

# Applications of the Laplacian

Justin Solomon

MIT, Spring 2017



*Review:*

# Rough Intuition: Spectral Geometry

[http://pngimg.com/upload/hammer\\_PNG3886.png](http://pngimg.com/upload/hammer_PNG3886.png)



You can learn a lot  
about a shape by  
**hitting it** (lightly)  
**with a hammer!**

*Review:*

# Rough Definition

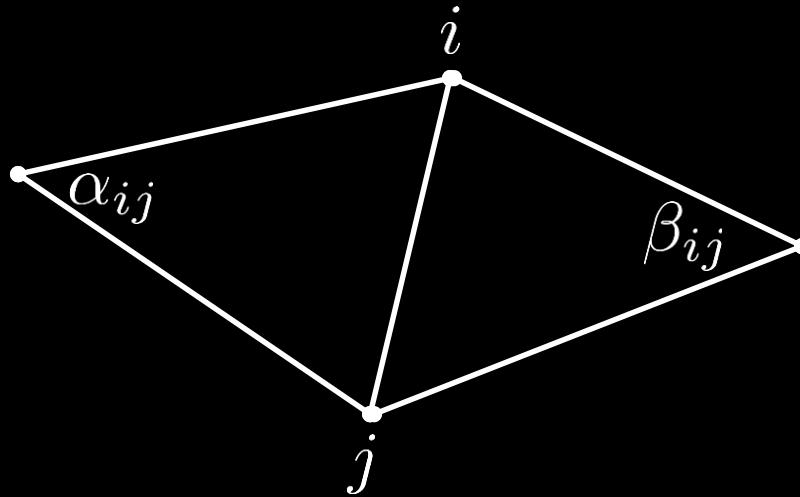
What can you learn about its shape from  
vibration frequencies and  
oscillation patterns?

$$\Delta f = \lambda f$$

*Review:*

# THE COTANGENT LAPLACIAN

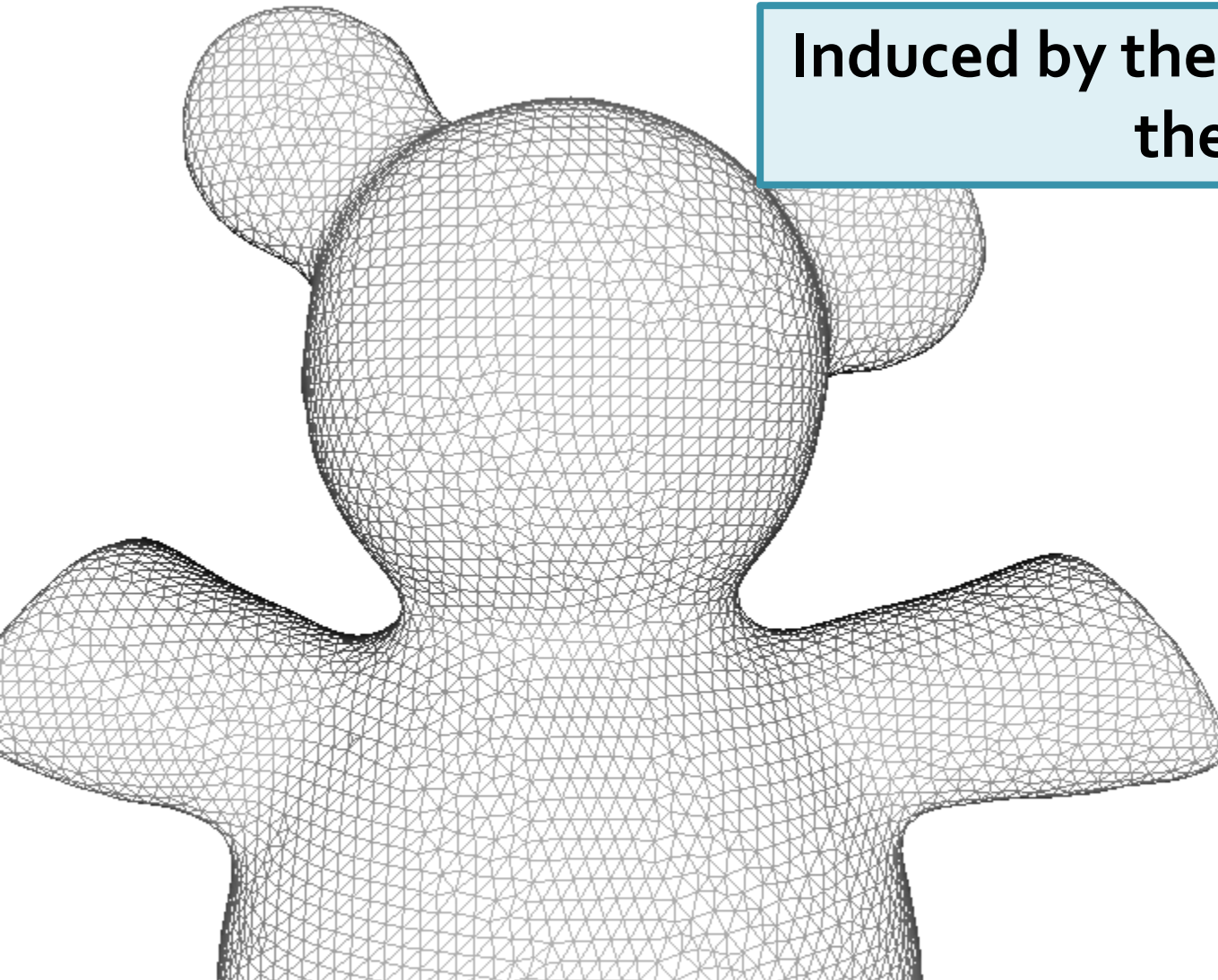
$$L_{ij} = \begin{cases} \frac{1}{2} \sum_{i \sim k} (\cot \alpha_{ik} + \cot \beta_{ik}) & \text{if } i = j \\ -\frac{1}{2} (\cot \alpha_{ij} + \cot \beta_{ij}) & \text{if } i \sim j \\ 0 & \text{otherwise} \end{cases}$$



*Key property:*

# Sparsity

Induced by the **connectivity** of the triangle mesh.



# Our Next Topic

*Discrete Laplacian operators:*

## What are they good for?

- Useful properties of the Laplacian
- Applications in graphics/shape analysis
  - Applications in machine learning

*A quick survey:  
A popular field!*

# Our Next Topic

*Discrete Laplacian operators:*

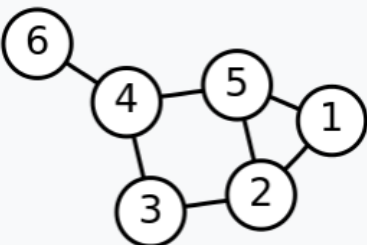
## What are they good for?

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*A quick survey:  
A popular field!*

# One Object, Many Interpretations

$$L_{vw} = A - D = \begin{cases} 1 & \text{if } v \sim w \\ -\text{degree}(v) & \text{if } v = w \\ 0 & \text{otherwise} \end{cases}$$

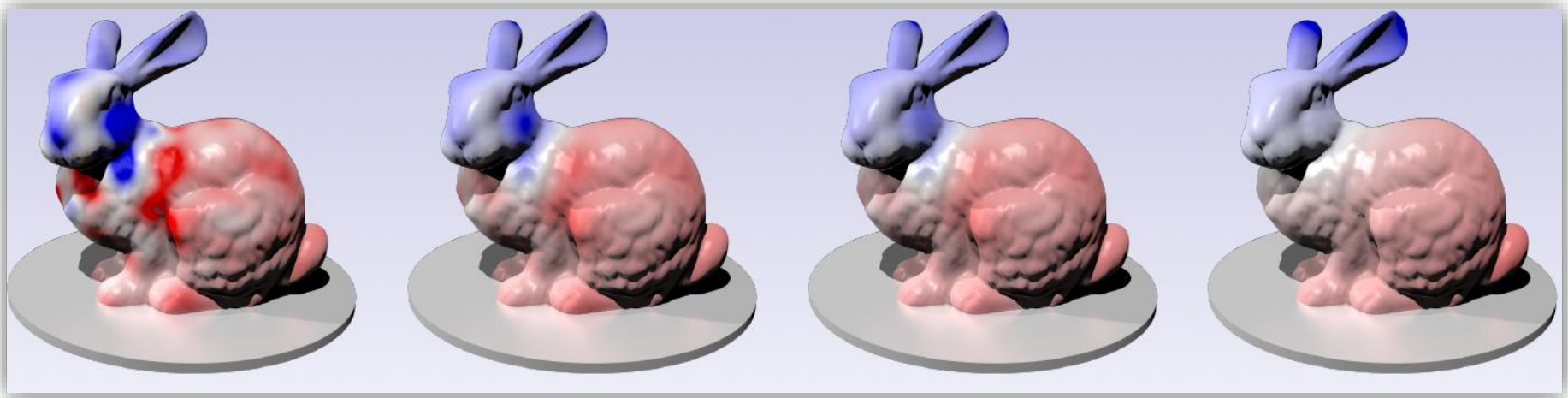
Labeled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

[https://en.wikipedia.org/wiki/Laplacian\\_matrix](https://en.wikipedia.org/wiki/Laplacian_matrix)

## Deviation from neighbors



# One Object, Many Interpretations



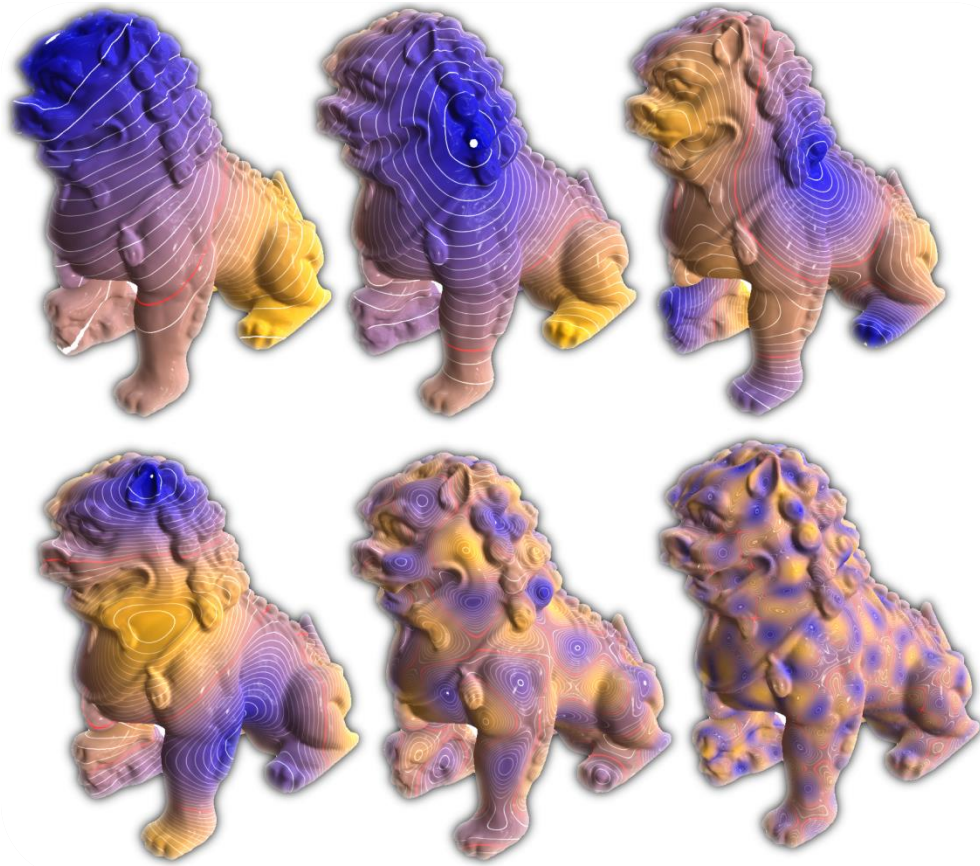
Decreasing  $E$

$$E[f] := \int_S \|\nabla f\|_2^2 dA = - \int_S f(x) \Delta f(x) dA(x)$$

Images made by E. Vouga

**Dirichlet energy: Measures smoothness**

# One Object, Many Interpretations



$$\Delta \psi_i = \lambda_i \psi_i$$

**Vibration modes of  
surface (not volume!)**

[http://alice.loria.fr/publications/papers/zoo8/ManifoldHarmonics//photo/dragon\\_mhb.png](http://alice.loria.fr/publications/papers/zoo8/ManifoldHarmonics//photo/dragon_mhb.png)

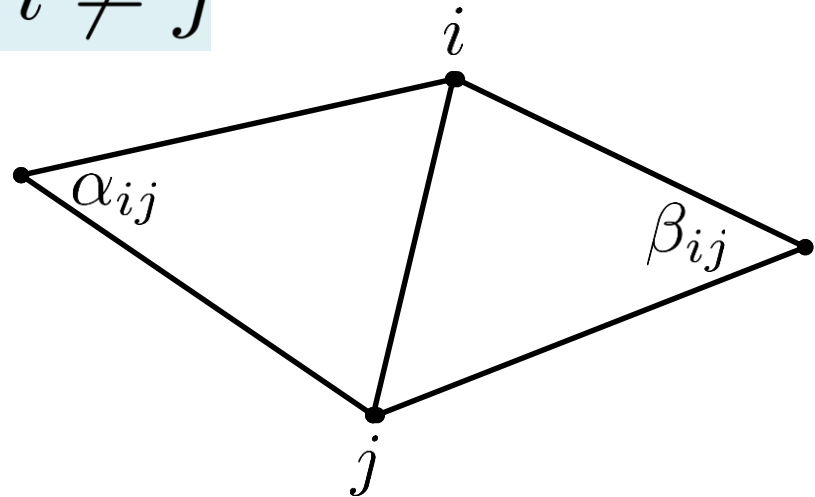
## Vibration modes

# Key Observation (in discrete case)

$$L_{ij} = \begin{cases} \frac{1}{2} \sum_{i \sim k} (\cot \alpha_{ik} + \cot \beta_{ik}) & \text{if } i = j \\ -\frac{1}{2} (\cot \alpha_{ij} + \cot \beta_{ij}) & \text{if } i \sim j \\ 0 & \text{otherwise} \end{cases}$$

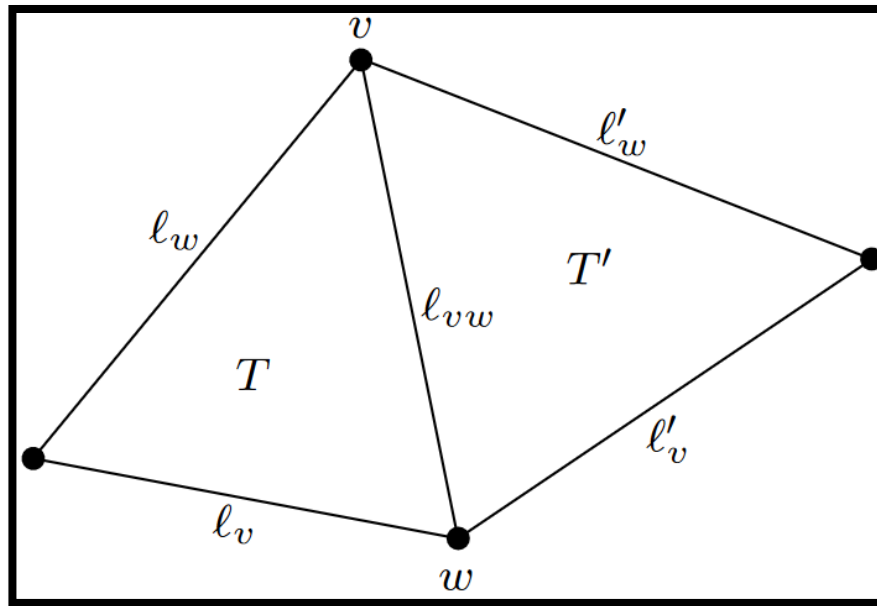
$$M_{ij} = \begin{cases} \frac{\text{one-ring area}}{6} & \text{if } i = j \\ \frac{\text{adjacent area}}{12} & \text{if } i \neq j \end{cases}$$

Can be written in  
terms of angles  
and areas!



# After (More) Trigonometry

$$L_{vw} = \frac{1}{8} \begin{cases} -\sum_{u \sim v} L_{uv} & \text{when } v = w \\ \mu(T)^{-1}(\ell_{vw}^2 - \ell_v^2 - \ell_w^2) & \text{when } v \sim w \\ +\mu(T')^{-1}(\ell_{vw}^2 - \ell'_v{}^2 - \ell'_w{}^2) & \\ 0 & \text{otherwise} \end{cases}$$



Image/formula in "Functional Characterization of Intrinsic and Extrinsic Geometry," TOG 2017 (Corman et al.)

**Laplacian only depends on edge lengths**

# Isometry

[ahy-som-i-tree]:

Bending without stretching.



# Lots of Interpretations

Global isometry

$$d_1(x, y) = d_2(f(x), f(y))$$

Local isometry

$$\begin{aligned} g_1 &= f^* g_2 \\ g_1(v, w) &= g_2(f_* v, f_* w) \end{aligned}$$

# Intrinsic Techniques



<http://www.revedreams.com/crochet/yarncrochet/nonorientable-crochet/>

## Isometry invariant



# Isometry Invariance: Hope





# Isometry Invariance: Reality

"Rigidity"



<http://www.4tnz.com/content/got-toilet-paper>

**Few shapes *can* deform isometrically**

# Isometry Invariance: Reality

Behavior for  
approximate isometry  
is important, too!

<http://www.4tnz.com/content/got-toilet-paper>

Few shapes *can* deform isometrically

# Useful Fact

Graphical Models 74 (2012) 121–129



Contents lists available at SciVerse ScienceDirect

## Graphical Models

journal homepage: [www.elsevier.com/locate/gmod](http://www.elsevier.com/locate/gmod)



### Discrete heat kernel determines discrete Riemannian metric

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#### ARTICLE INFO

##### Article history:

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Discrete heat kernel

Discrete Riemannian metric

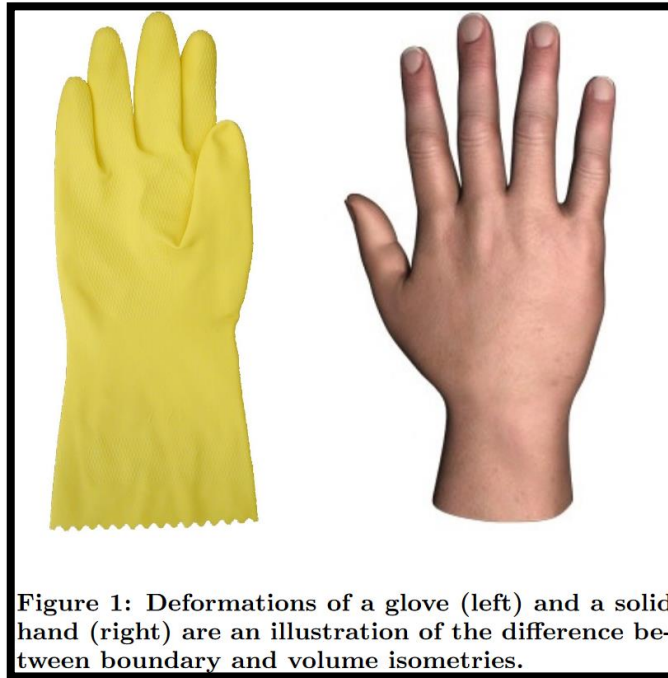
Laplace–Beltrami operator

Legendre duality principle

#### ABSTRACT

The Laplace–Beltrami operator of a smooth Riemannian manifold is determined by the Riemannian metric. Conversely, the heat kernel constructed from the eigenvalues and eigenfunctions of the Laplace–Beltrami operator determines the Riemannian metric. This work proves the analogy on Euclidean polyhedral surfaces (triangle meshes), that the discrete heat kernel and the discrete Riemannian metric (unique up to a scaling) are mutually determined by each other. Given a Euclidean polyhedral surface, its Riemannian metric is represented as edge lengths, satisfying triangle inequalities on all faces. The Laplace–Beltrami operator is formulated using the cotangent formula, where the edge weight is defined as the sum of the cotangent of angles against the edge. We prove that the edge

# Beware



But calculations  
on a volume are  
expensive!

*Image from:* Raviv et al. "Volumetric Heat Kernel Signatures." 3DOR 2010.

# Not the same.

# Why Study the Laplacian?

- **Encodes intrinsic geometry**

Edge lengths on triangle mesh, Riemannian metric on manifold

- **Multi-scale**

Filter based on frequency

- **Geometry through linear algebra**

Linear/eigenvalue problems, sparse positive definite matrices

- **Connection to physics**

Heat equation, wave equation, vibration, ...

# Our Next Topic

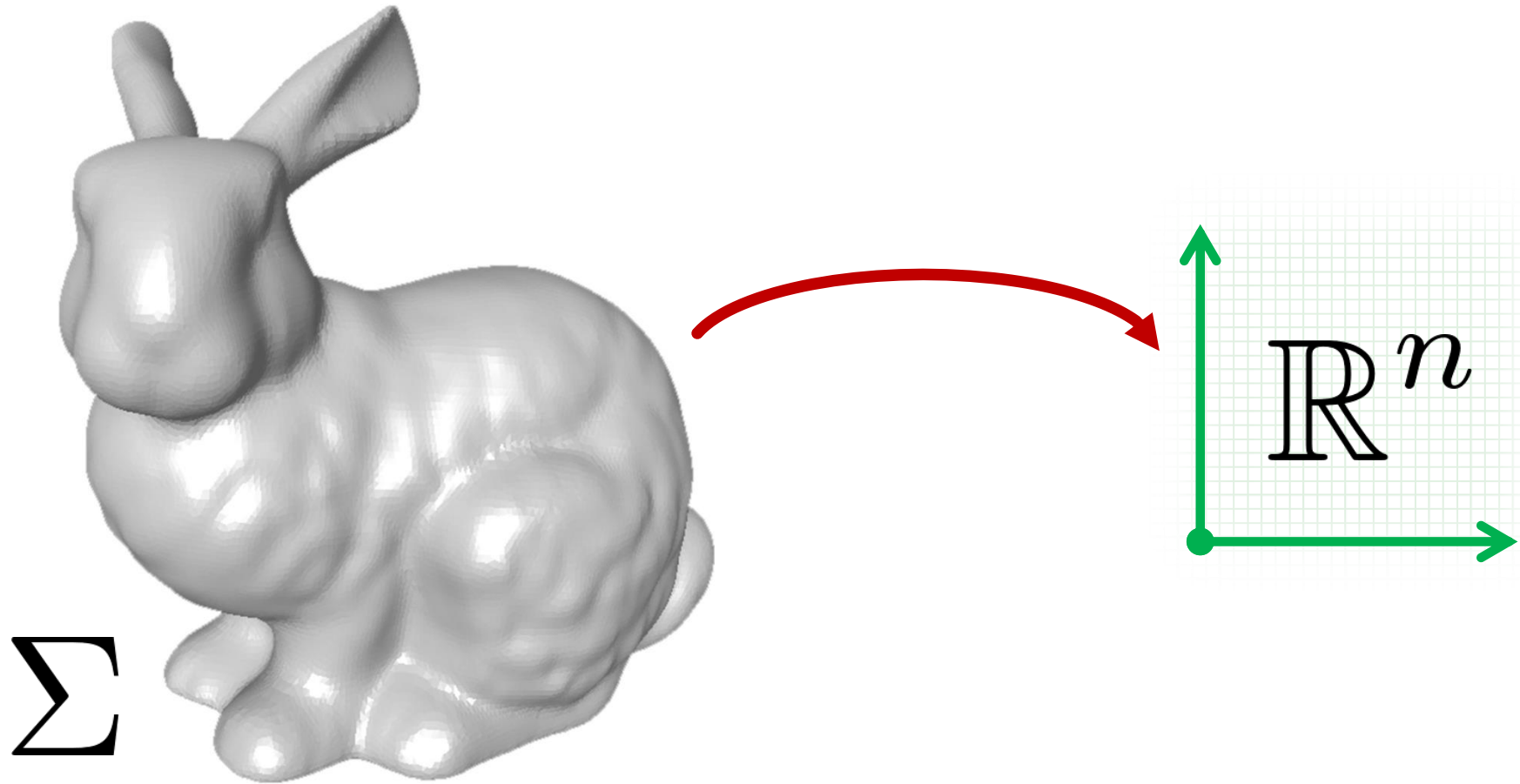
*Discrete Laplacian operators:*

## What are they good for?

- Useful properties of the Laplacian
- Applications in graphics/shape analysis
  - Applications in machine learning

*A quick survey:  
A popular field!*

# Example Task: Shape Descriptors



[http://liris.cnrs.fr/meshbenchmark/images/fig\\_attacks.jpg](http://liris.cnrs.fr/meshbenchmark/images/fig_attacks.jpg)

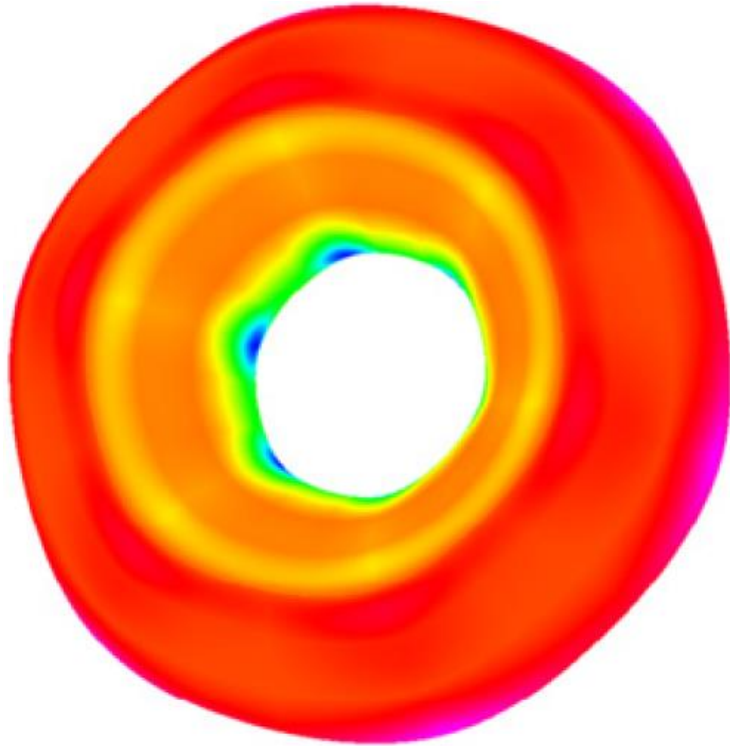
**Pointwise quantity**

# Descriptor Tasks

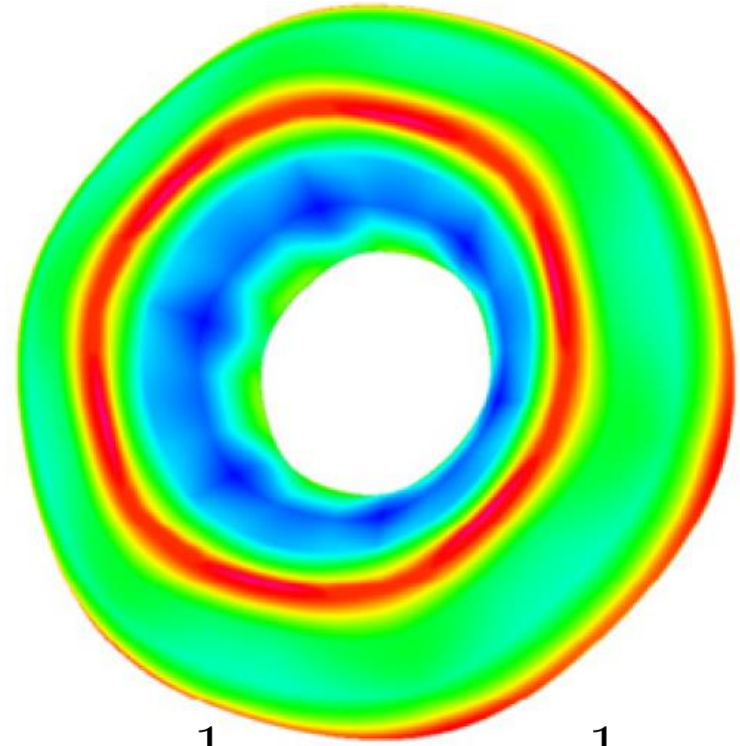
- **Characterize local geometry**  
Feature/anomaly detection
- **Describe point's role on surface**  
Symmetry detection, correspondence



# Descriptors We've Seen Before



$$K := \kappa_1 \kappa_2 = \det \mathbb{I}$$



$$H := \frac{1}{2}(\kappa_1 + \kappa_2) = \frac{1}{2} \operatorname{tr} \mathbb{I}$$

<http://www.sciencedirect.com/science/article/pii/S0010448510001983>

## Gaussian and mean curvature

# Desirable Properties

- **Distinguishing**

Provides useful information about a point

- **Stable**

Numerically and geometrically

- **Intrinsic**

No dependence on embedding

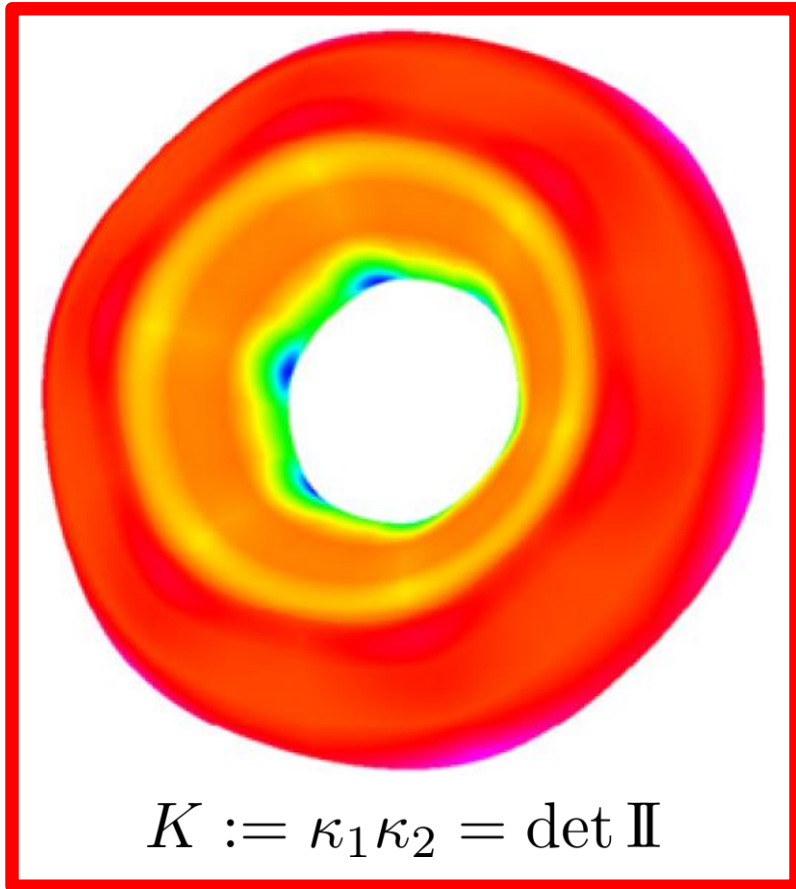
*Sometimes  
undesirable!*

# Intrinsic Descriptors

*Invariant under*

- Rigid motion
- Bending without stretching

# Intrinsic Descriptor



**Theorema Egregium**  
("Totally Awesome  
Theorem"):  
**Gaussian curvature**  
is **intrinsic**.

<http://www.sciencedirect.com/science/article/pii/S0010448510001983>

## Gaussian curvature

# End of the Story?

*Noisy!*

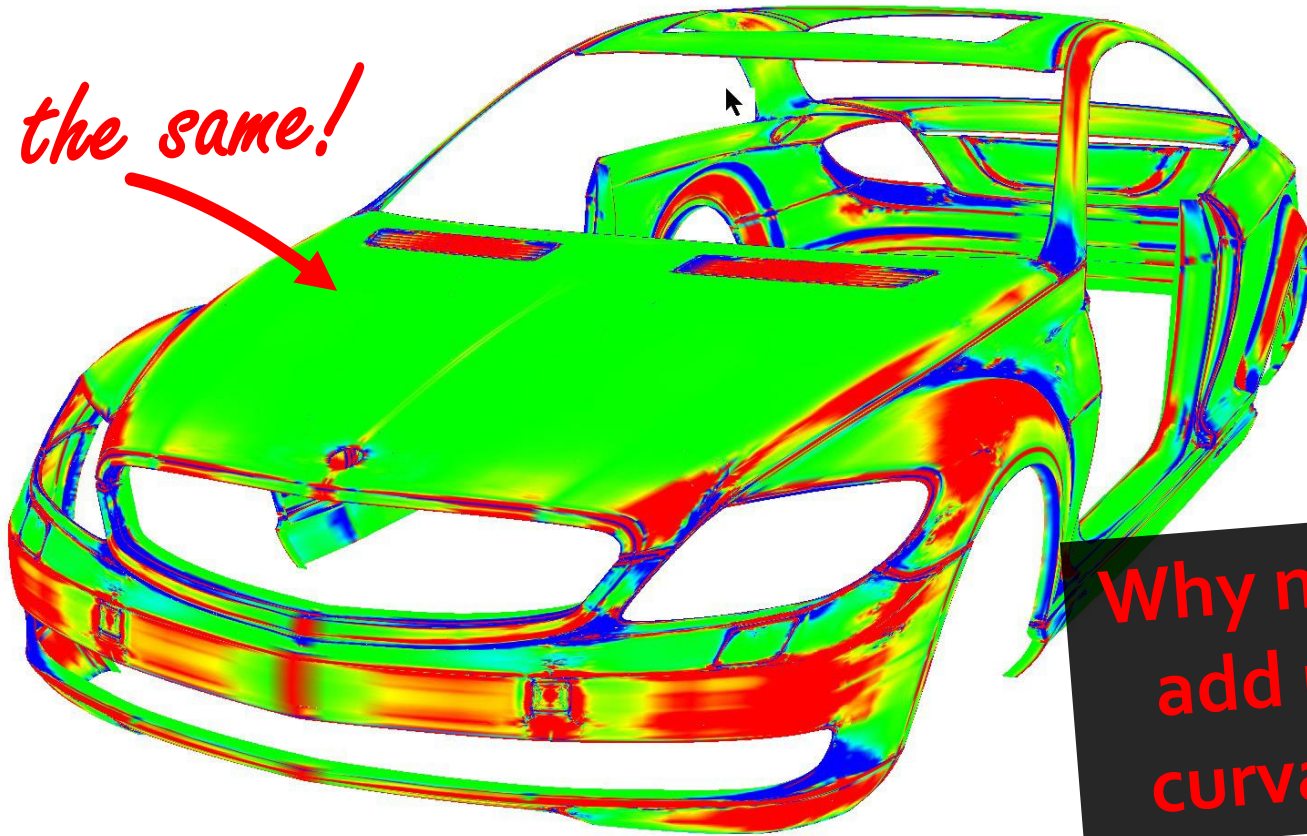


$$K = \kappa_1 \kappa_2$$

**Second derivative quantity**

# End of the Story?

*Looks the same!*



Why not just  
add mean  
curvature?

<http://www.integrityware.com/images/MercedesGaussianCurvature.jpg>

# Non-unique

# Desirable Properties

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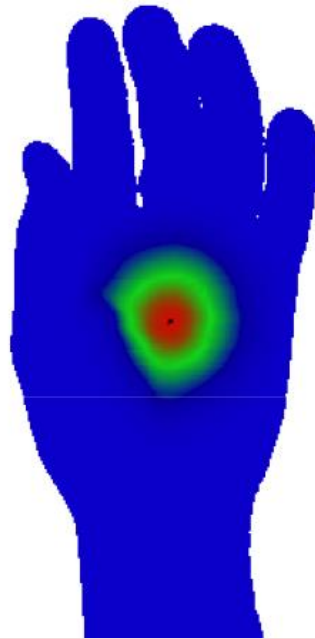
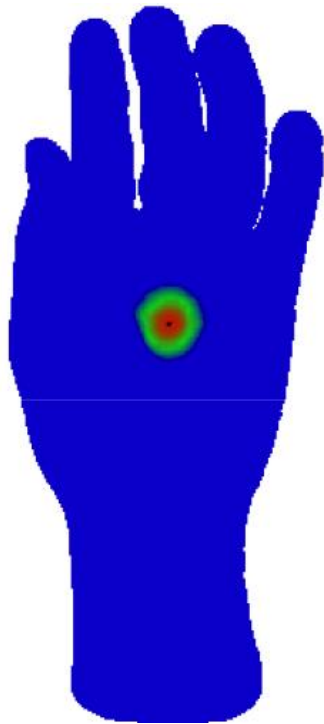
**Incorporates neighborhood information** in an intrinsic fashion

**Stable** under small deformation

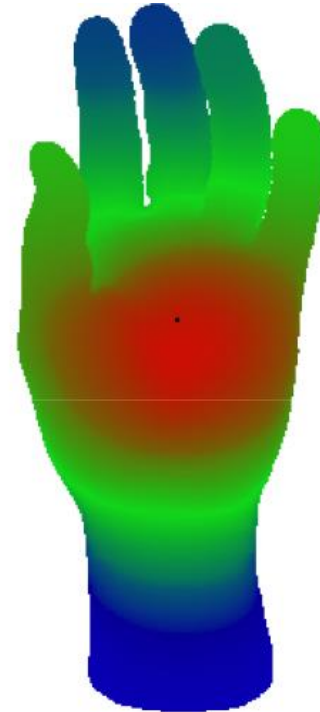


*Recall:*

# Connection to Physics



$$\frac{\partial u}{\partial t} = -\Delta u$$



[http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11\\_shape\\_matching.pdf](http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf)

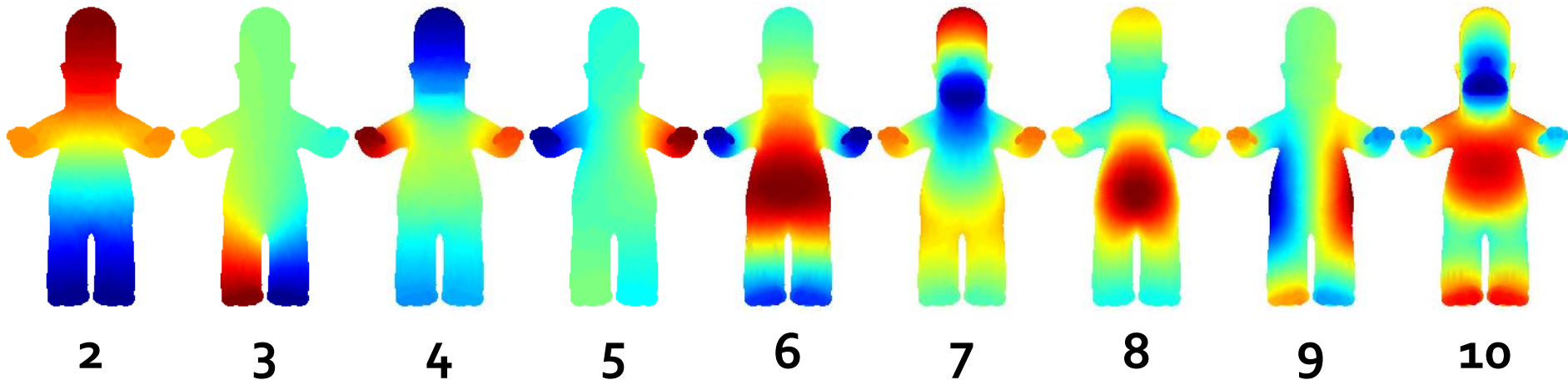
## Heat equation



# Intrinsic Observation

Heat diffusion patterns are not affected if you bend a surface.

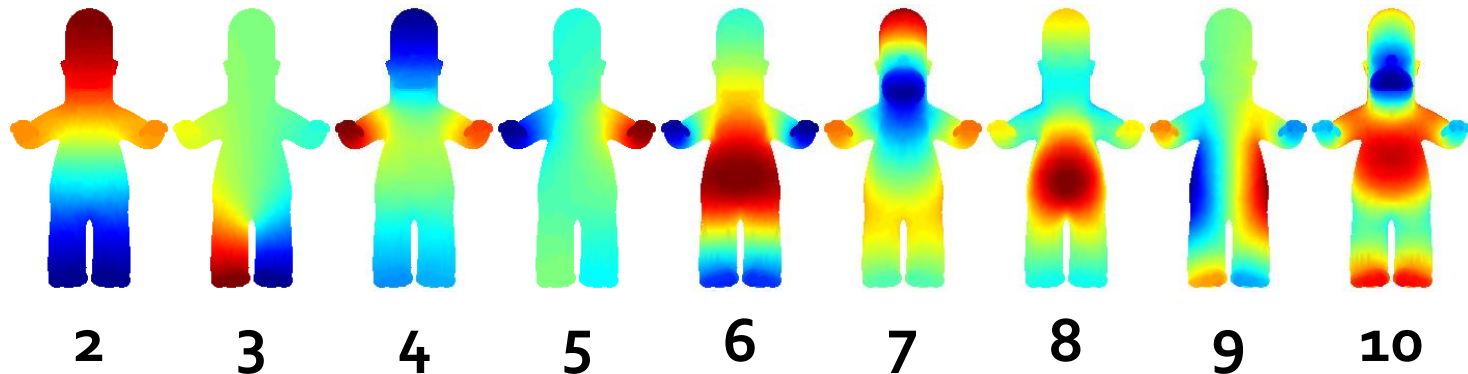
# Global Point Signature



$$\text{GPS}(p) := \left( -\frac{1}{\sqrt{\lambda_1}} \phi_1(p), -\frac{1}{\sqrt{\lambda_2}} \phi_2(p), -\frac{1}{\sqrt{\lambda_3}} \phi_3(p), \dots \right)$$

“Laplace-Beltrami Eigenfunctions for Deformation Invariant Shape Representation”  
Rustamov, SGP 2007

# Global Point Signature

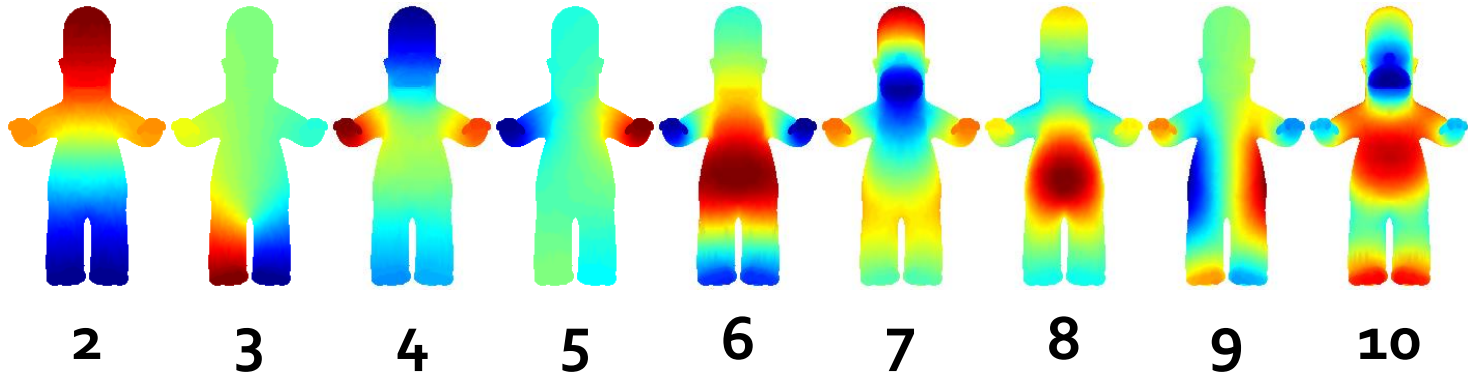


$$\text{GPS}(p) := \left( -\frac{1}{\sqrt{\lambda_1}} \phi_1(p), -\frac{1}{\sqrt{\lambda_2}} \phi_2(p), -\frac{1}{\sqrt{\lambda_3}} \phi_3(p), \dots \right)$$

If surface does not **self-intersect**, neither does the GPS embedding.

Proof: Laplacian eigenfunctions span  $L^2(\Sigma)$ ; if  $\text{GPS}(p) = \text{GPS}(q)$ , then all functions on  $\Sigma$  would be equal at  $p$  and  $q$ .

# Global Point Signature



$$\text{GPS}(p) := \left( -\frac{1}{\sqrt{\lambda_1}} \phi_1(p), -\frac{1}{\sqrt{\lambda_2}} \phi_2(p), -\frac{1}{\sqrt{\lambda_3}} \phi_3(p), \dots \right)$$

**GPS is isometry-invariant.**

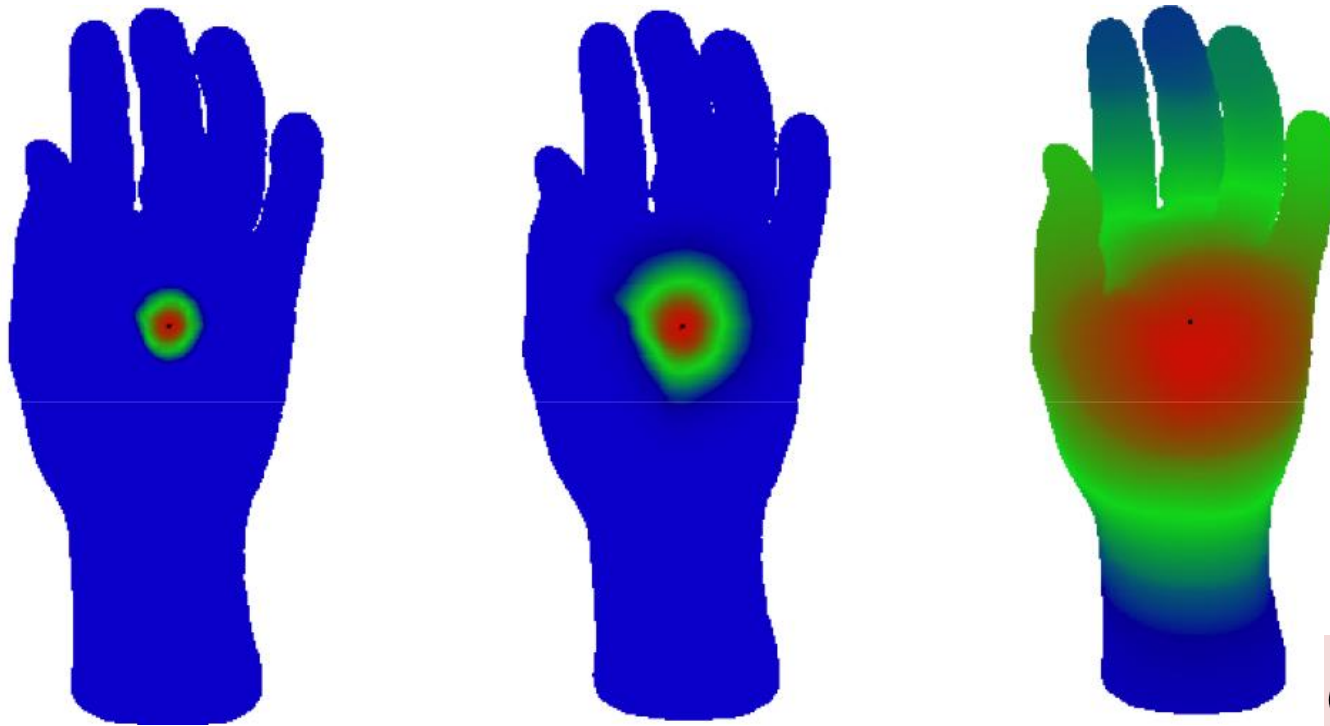
Proof: Comes from the Laplacian.

# Drawbacks of GPS

- Assumes **unique**  $\lambda$ 's
- Potential for eigenfunction “**switching**”
- **Nonlocal** feature

*New idea:*

# PDE Applications of the Laplacian



$$\frac{\partial u}{\partial t} = -\Delta u$$

[http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11\\_shape\\_matching.pdf](http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf)

## Heat equation

# PDE Applications of the Laplacian




$$\frac{\partial^2 u}{\partial t^2} = -i\Delta u$$

Image courtesy G. Peyré

## Wave equation

# PDE Applications of the Laplacian



Use this behavior to  
characterize shape.

$$\frac{\partial^2 u}{\partial t^2} = -i\Delta u$$

Image courtesy G. Peyré

## Wave equation



# Solutions in the LB Basis

$$\frac{\partial u}{\partial t} = -\Delta u$$

**Heat equation**

$$u = \sum_{n=0}^{\infty} a_n e^{-\lambda_n t} \phi_n(x)$$

$$a_n = \int_{\Sigma} u_0(x) \cdot \phi_n(x) dA$$

# Heat Kernel Signature (HKS)

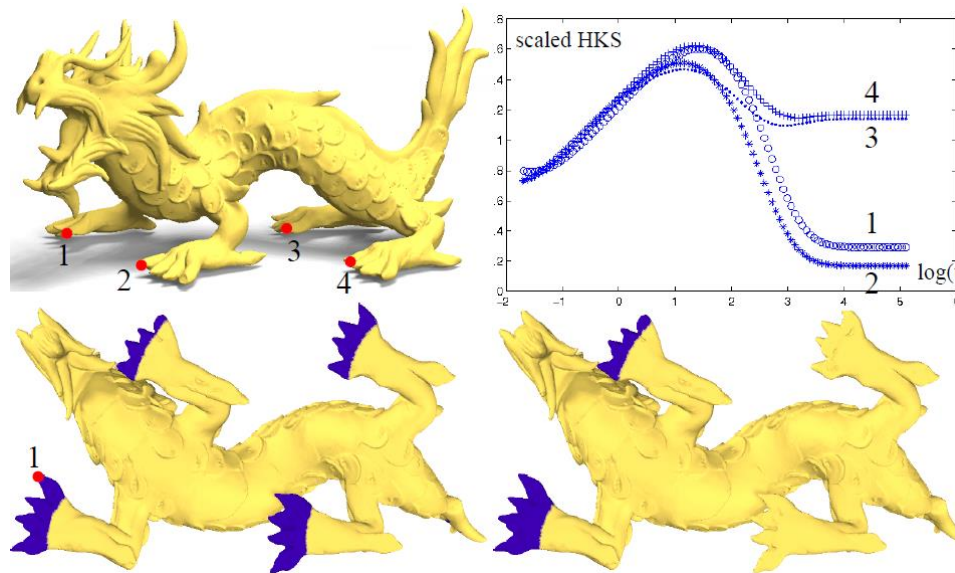
$$k_t(x, x) = \sum_{n=0}^{\infty} e^{-\lambda_n t} \phi_n(x)^2$$

Continuous function of  $t \in [0, \infty)$

**How much heat  
diffuses from  $x$  to  
itself in time  $t$ ?**

# Heat Kernel Signature (HKS)

$$k_t(x, x) = \sum_{n=0}^{\infty} e^{-\lambda_n t} \phi_n(x)^2$$



“A concise and provably informative multi-scale signature based on heat diffusion”  
Sun, Ovsjanikov, and Guibas; SGP 2009

# Heat Kernel Signature (HKS)

$$k_t(x, x) = \sum_{n=0}^{\infty} e^{-\lambda_n t} \phi_n(x)^2$$

**Good properties:**

- Isometry-invariant
- Multiscale
- Not subject to switching
- Easy to compute
- Related to curvature at small scales

# Heat Kernel Signature (HKS)

$$k_t(x, x) = \sum_{n=0}^{\infty} e^{-\lambda_n t} \phi_n(x)^2$$

## Bad properties:

- Issues remain with repeated eigenvalues
- Theoretical guarantees require (near-)isometry

# Wave Kernel Signature (WKS)

$$\text{WKS}(E, x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\psi_E(x, t)|^2 dt = \sum_{n=0}^{\infty} \phi_n(x)^2 f_E(\lambda_n)^2$$

**Initial energy  
distribution**



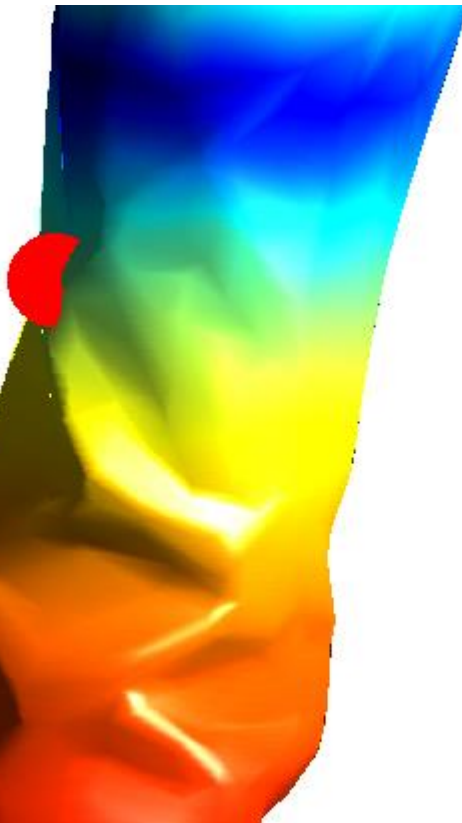
**Average probability over  
time that particle is at x.**



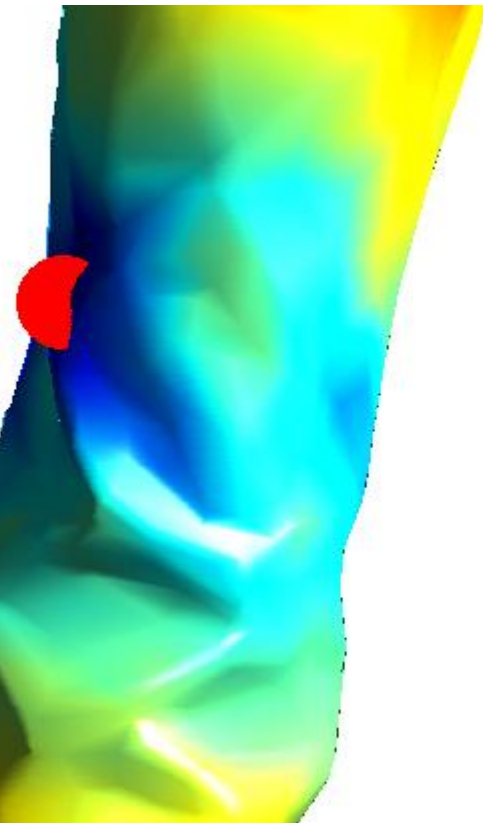
“The Wave Kernel Signature: A Quantum Mechanical Approach to Shape Analysis”  
Aubry, Schlickewei, and Cremers; ICCV Workshops 2012

# Wave Kernel Signature (WKS)

$$\text{WKS}(E, x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\psi_E(x, t)|^2 dt = \sum_{n=0}^{\infty} \phi_n(x)^2 f_E(\lambda_n)^2$$



HKS



WKS

# Wave Kernel Signature (WKS)

$$\text{WKS}(E, x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\psi_E(x, t)|^2 dt = \sum_{n=0}^{\infty} \phi_n(x)^2 f_E(\lambda_n)^2$$

## Good properties:

- [Similar to HKS]
- Localized in frequency
- Stable under some non-isometric deformation
- Some multi-scale properties



# Wave Kernel Signature (WKS)

$$\text{WKS}(E, x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\psi_E(x, t)|^2 dt = \sum_{n=0}^{\infty} \phi_n(x)^2 f_E(\lambda_n)^2$$

**Bad properties:**

- [Similar to HKS]
- Can filter out *large*-scale features

# Many Others

Lots of **spectral descriptors** in  
terms of Laplacian  
eigenstructure.

# Combination with Machine Learning

$$p(x) = \sum_k f(\lambda_k) \phi_k^2(x)$$

Learn  $f$  rather than defining it

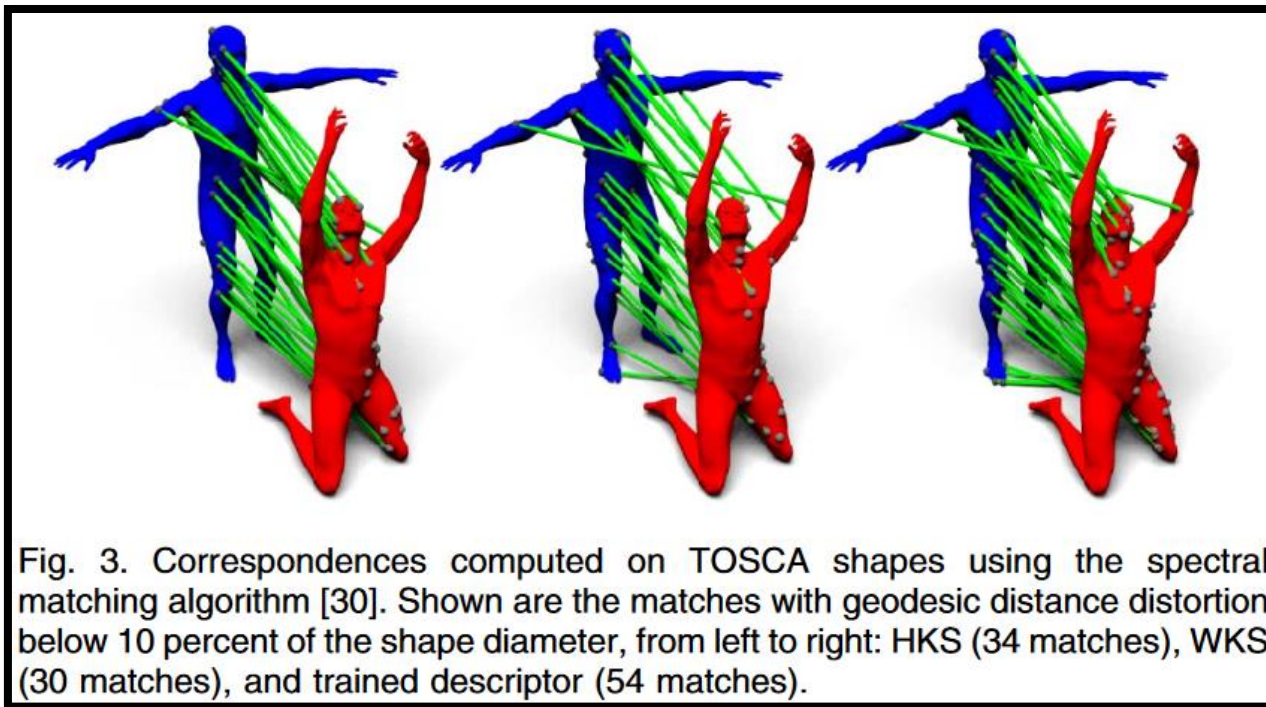


Fig. 3. Correspondences computed on TOSCA shapes using the spectral matching algorithm [30]. Shown are the matches with geodesic distance distortion below 10 percent of the shape diameter, from left to right: HKS (34 matches), WKS (30 matches), and trained descriptor (54 matches).

Learning Spectral Descriptors for Deformable Shape Correspondence

Litman and Bronstein; PAMI 2014

# Application: Feature Extraction

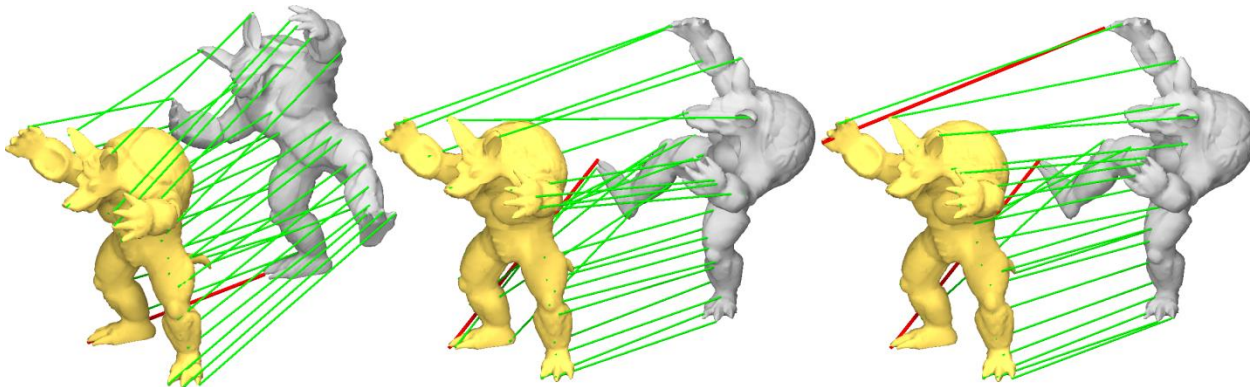
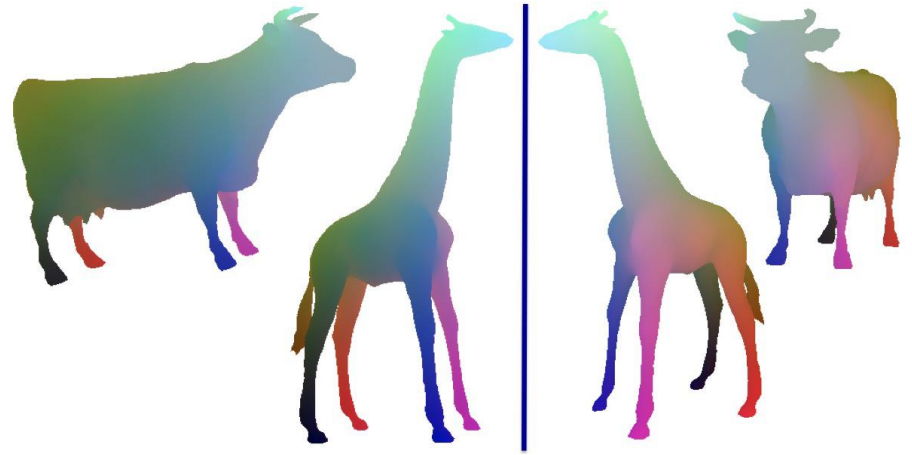
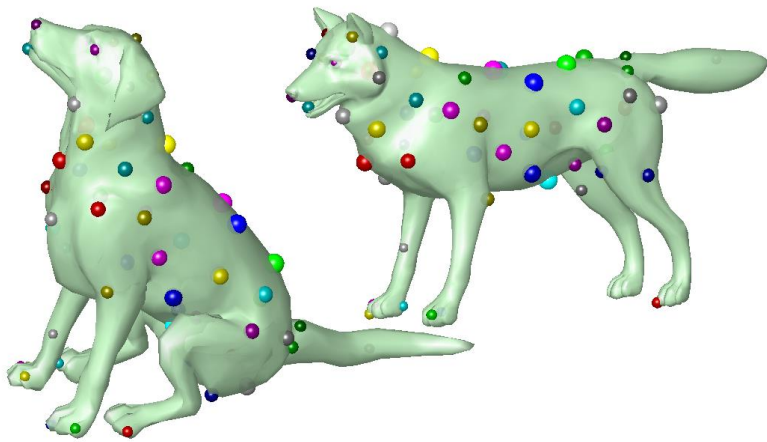


Maxima of  $k_t(x, x)$  over  $x$  for large  $t$ .

A Concise and Provably Informative Multi-Scale Signature Based on Heat Diffusion  
Sun, Ovsjanikov, and Guibas; SGP 2009

**Feature points**

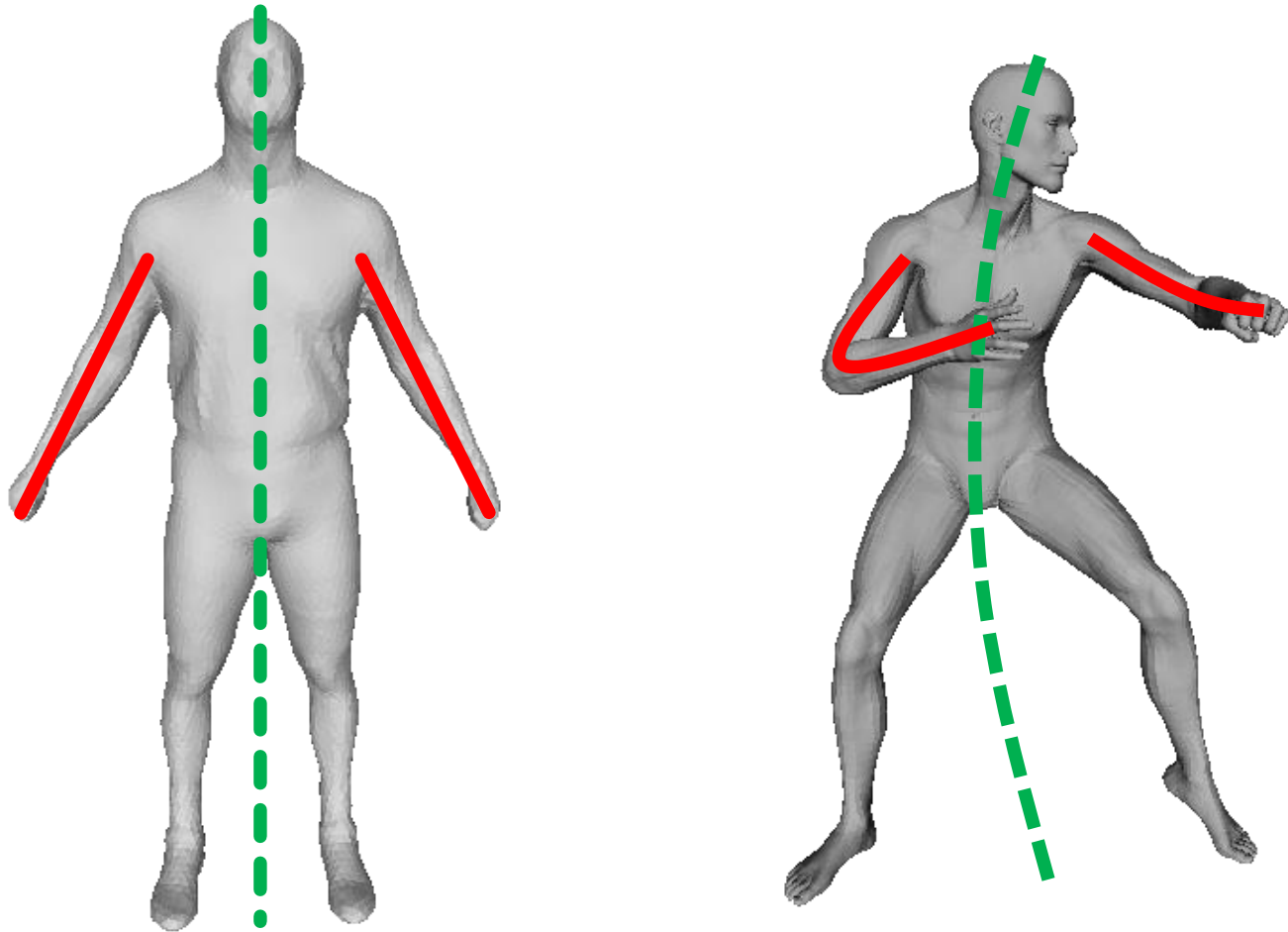
# Preview: Correspondence



# Descriptor Matching

Simply match **closest points** in  
descriptor space.

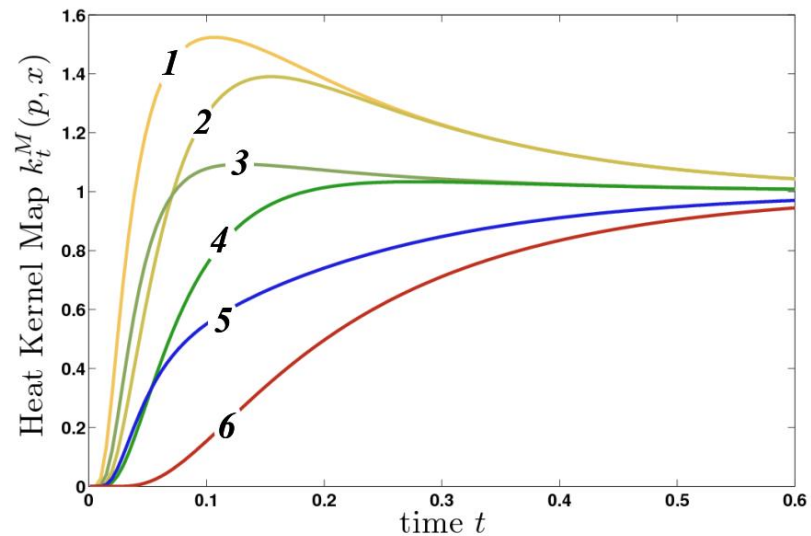
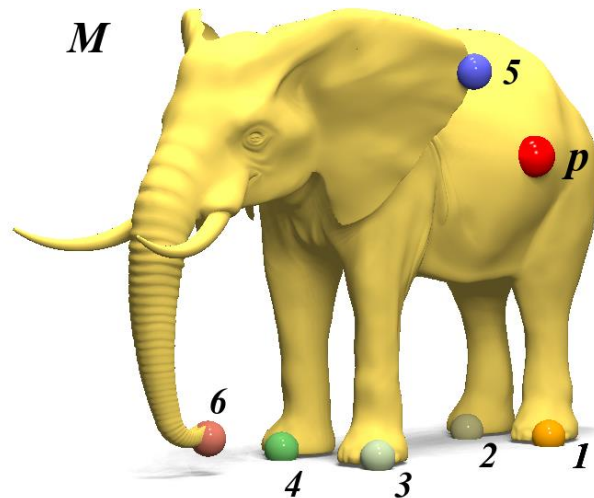
# Descriptor Matching Problem



Symmetry



# Heat Kernel Map



$$\text{HKM}_p(x, t) := k_t(p, x)$$

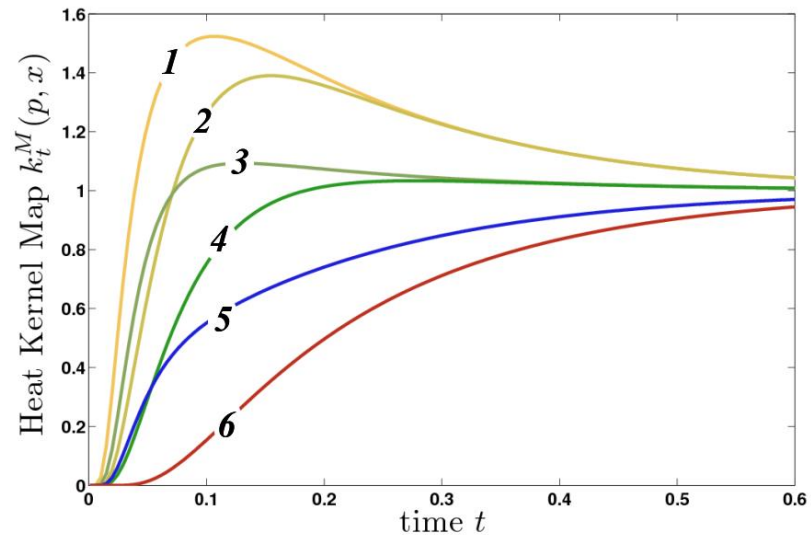
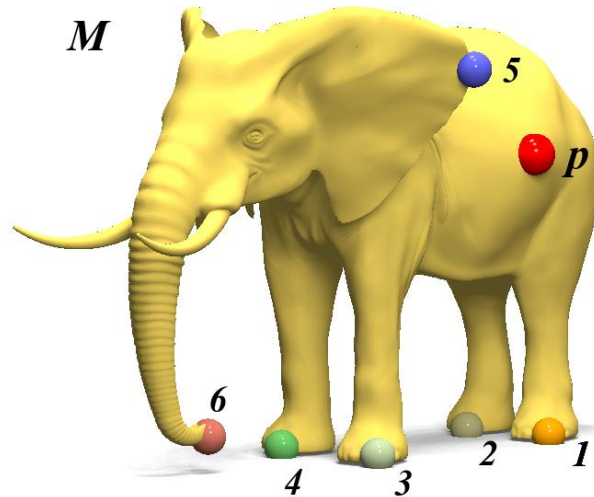
How much heat diffuses from  $p$  to  $x$  in time  $t$ ?

One Point Isometric Matching with the Heat Kernel

Ovsjanikov et al. 2010



# Heat Kernel Map



$$\text{HKM}_p(x, t) := k_t(p, x)$$

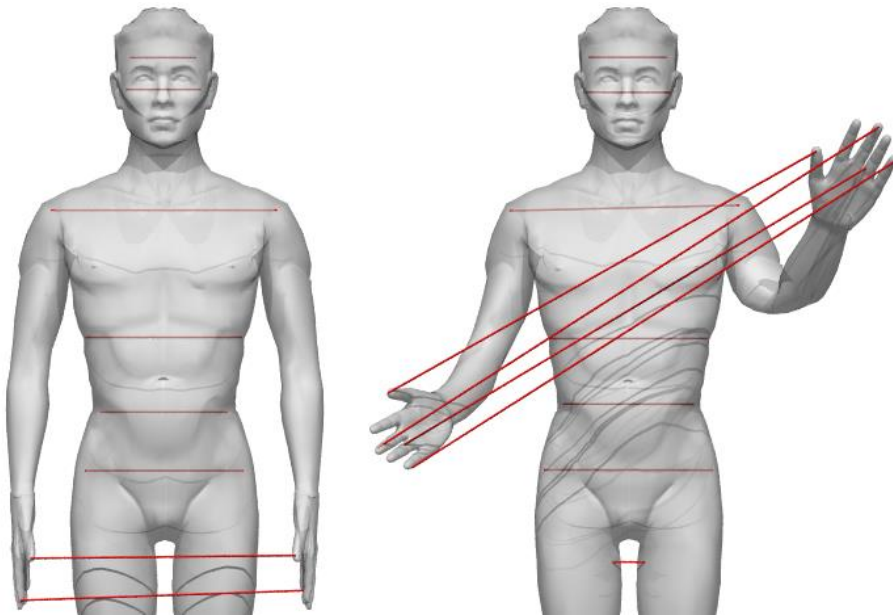
**Theorem:** Only have to match one point!

One Point Isometric Matching with the Heat Kernel

Ovsjanikov et al. 2010

*KNN*

# Self-Map: Symmetry



Intrinsic **symmetries**  
become **extrinsic** in  
GPS space!

Global Intrinsic Symmetries of Shapes  
Ovsjanikov, Sun, and Guibas 2008

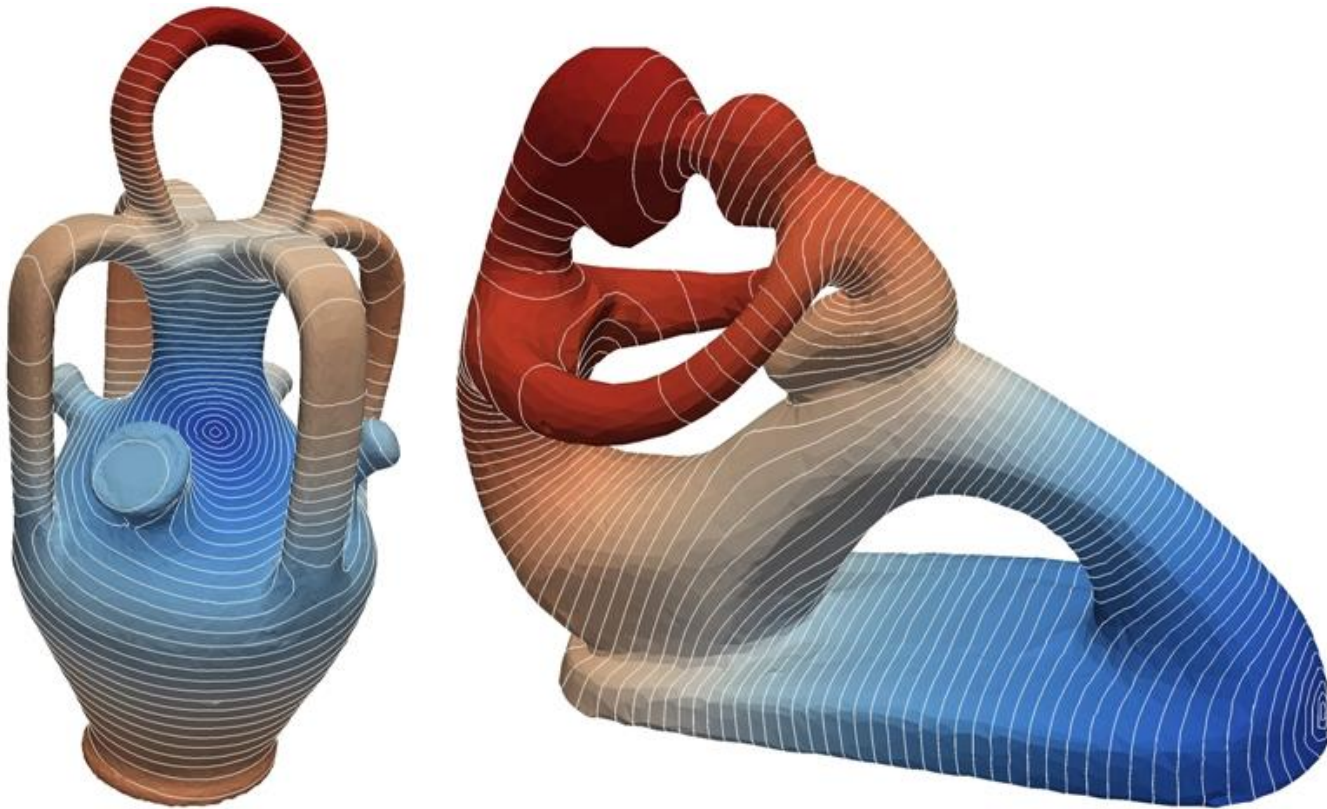
**“Discrete intrinsic” symmetries**

# All Over the Place

**Laplacians appear everywhere  
in shape analysis and  
geometry processing.**

# Biharmonic Distances

$$d_b(p, q) := \|g_p - g_q\|_2, \text{ where } \Delta g_p = \delta_p$$



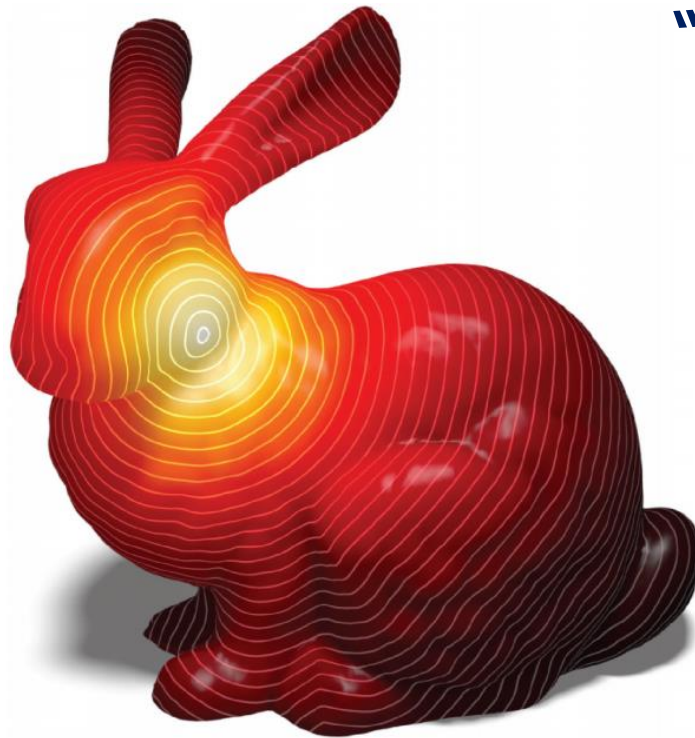
“Biharmonic distance”

Lipman, Rustamov & Funkhouser, 2010

# Geodesic Distances

$$d_g(p, q) = \lim_{t \rightarrow 0} \sqrt{-4t \log k_{t,p}(q)}$$

“Varadhan’s Theorem”



“Geodesics in heat”

Crane, Weischedel, and Wardetzky; TOG 2013



# Alternative to Eikonal Equation

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## Algorithm 1 The Heat Method

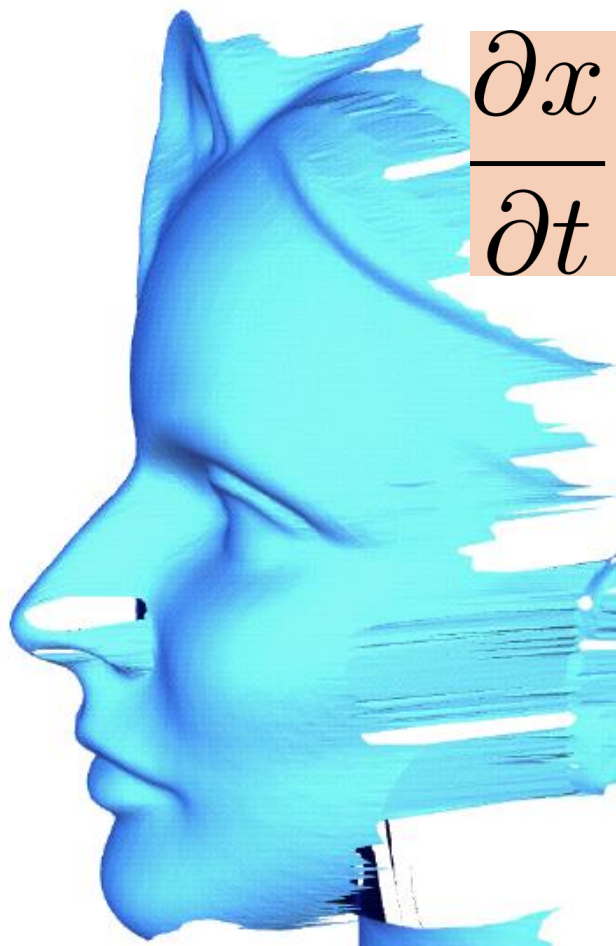
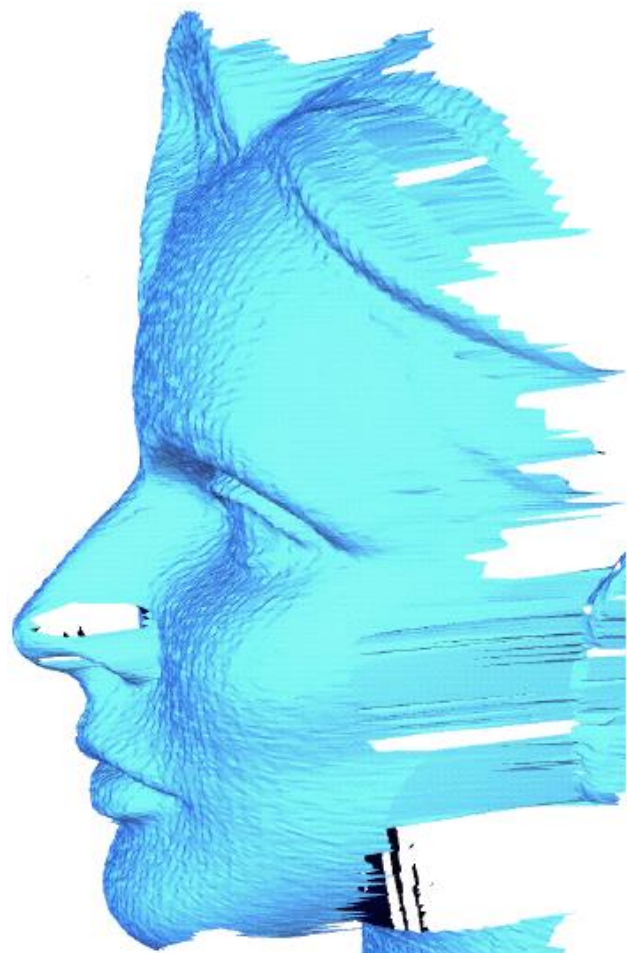
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- I. Integrate the heat flow  $\dot{u} = \Delta u$  for time  $t$ .
  - II. Evaluate the vector field  $X = -\nabla u / |\nabla u|$ .
  - III. Solve the Poisson equation  $\Delta \phi = \nabla \cdot X$ .
- 



Crane, Weischedel, and Wardetzky. "Geodesics in Heat." TOG, 2013.

# Implicit Fairing: Mean Curvature Flow



$$\frac{\partial x}{\partial t} = \Delta(x) \cdot x$$

“Implicit fairing of irregular meshes using diffusion and curvature flow”

Desbrun et al., 1999

# Useful Technique

$$\frac{\partial f}{\partial t} = -\Delta f \text{ (heat equation)}$$

$$\rightarrow M \frac{\partial f}{\partial t} = Lf \text{ after discretization in space}$$

$$\rightarrow M \frac{f_T - f_0}{T} = Lf_T \text{ after time discretization}$$

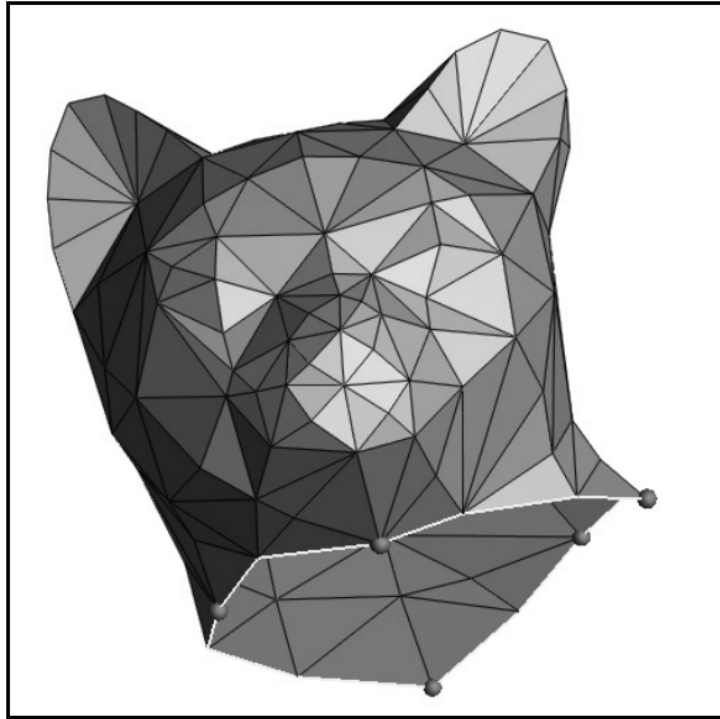
Choice: Evaluate at time T

Unconditionally stable, but not necessarily accurate for large T!

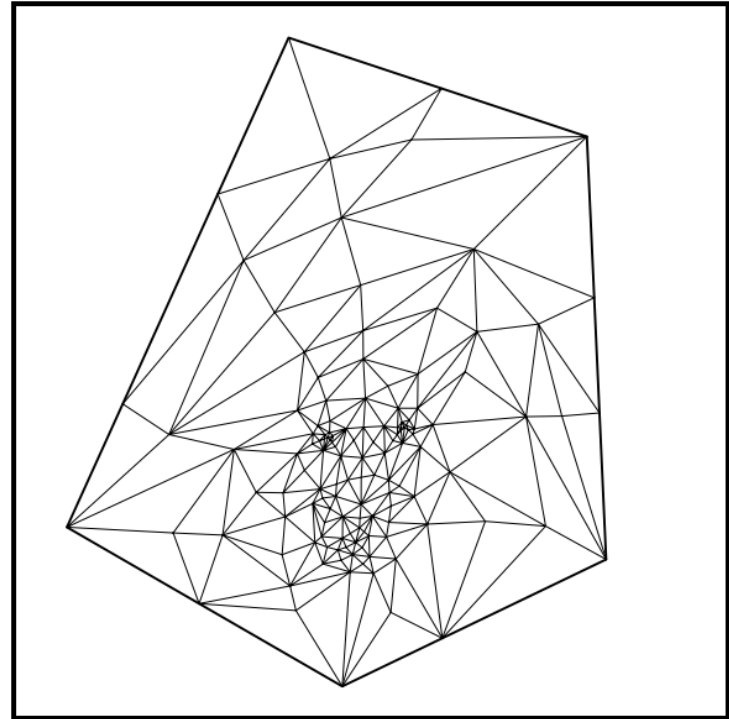
## Implicit time stepping



# Parameterization: Harmonic Map



(a) Original mesh tile



(b) Harmonic embedding

Recall:  
Mean value principle

**"Multiresolution analysis of arbitrary meshes"**

Eck et al., 1995 (and many others!)

# Others

- **Shape retrieval from Laplacian eigenvalues**

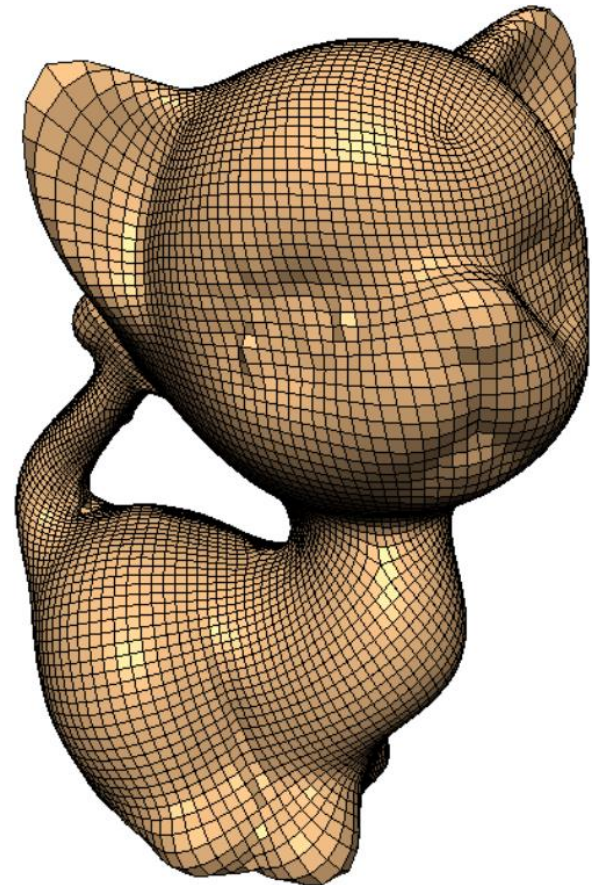
“Shape DNA” [Reuter et al., 2006]

- **Quadrangulation**

Nodal domains [Dong et al., 2006]

- **Surface deformation**

“As-rigid-as-possible” [Sorkine & Alexa, 2007]



# Our Next Topic

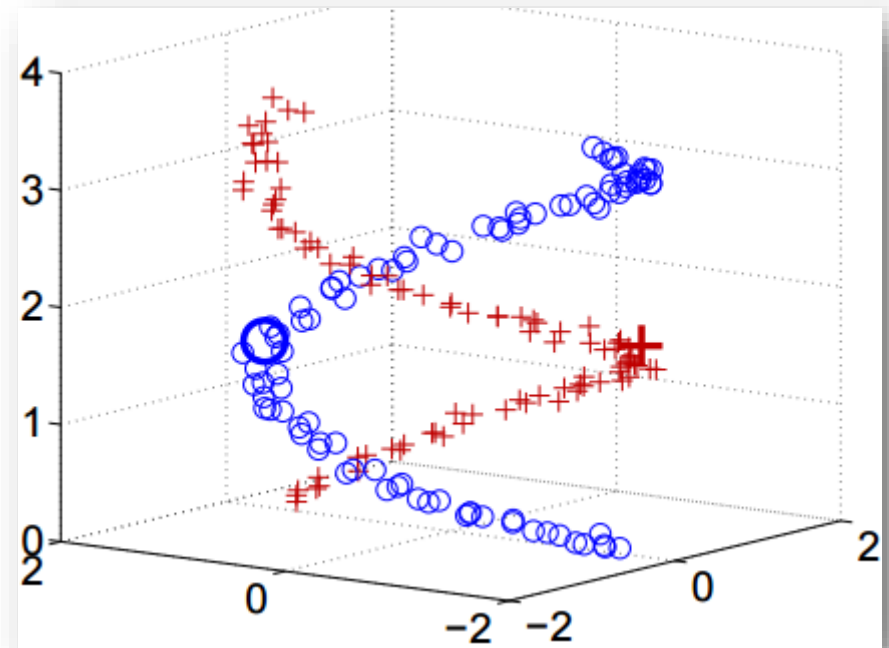
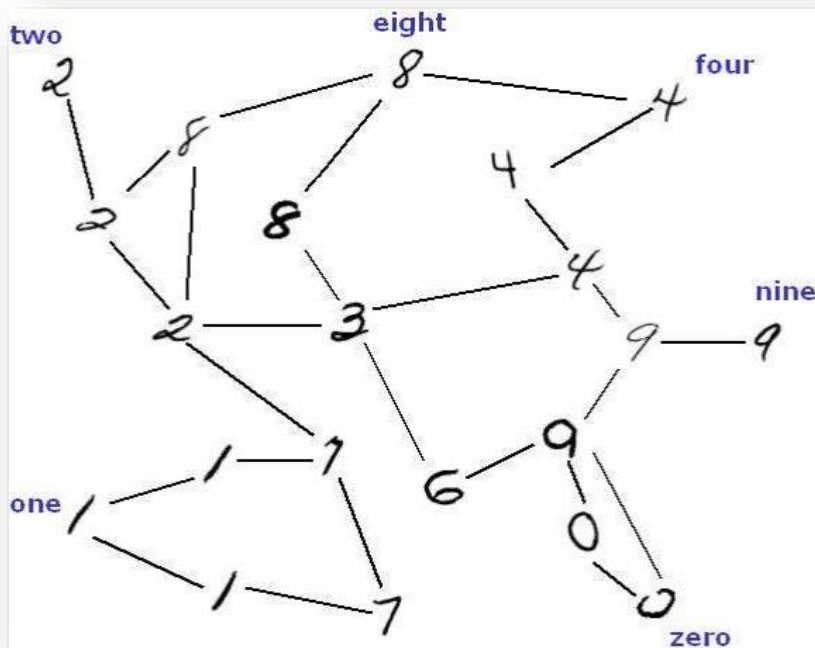
*Discrete Laplacian operators:*

## What are they good for?

- Useful properties of the Laplacian
- Applications in graphics/shape analysis
  - Applications in machine learning

*A quick survey:  
A popular field!*

# Semi-Supervised Learning



“Semi-supervised learning using Gaussian fields and harmonic functions”

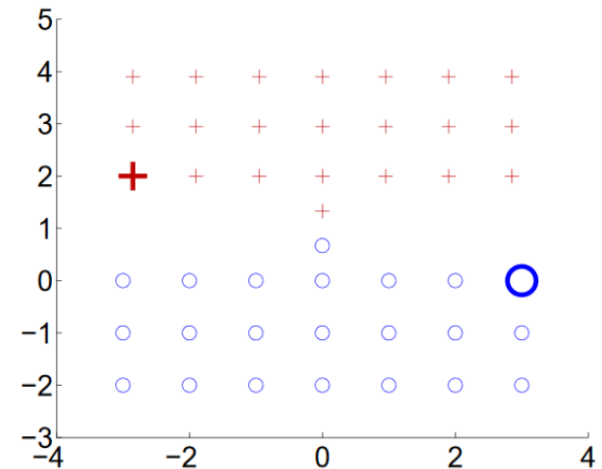
Zhu, Ghahramani, & Lafferty 2003

# Semi-Supervised Technique

Given:  $\ell$  labeled points  $(x_1, y_1), \dots, (x_\ell, y_\ell); y_i \in \{0, 1\}$   
 $u$  unlabeled points  $x_{\ell+1}, \dots, x_{\ell+u}; \ell \ll u$

$$\begin{aligned} \min \quad & \frac{1}{2} \sum_{ij} w_{ij} (f(i) - f(j))^2 \\ \text{s.t.} \quad & f(k) \text{ fixed } \forall k \leq \ell \end{aligned}$$

Dirichlet energy  $\rightarrow$  Linear system of equations (Poisson)



# Related Method

- **Step 1:**  
Build  $k$ -NN graph
- **Step 2:**  
Compute  $p$  smallest Laplacian eigenvectors
- **Step 3:**  
Solve semi-supervised problem in subspace

“Using Manifold Structure for Partially Labelled Classification”

Belkin and Niyogi; NIPS 2002

# Buyer Beware: Ill-Posed in Limit?

## Semi-Supervised Learning with the Graph Laplacian: The Limit of Infinite Unlabelled Data

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### Abstract

We study the behavior of the popular Laplacian Regularization method for Semi-Supervised Learning at the regime of a fixed number of labeled points but a large

Potential fix:  
**Higher-order  
operators**

*Aside:*  
**Common Misconception**

$$\min_f E[f] \text{ s.t. } f(p) = \text{const.}$$



**Point constraints are ill-advised**

# Manifold Regularization

Regularized learning:  $\arg \min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} V(f(x_i), y_i) + \gamma \|f\|^2$

Loss function                      Regularizer

Dirichlet energy

$$\|f\|_I^2 := \int \|\nabla f(x)\|^2 dx \approx f^\top L f$$

**“Manifold Regularization:  
A Geometric Framework for Learning from Labeled and Unlabeled Examples”**  
Belkin, Niyogi, and Sindhwani; JMLR 2006



# Examples of Manifold Regularization

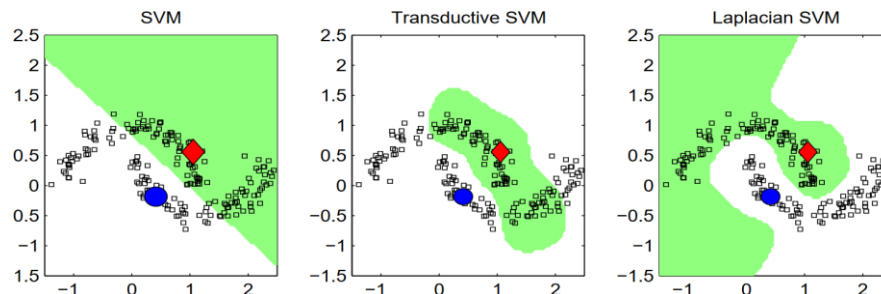
- Laplacian-regularized least squares (**LapRLS**)

$$\arg \min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} (f(x_i) - y_i)^2 + \gamma \|f\|_I^2 + \text{Other}[f]$$

- Laplacian support vector machine (**LapSVM**)

$$\arg \min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} \max(0, 1 - y_i f(x_i)) + \gamma \|f\|_I^2 + \text{Other}[f]$$

“On Manifold Regularization”  
Belkin, Niyogi, Sindhwani; AISTATS 2005



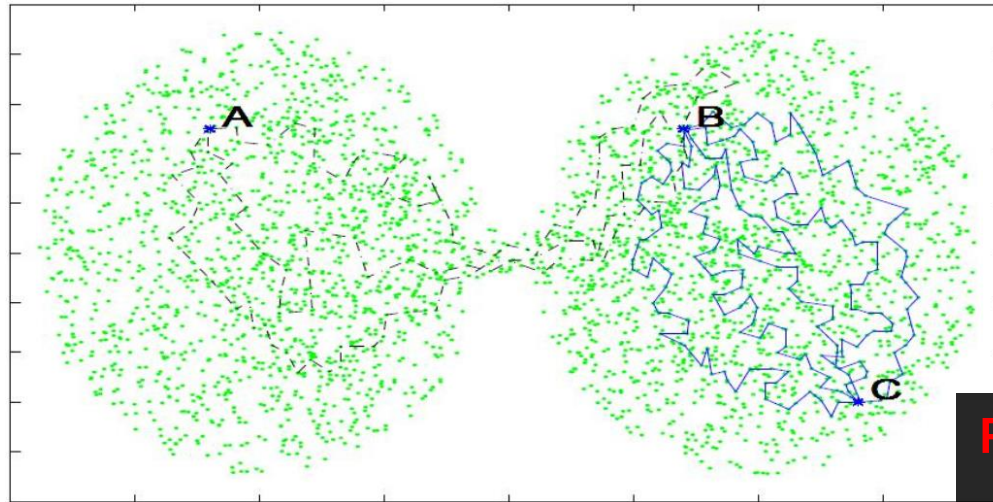
# Diffusion Maps

Embedding from first  $k$  eigenvalues/vectors:

$$\Psi_t(x) := (\lambda_1^t \psi_1(x), \lambda_2^t \psi_2(x), \dots, \lambda_k^t \psi_k(x))$$

*Roughly:*

$|\Psi_t(x) - \Psi_t(y)|$  is probability that  $x, y$  diffuse to the same point in time  $t$ .



**Robust to sampling  
and noise**

“Diffusion Maps”

Coifman and Lafon; Applied and Computational Harmonic Analysis, 2006



# Applications of the Laplacian

Justin Solomon

MIT, Spring 2017

