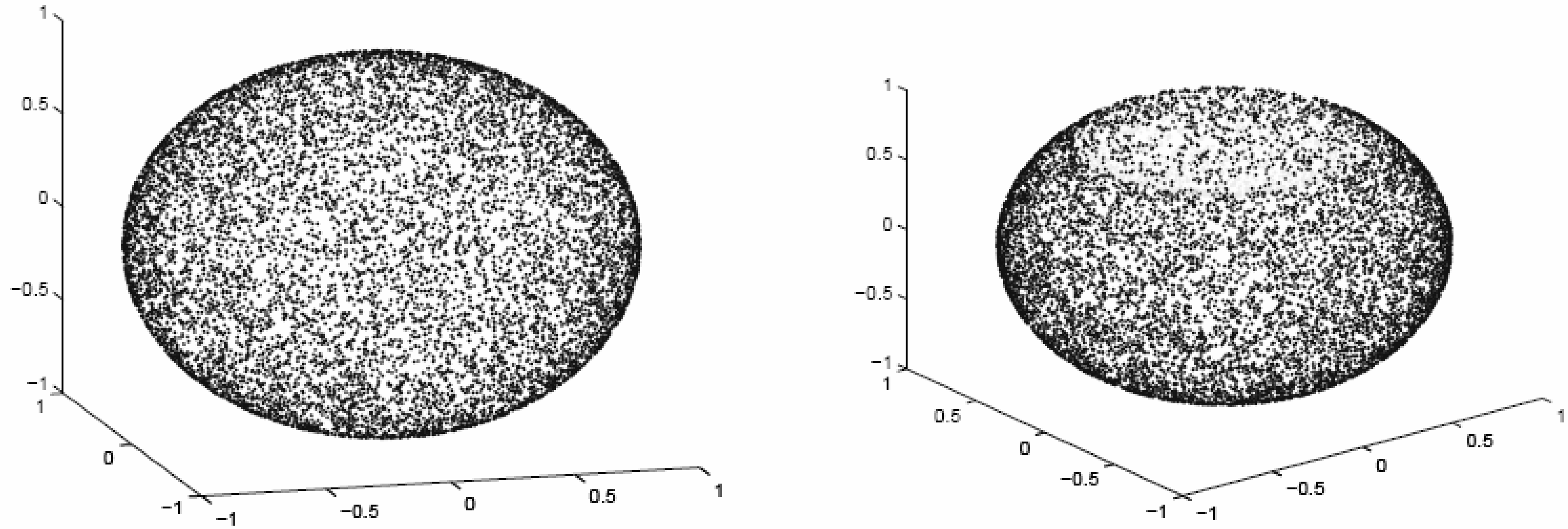
- Edge-type singularity
  - $\partial_{\mathbf{n}_1}\phi_t|_{\Omega_1}(x_0) = \partial_{\mathbf{n}_2}\phi_t|_{\Omega_2}(x_0)$
- Conjecture:
  - Eigenvalues and eigenfunctions of two isometric singular manifolds are the same.

Examples



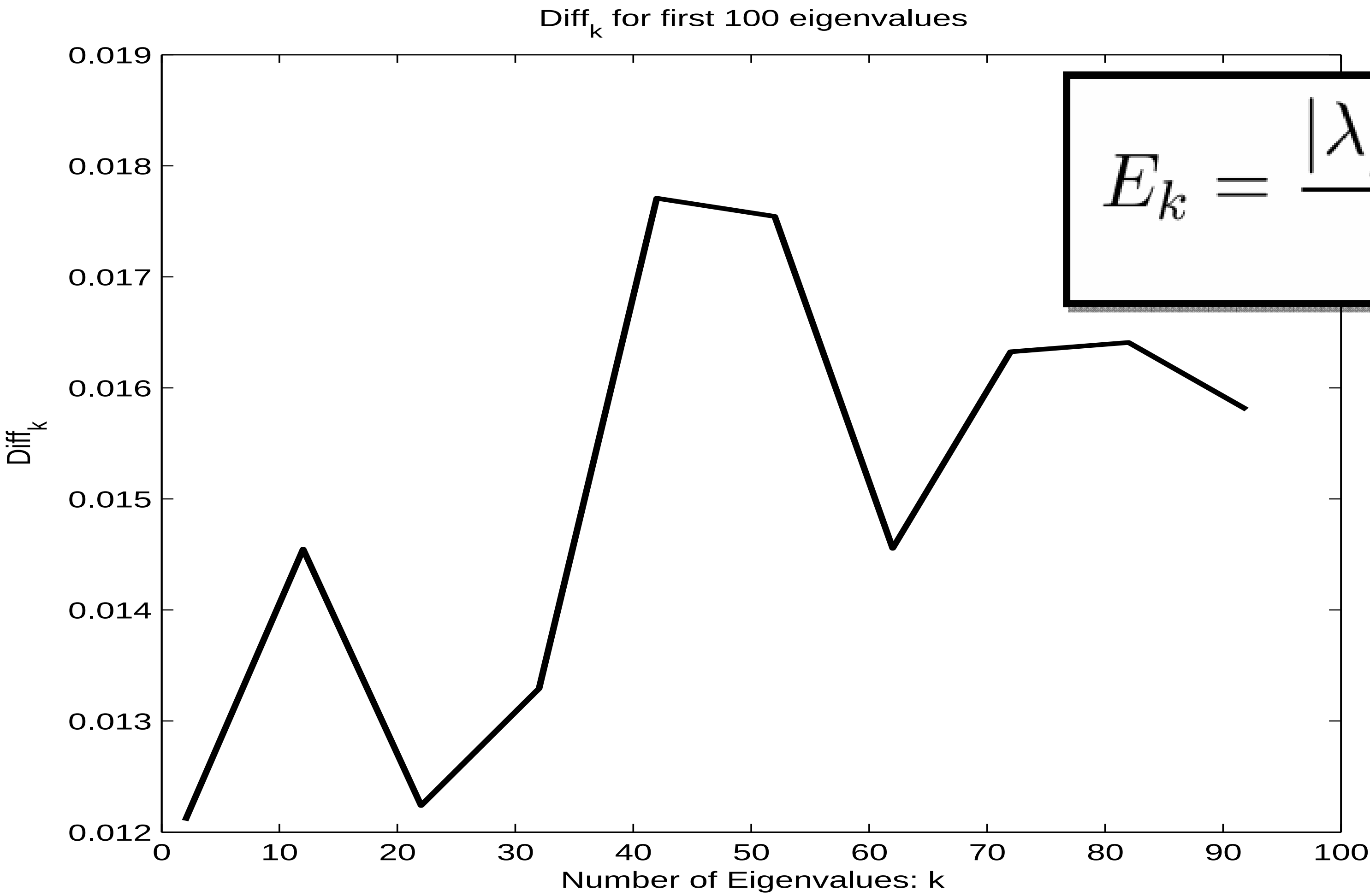
(a) Ω_1 (b) Ω_2

Figure 5: 2nd-17th eigenvectors of the graph Laplace matrices of the two manifolds Ω_1 and Ω_2



(a) S_1 (b) S_2

Figure 6: Unit sphere S_1 (left), and unit sphere with the top "sliced and flipped" S_2 (right).



$$E_k = \frac{|\lambda_k^1 - \lambda_k^2|}{|\lambda_k^1|}$$

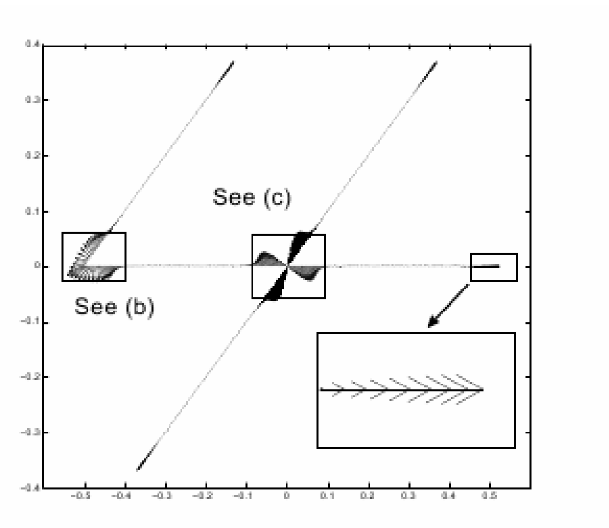
Summary and Other Discussions

- Initial study of the behavior of weighted Graph Laplacian on singular manifolds
  - Lightweight structure, geometry information it captures

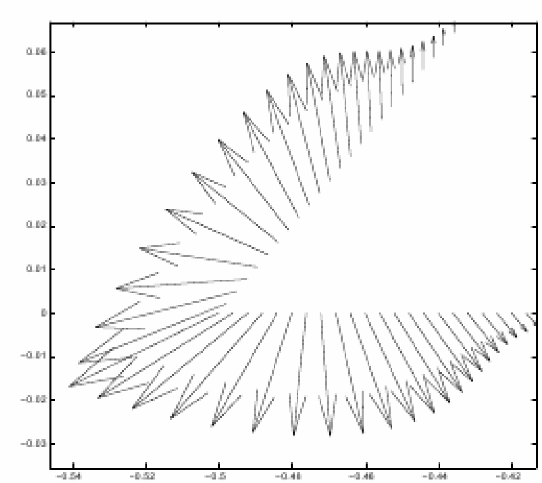
- Behavior of its eigenfunctions
- Potential applications:
  - Feature curve reconstruction for surface models from point samples
  - Better de-noising or classification algorithms ?
- Learning collection of linear subspaces ?
- Combining with stratification learning ?

Examples

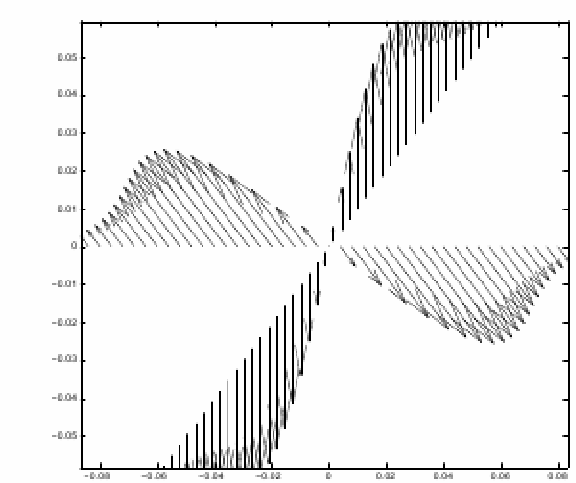
- Apply L_t to ambient space coordinate functions
  - induces a vector field



Input Data



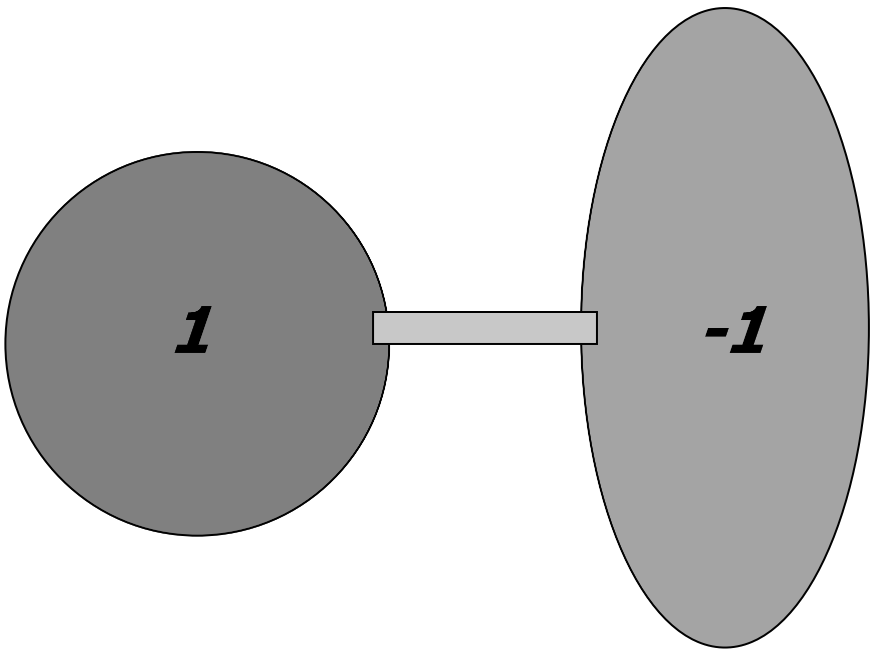
Edge-singularity



Intersectoin-singularity

Example: I

- Clustering:



- $\Delta f = 0$ if f is constant on each component
- Take Eigenfunction corresponding to 0 Eigenvalue
- Segmentation etc

Example II:

- Smoothing

- Eigenfunctions form a basis for functions on manifold
- Relation to Heat

- Levy: Laplace-beltrami eigenfunctions: Towards an algorithm that understands geometry. In *IEEE SMI, invited talk (2006)*
- Sorkine. Differential representations for mesh processing. *Computer Graphics Forum*, (2006).
- Zhang, Van Kaick, Dyer: Spectral mesh processing. *Computer Graphics Forum,* (2009).