Laplacian Operators

Justin Solomon

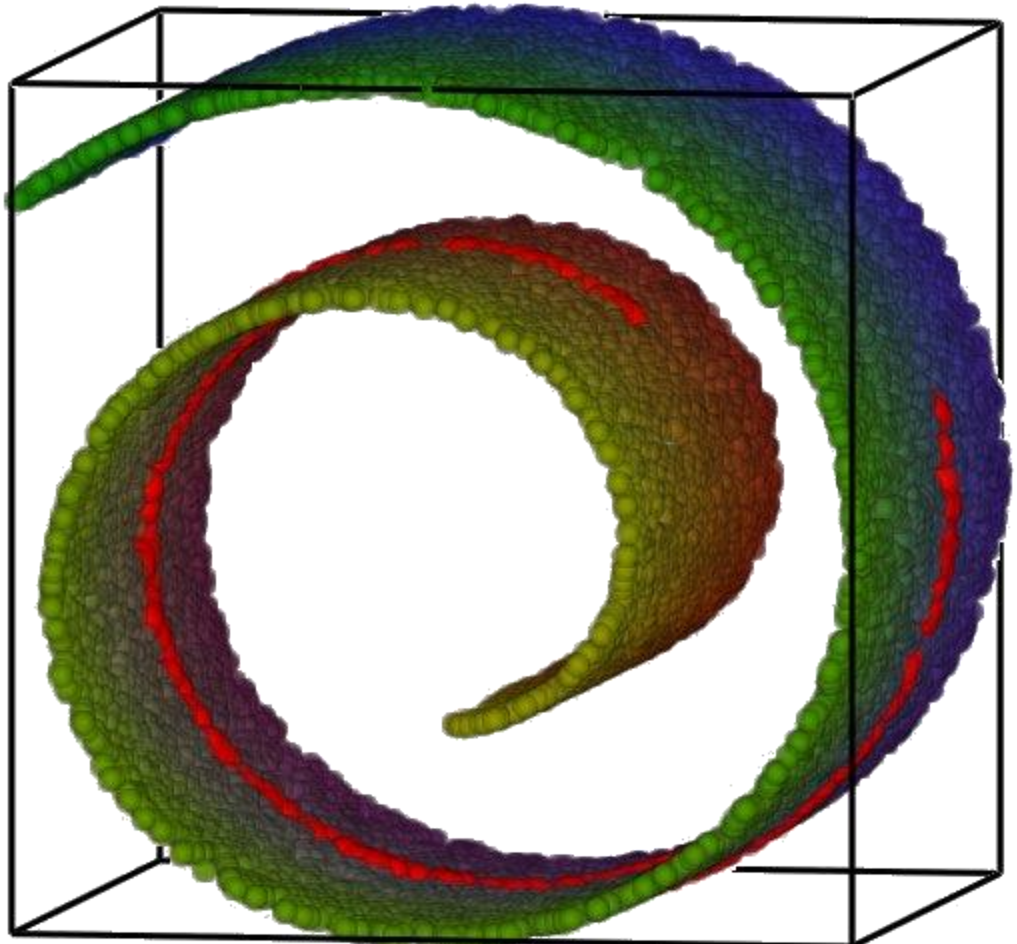
MLSS 2019

MIT EECS

https://tinyurl.com/solomon-mlss-2019

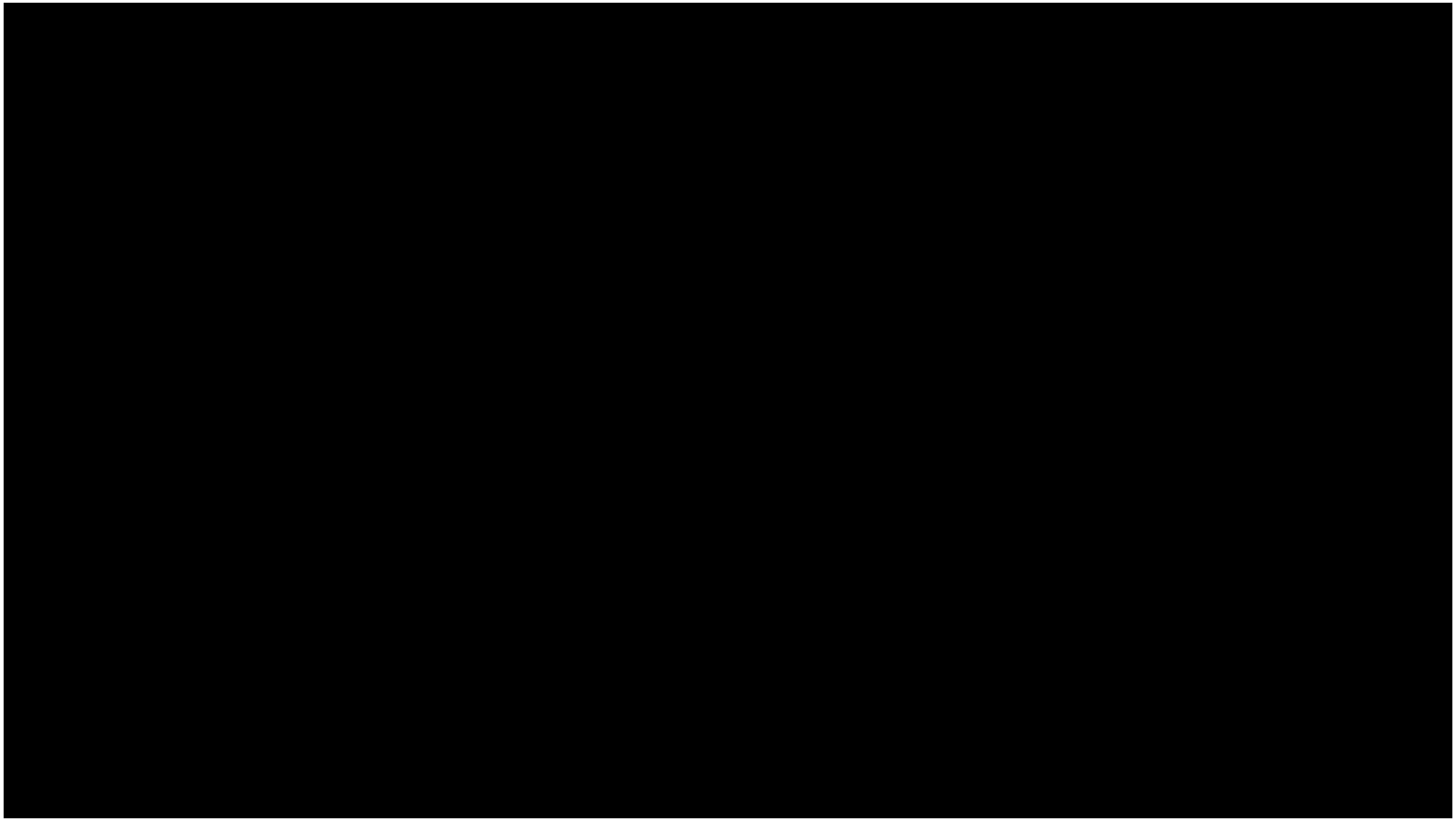

WARNING
SIGN
MISTAKES
LIKELY

Manifold Learning



What is the dimensionality?

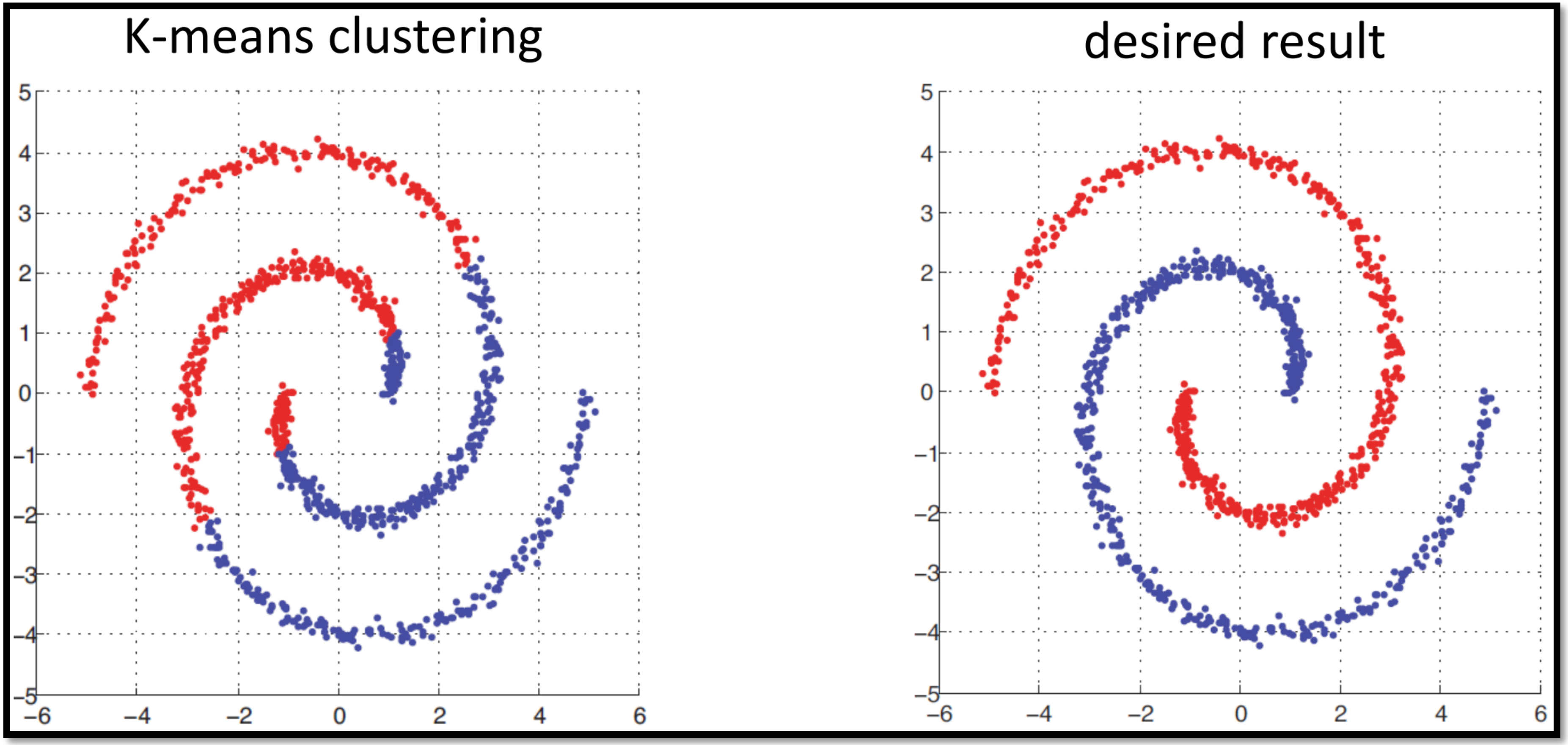
Example



https://www.youtube.com/watch?v=8d80Dbd2BwY

Video courtesy Roy Lederman

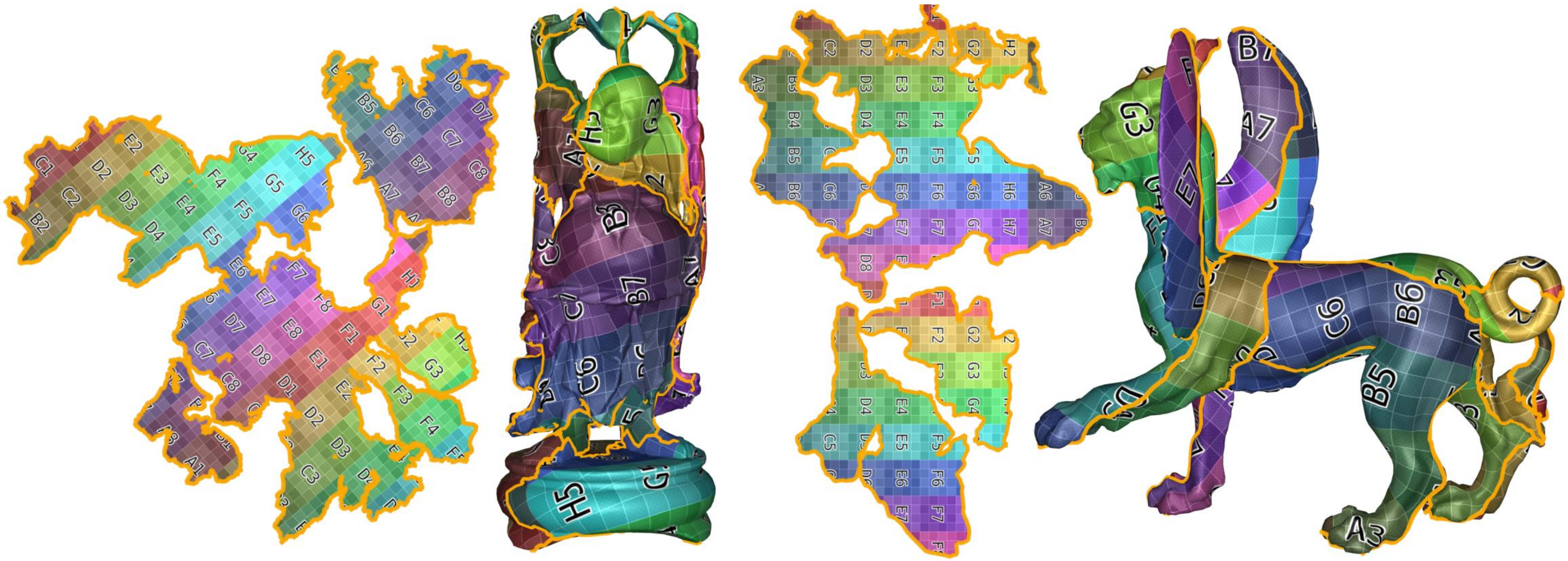
Typical Challenges



https://trevorcohn.github.io/comp90051-2017/slides/16_manifold_learning.pdf

Problematic approach:

Parameterization and Embedding

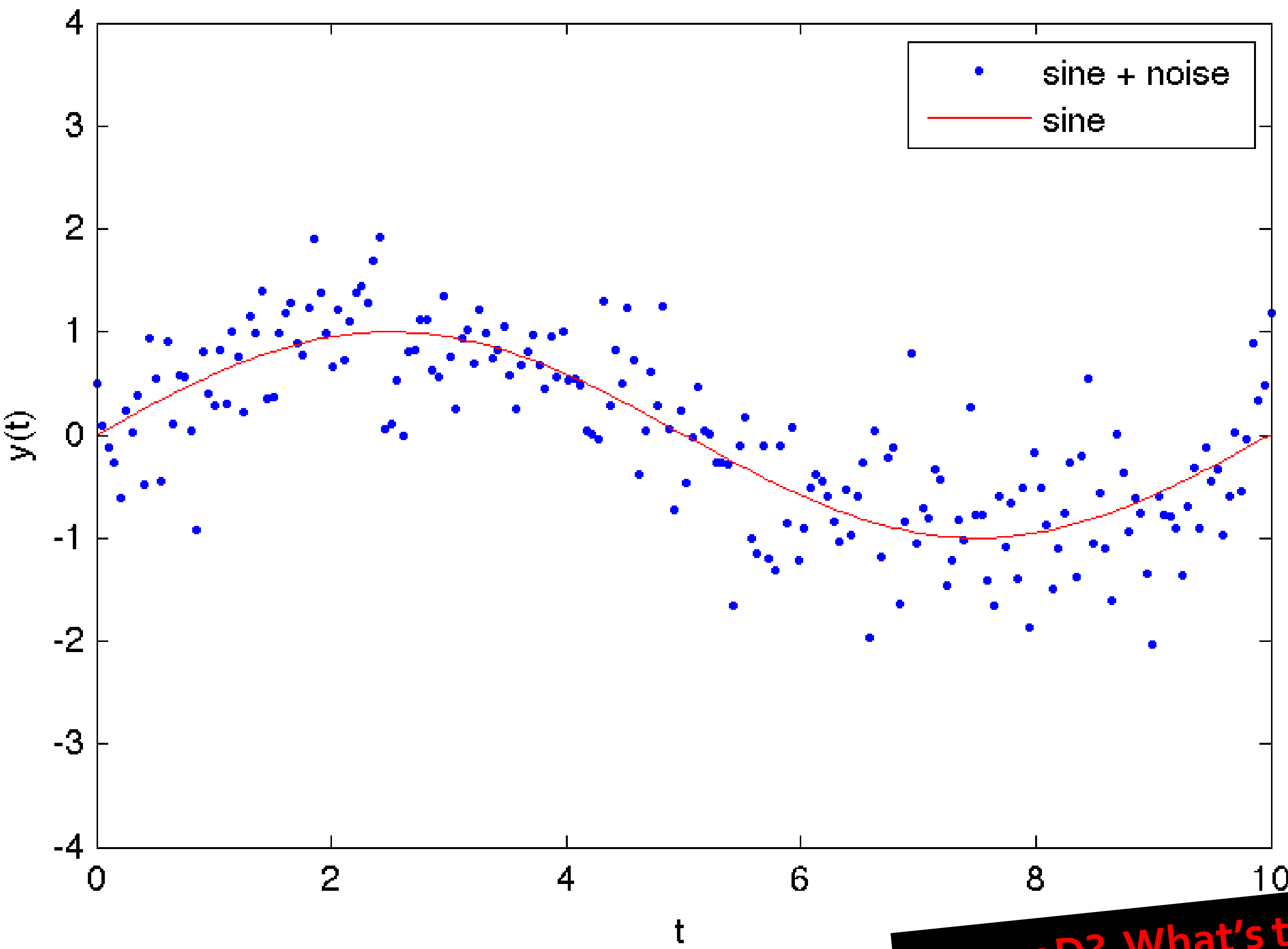


Where do you cut?
What is the dimension?
Are gaps OK?

Image from [Li, Kaufman, Kim, Solomon, & Sheffer 2018]

Additional challenge:

No Connectivity

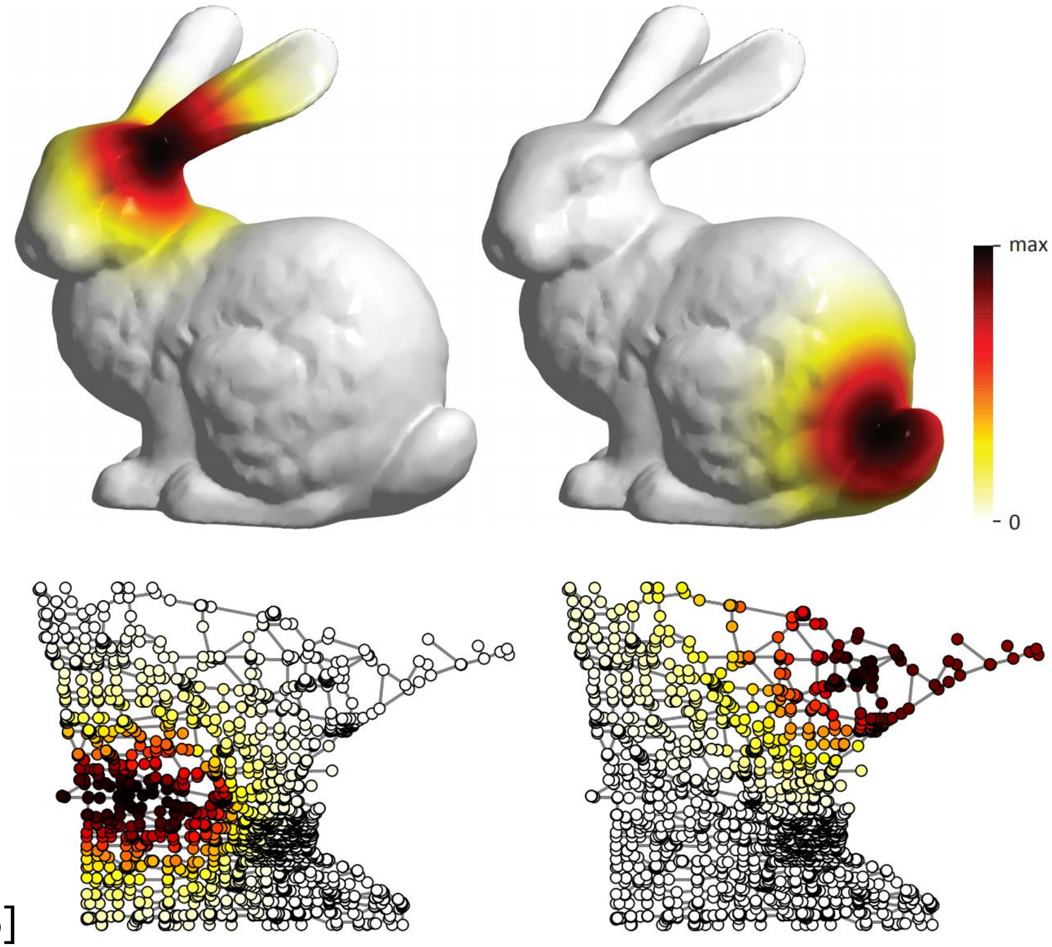


1D or 2D? What's the manifold?

Q:

Can we perform learning directly on manifold-shaped data?

Initial Motivation



[Bronstein et al. 2016]

Diffusion to move information around

Historical Motivation

CAN ONE HEAR THE SHAPE OF A DRUM?

MARK KAC, The Rockefeller University, New York

To George Eugene Uhlenbeck on the occasion of his sixty-fifth birthday

"La Physique ne nous donne pas seulement l'occasion de résoudre des problèmes . . . , elle nous fait presentir la solution." H. POINCARÉ.

Before I explain the title and introduce the theme of the lecture I should like to state that my presentation will be more in the nature of a leisurely excursion than of an organized tour. It will not be my purpose to reach a specified destination at a scheduled time. Rather I should like to allow myself on many occasions the luxury of stopping and looking around. So much effort is being spent on streamlining mathematics and in rendering it more efficient, that a solitary transgression against the trend could perhaps be forgiven.

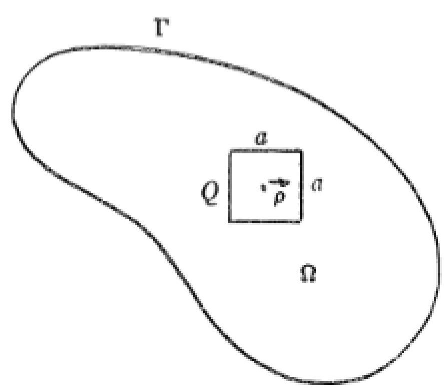
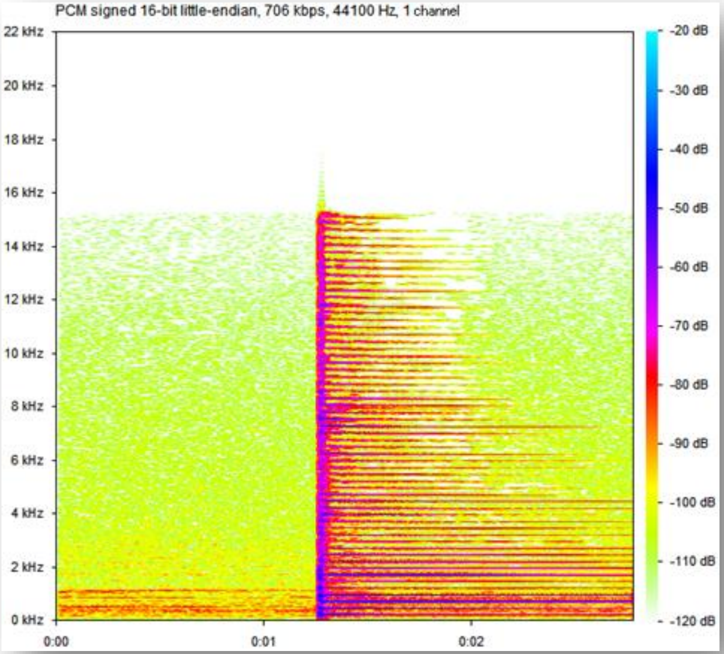


FIG. 1

An Experiment

Is this possible?

Unreasonable to Ask?

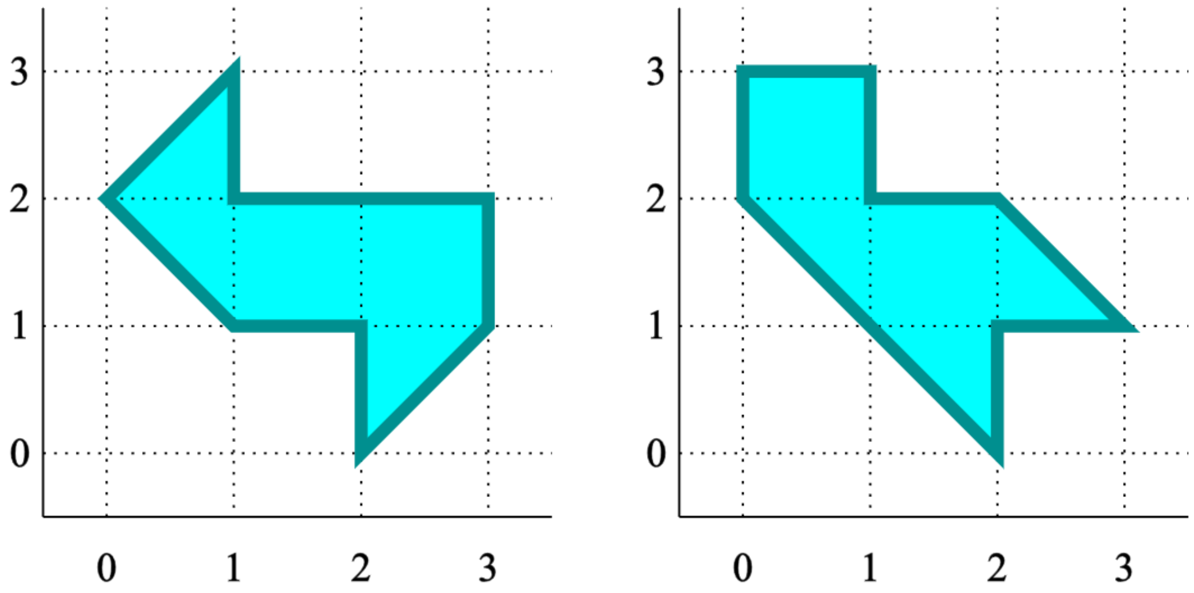


Length of string

http://www.takamine.com/templates/default/images/gclassical.png
http://firsttimeprogrammer.blogspot.com/2015/05/spectrogram-representation-of-b-note.html

Spoiler Alert

Extra credit: Make these!



"No, but…"

- Has to be a weird drum
- Spectrum tells you a lot!

https://en.wikipedia.org/wiki/Hearing_the_shape_of_a_drum

Rough Intuition

http://pngimg.com/upload/hammer_PNG3886.png

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

Works for manifolds too!

Broader Theme

If we can approximate the data manifold Laplacian,

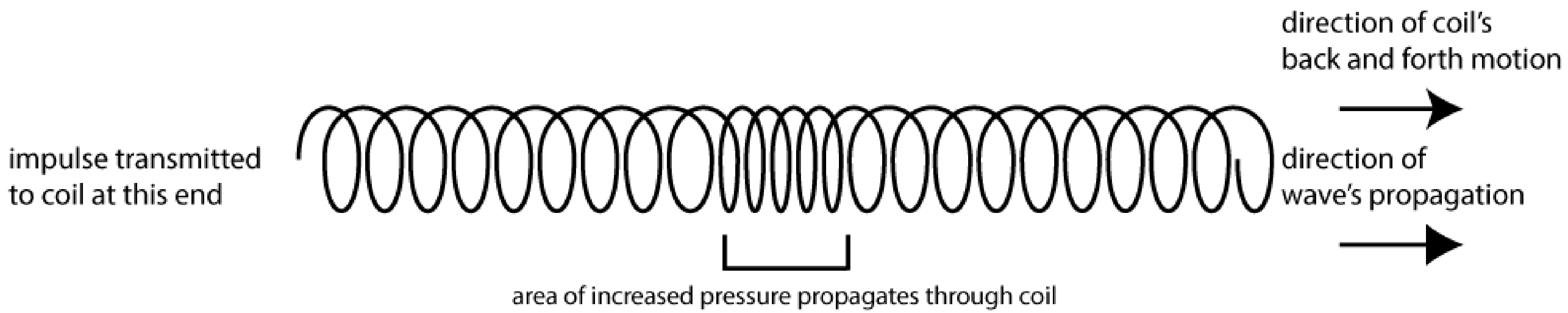
how can we use it?

$$\Delta$$

Introducing Laplacians

- Line segments
- Regions in $\mathbb{R}^n$
- Graphs
- Surfaces/manifolds

1D Transverse Wave



$$u_{tt} - c^2 u_{xx} = 0$$

Minus Second Derivative Operator

"Dirichlet boundary conditions"

$$\{f(\cdot) \in C^\infty([a,b]) : f(0) = f(\ell) = 0\}$$

$$\boxed{\mathcal{L}[\cdot] : u \mapsto -\frac{\partial^2 u}{\partial x^2}}$$

On the board: Interpretation as positive (semi-)definite operator.

Eigenfunctions:

$$\phi_k(x) = \sqrt{\frac{2}{\ell}} \sin\left(\frac{\pi k x}{\ell}\right), \quad \lambda_k = \left(\frac{\pi k}{\ell}\right)^2$$

Can you hear the length of an interval?

$$\lambda_k = \left(\frac{\pi k}{\ell}\right)^2$$

Yes!

Our Progression

- Line segments
- Regions in $\mathbb{R}^n$
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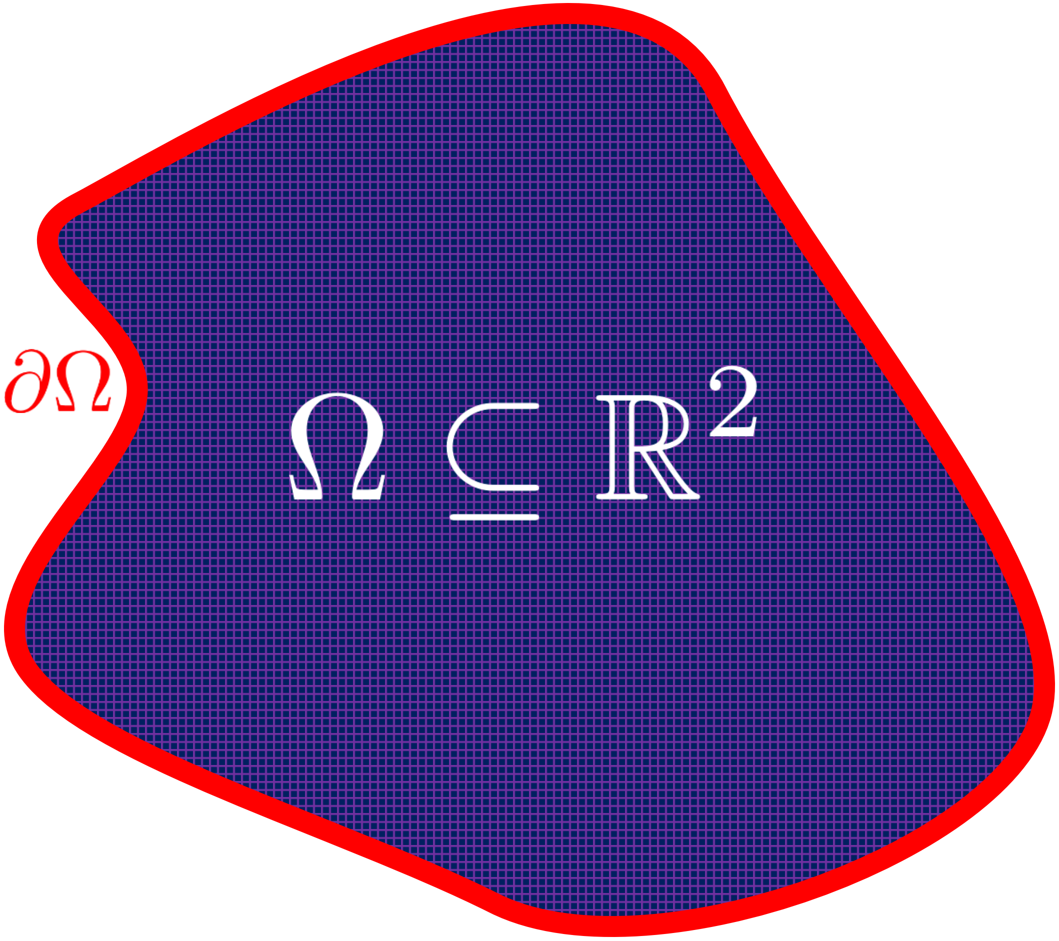
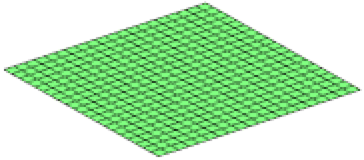
Planar Region



Wave equation:

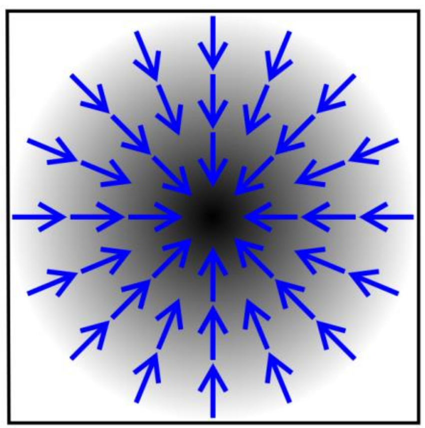
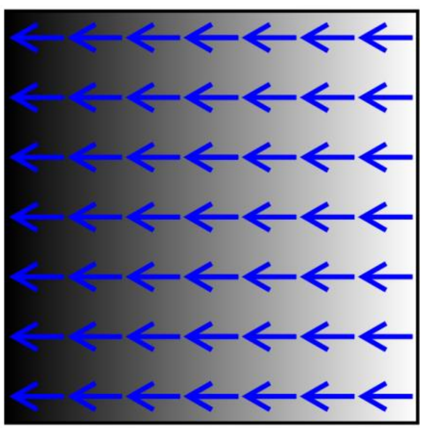
$$\frac{\partial^2 u}{\partial t^2} = -\Delta u$$

$$\Delta := -\sum_i \frac{\partial^2}{\partial x_i^2}$$



Typical Notation

$$\text{“}\Delta = -\underbrace{\nabla \cdot}_{\text{divergence}} \underbrace{\nabla}_{\text{gradient}}\text{”}$$

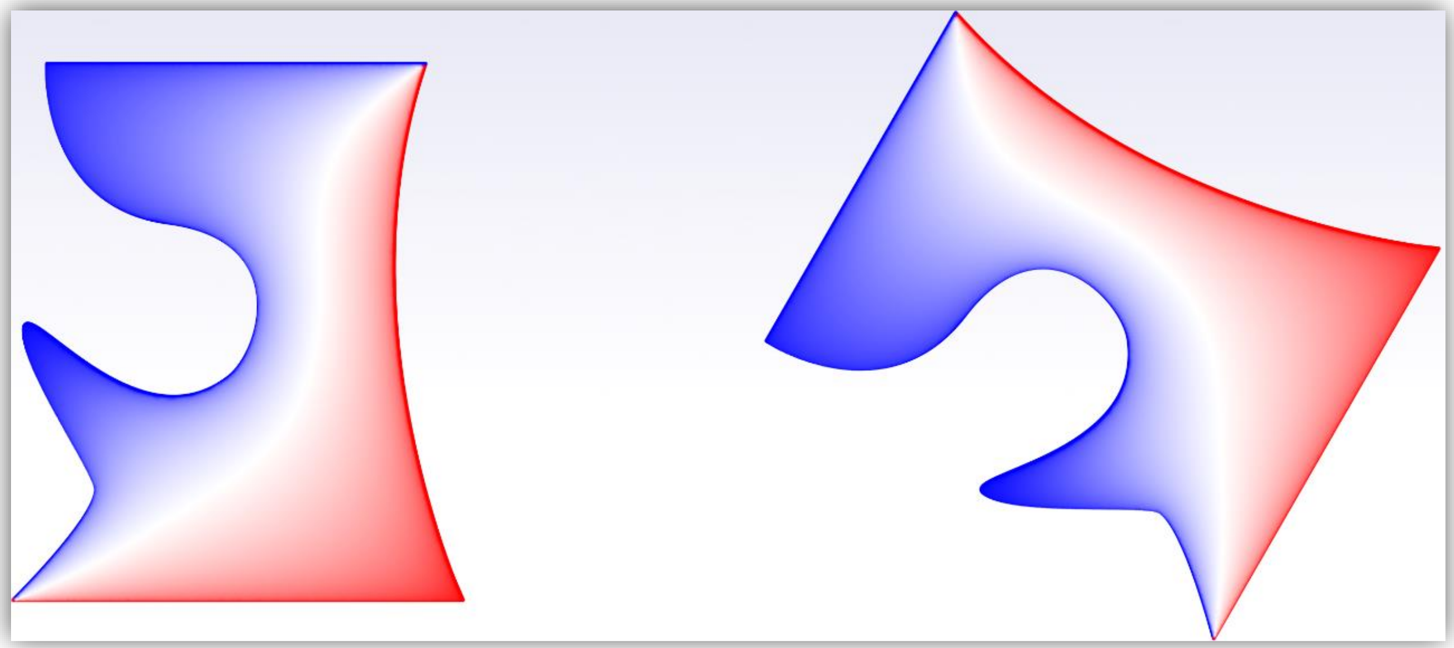
 

Gradient operator:

$$\nabla := \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \cdots, \frac{\partial}{\partial x_n} \right)$$

http://www.gamasutra.com/db_area/images/feature/4164/figy.png, https://en.wikipedia.org/wiki/Gradient

Intrinsic Operator

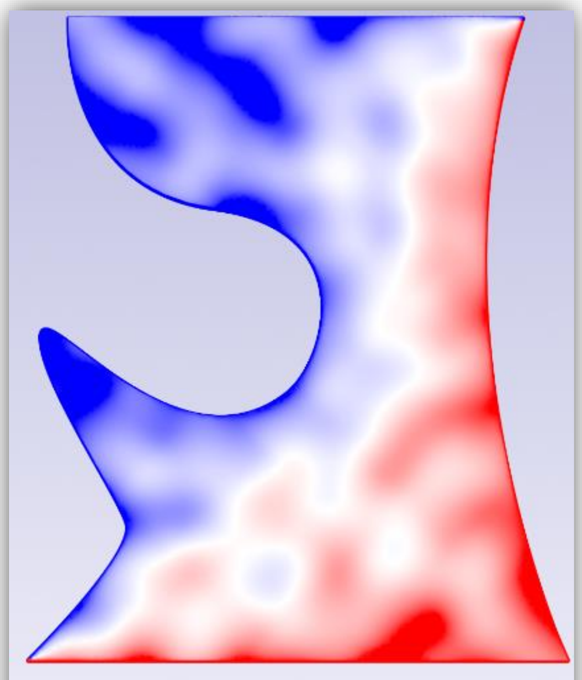


Images made by E. Vouga

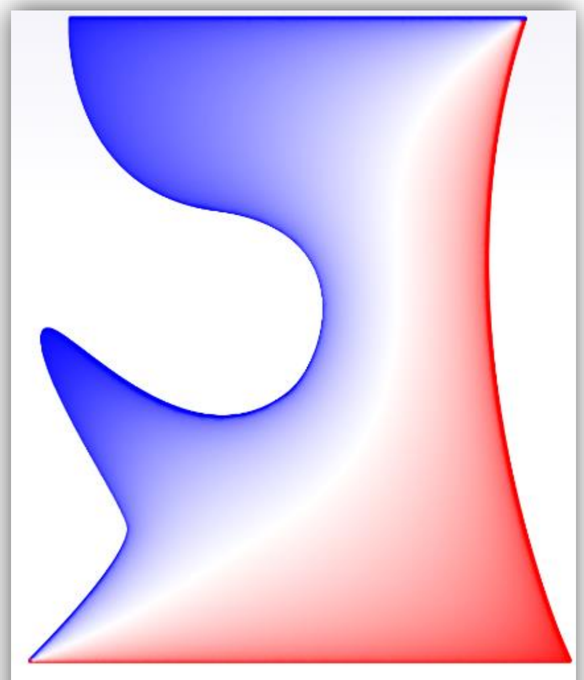
Coordinate-independent (important!)

Dirichlet Energy

$$E[u] := \frac{1}{2}\int_\Omega \|\nabla u(\mathbf{x})\|_2^2 \, dA(\mathbf{x})$$



non-smooth $f(x)$



solution $\Delta f = 0$

$$\min_{u(\mathbf{x}):\Omega\to\mathbb{R}} E[u]$$

$$\text{s.t. } u|_{\partial\Omega} \text{ prescribed}$$

$$\Downarrow$$

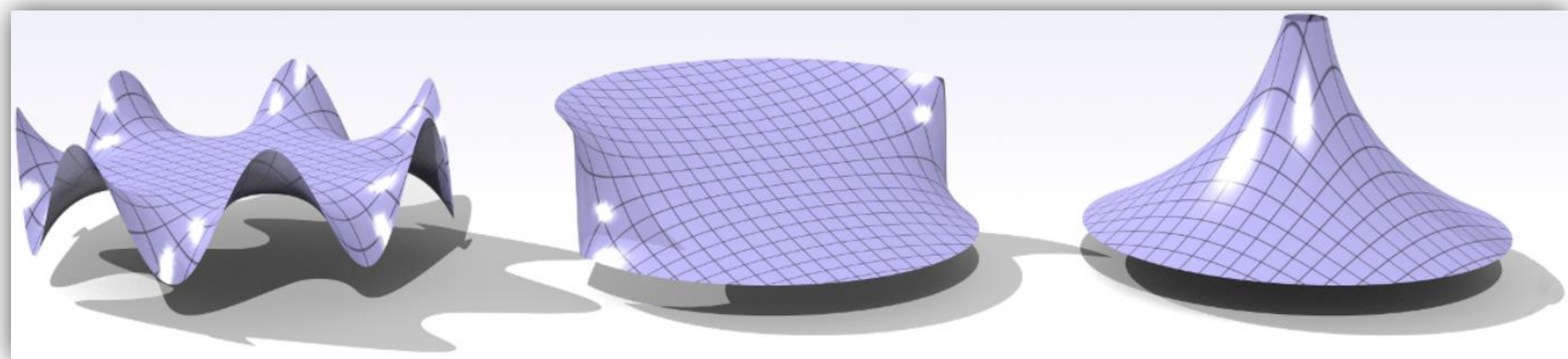
$$\Delta u \equiv 0$$

"Laplace equation"
"Harmonic function"

Images made by E. Vouga

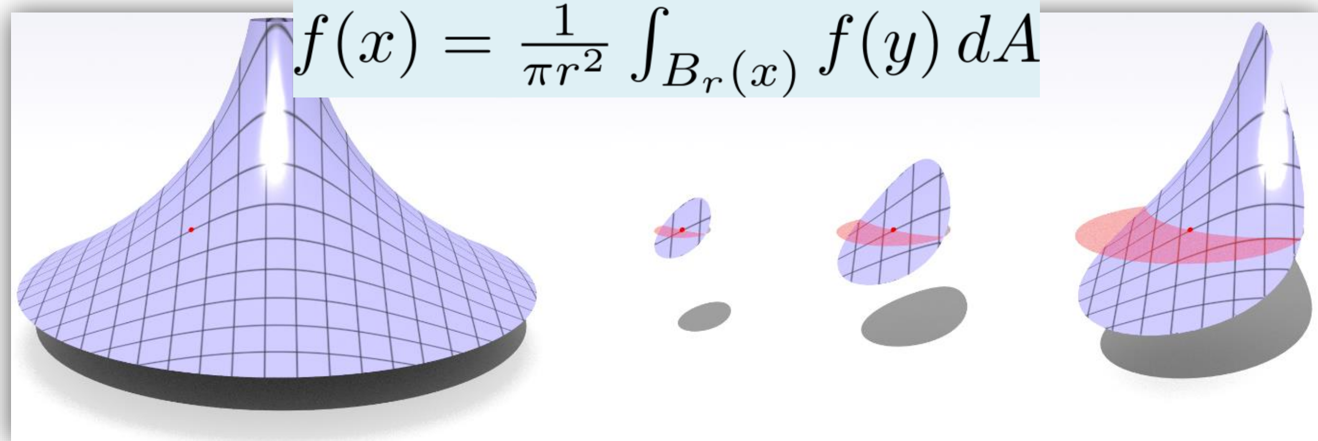
Harmonic Functions

$$\Delta f \equiv 0$$



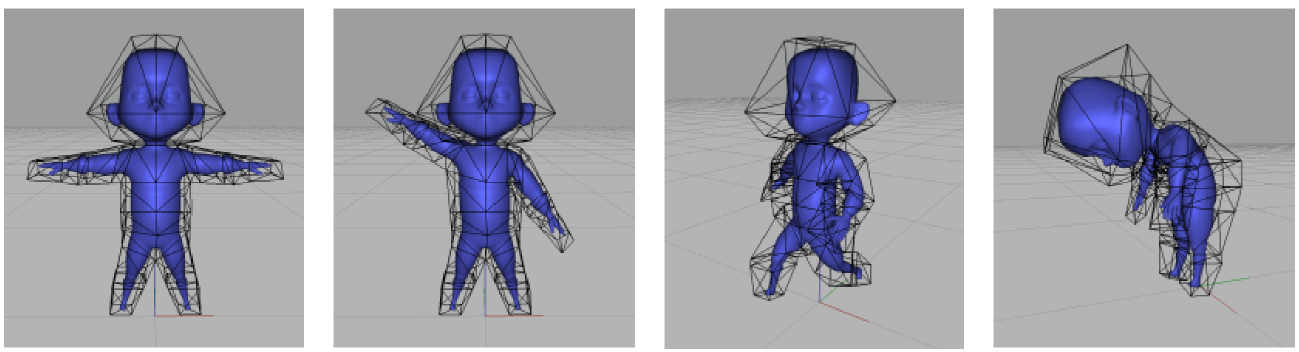
Mean value property:

$$f(x) = \frac{1}{\pi r^2} \int_{B_r(x)} f(y)\, dA$$



Images made by E. Vouga

Application



Harmonic Coordinates

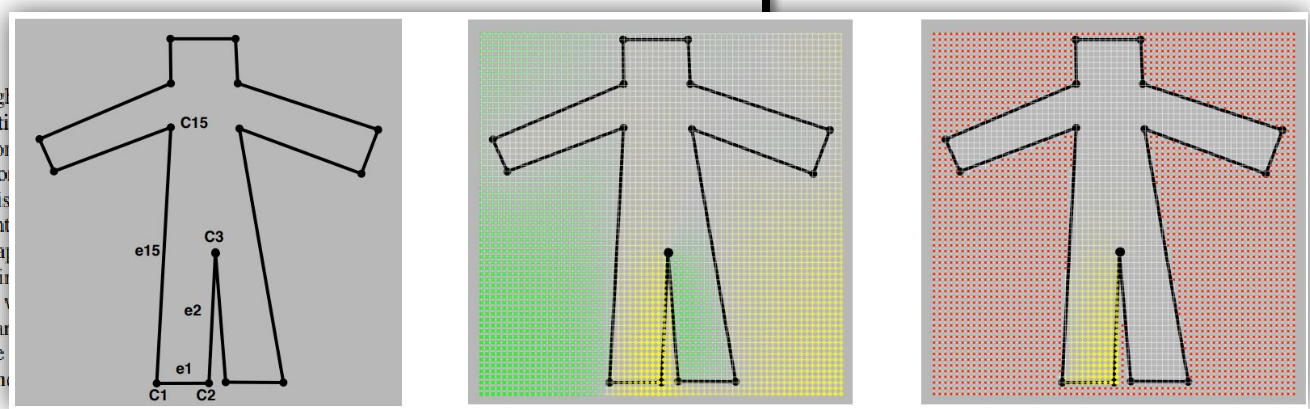
Tony DeRose Mark Meyer
Pixar Technical Memo #06-02
Pixar Animation Studios

(a) (b) (c) (d)

Figure 1: A character (shown in blue) being deformed by a cage (shown in black) using harmonic coordinates. (a) The character and cage at bind-time; (b) - (d) the deformed character corresponding to three different poses of the cage.

Abstract

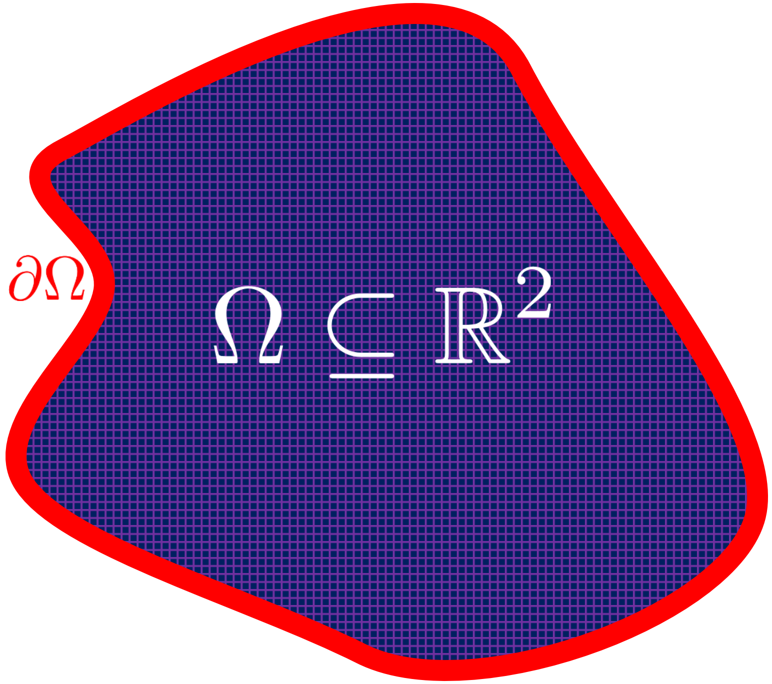
Generalizations of barycentric coordinates in two and hig
mensions have been shown to have a number of applicati
recent years, including finite element analysis, the definitior
patches (*n*-sided generalizations of Bézier surfaces), free-fo
formations, mesh parametrization, and interpolation. In this
we present a new form of *d* dimensional generalized barycent
ordinates. The new coordinates are defined as solutions to La
equation subject to carefully chosen boundary conditions. Si
lutions to Laplace's equation are called harmonic functions,
the new construction harmonic coordinates. We show that ha
coordinates possess several properties that make them more
tive than mean value coordinates when used to define two an
dimensional deformations.



Positivity, Self-Adjointness

$$\{f(\cdot) \in C^\infty(\Omega) : f|_{\partial\Omega} \equiv 0\}$$

"Dirichlet boundary conditions"



$$\mathcal{L}[f] := \Delta f$$

$$\langle f, g\rangle := \int_\Omega f(\mathbf{x})g(\mathbf{x})\,dA(\mathbf{x})$$

Check at home (Stokes' Theorem!):

1. **Positive:** $\langle f, \mathcal{L}[f]\rangle \geq 0$
2. **Self-adjoint:** $\langle f, \mathcal{L}[g]\rangle = \langle \mathcal{L}[f], g\rangle$

Aside:

Common Misconception

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

Point constraints are ill-advised

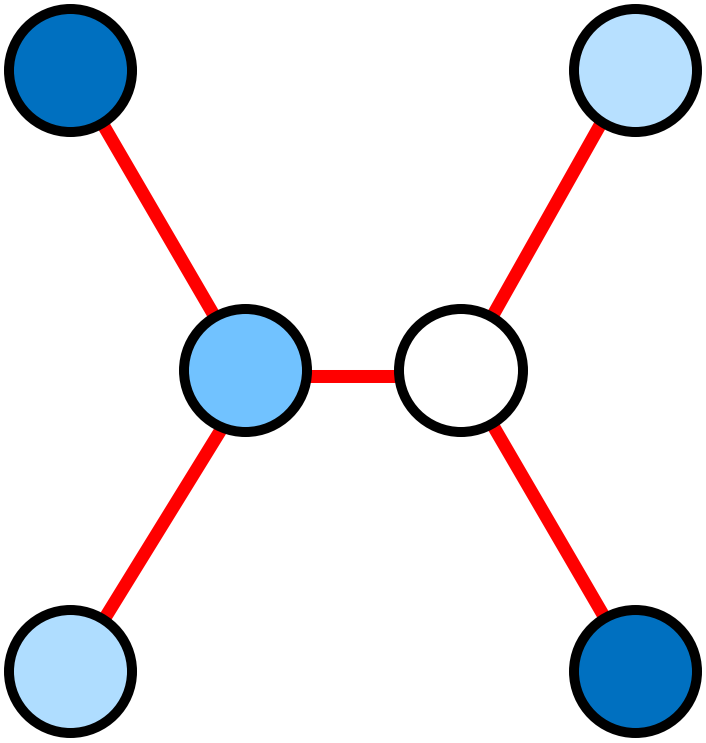
Our Progression

- Line segments
- Regions in $\mathbb{R}^n$
- Graphs
- Surfaces/manifolds

Basic Setup

- **Function:**

  One value per vertex



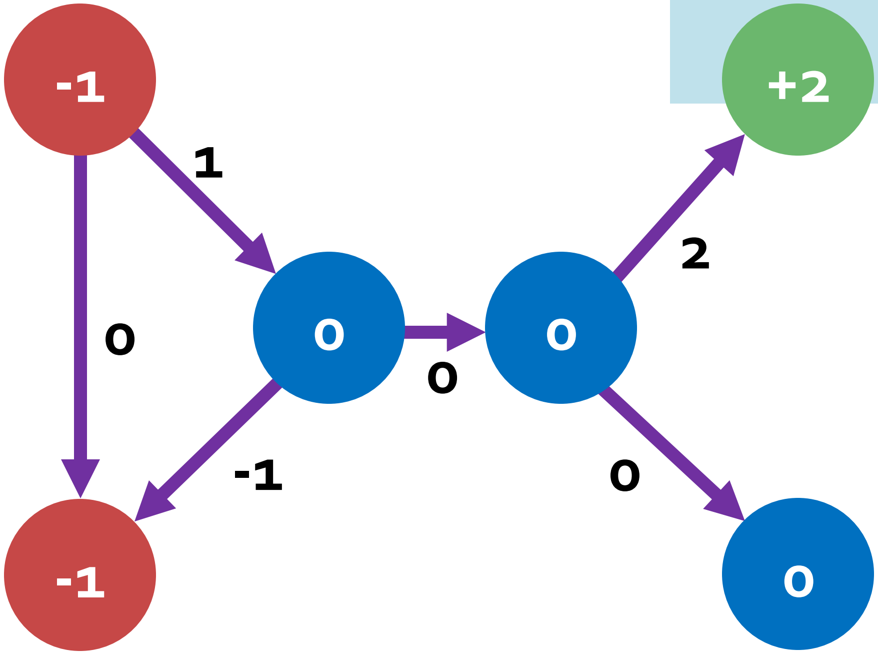
Q:

What is the
Dirichlet energy of a
function on a graph?

Differencing Operator

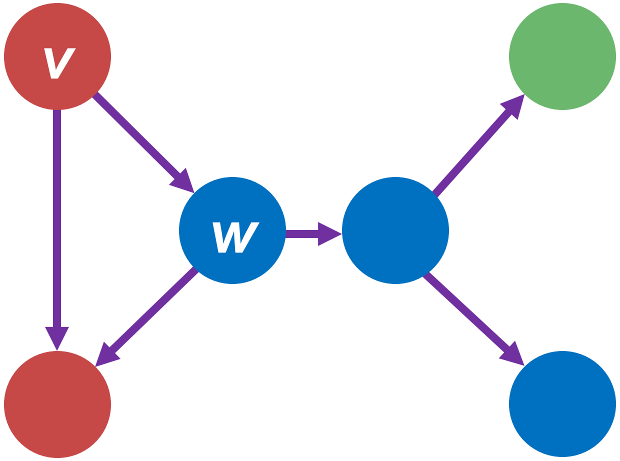
$$D_{ev} := \begin{cases} -1 & \text{if } E_{e1} = v \\ 1 & \text{if } E_{e2} = v \\ 0 & \text{otherwise} \end{cases}$$

$D \in \{-1, 0, 1\}^{|E| \times |V|}$



Orient edges arbitrarily

Dirichlet Energy on a Graph



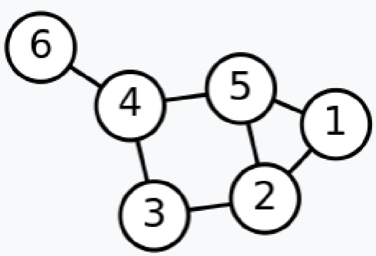
$$D_{ev} := \begin{cases} -1 & \text{if } E_{e1} = v \\ 1 & \text{if } E_{e2} = v \\ 0 & \text{otherwise} \end{cases}$$

$$E[f] := \|Df\|_2^2 = \sum_{(v,w)\in E} (f_v - f_w)^2$$

(Unweighted) Graph Laplacian

$$E[f] = \|Df\|_2^2 = f^\top (D^\top D) f := f^\top L f$$

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

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

- **Symmetric**
- **Positive semidefinite**

https://en.wikipedia.org/wiki/Laplacian_matrix

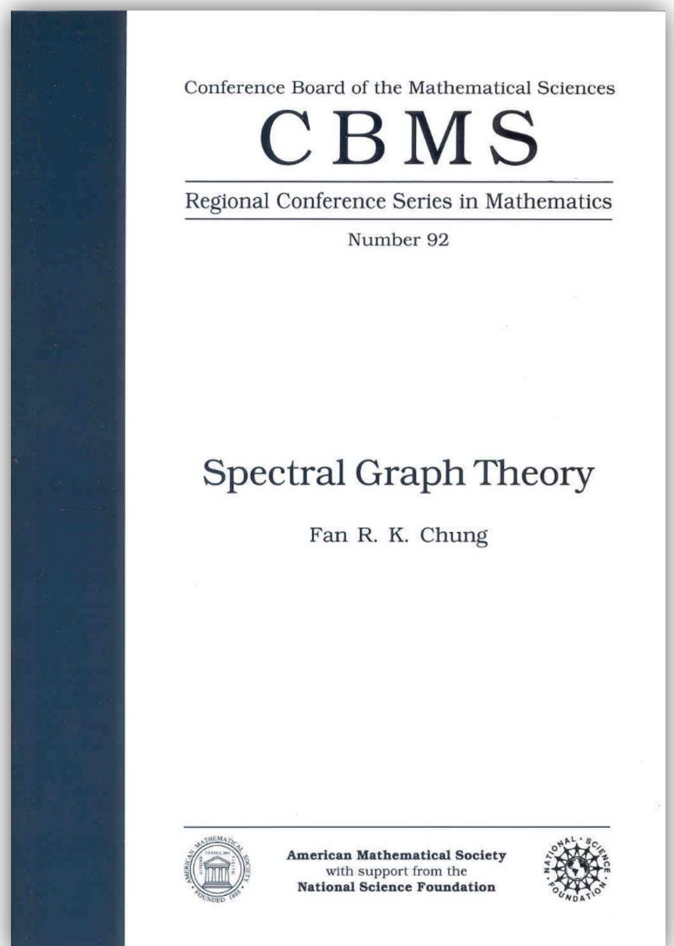
Mean Value Property

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

$$(Lx)_v = 0$$

Value at *v* is average of neighboring values

For More Information…



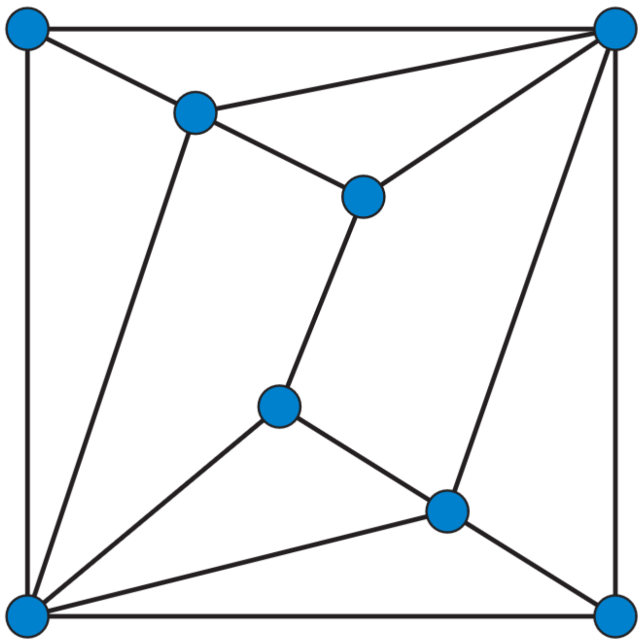
Graph Laplacian encodes lots of information!

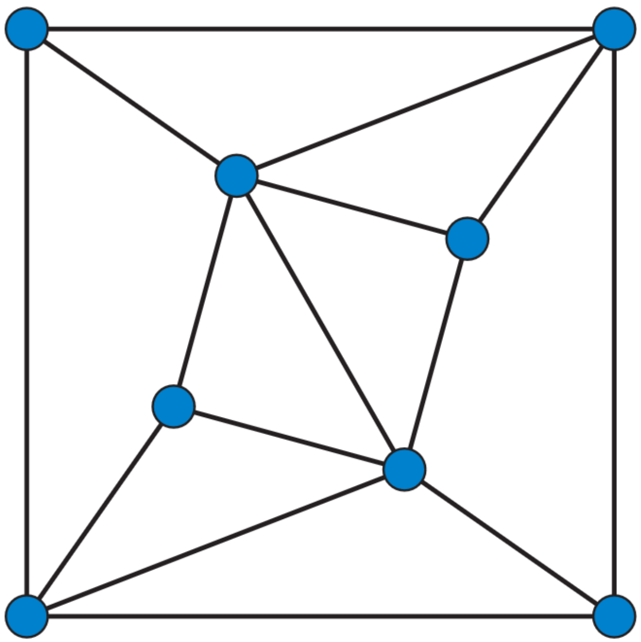
Example: Kirchoff's Theorem

Number of spanning trees equals

$$\frac{1}{n}\lambda_2\lambda_3\cdots\lambda_n$$

Hear the Shape of a Graph?





"Enneahedra"

No!

Our Progression

- Line segments
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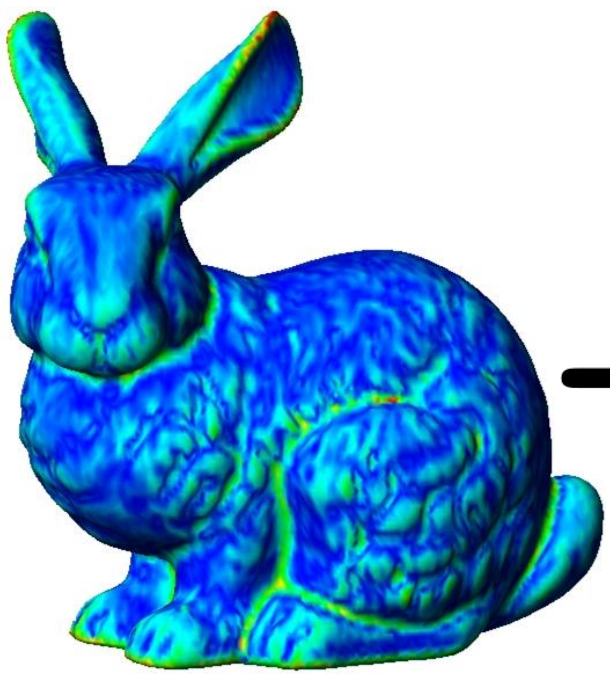
Recall:

Scalar Functions

$f :$  $\longrightarrow \mathbb{R}$

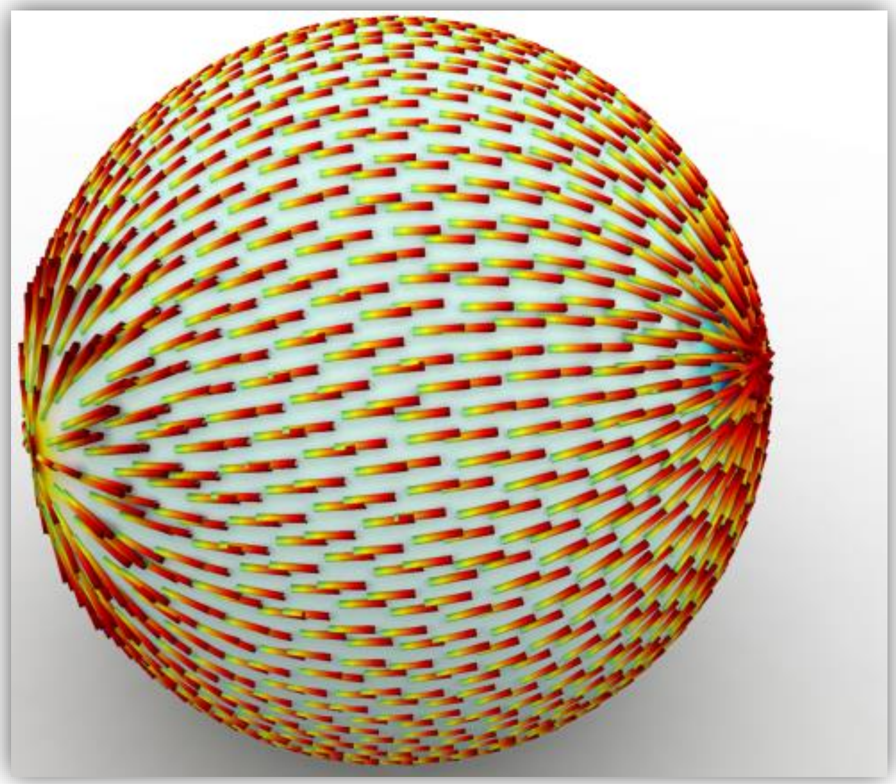
http://www.ieeta.pt/polymeco/Screenshots/PolyMeCo_OneView.jpg

Map points to real numbers

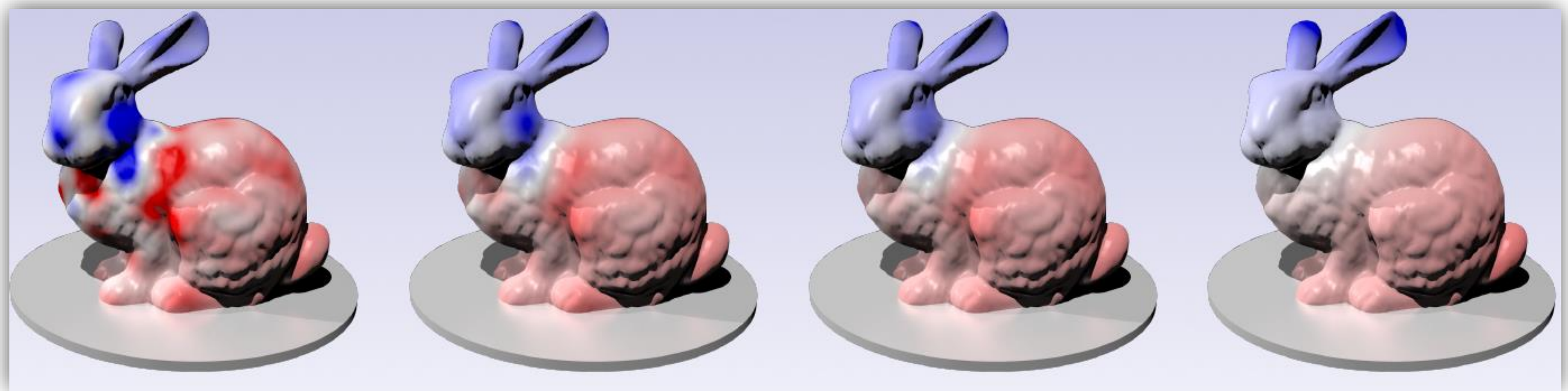
Recall:

Gradient Vector Field

Proposition 9.2. *For each* $\mathbf{p} \in \mathcal{M}$*, there exists a unique vector* $\nabla f(\mathbf{p}) \in T_{\mathbf{p}}\mathcal{M}$ *so that* $df_{\mathbf{p}}(\mathbf{v}) = \mathbf{v} \cdot \nabla f(\mathbf{p})$ *for all* $\mathbf{v} \in T_{\mathbf{p}}\mathcal{M}$.



Dirichlet Energy



Decreasing ***E***

$$E[f] := \int_S \|\nabla f\|_2^2 \, dA$$

Images made by E. Vouga

From Inner Product to Operator

$$\langle f, g \rangle_\Delta := \int_S \nabla f(x) \cdot \nabla g(x) \, dA$$
$$:= \langle f, \Delta g \rangle$$

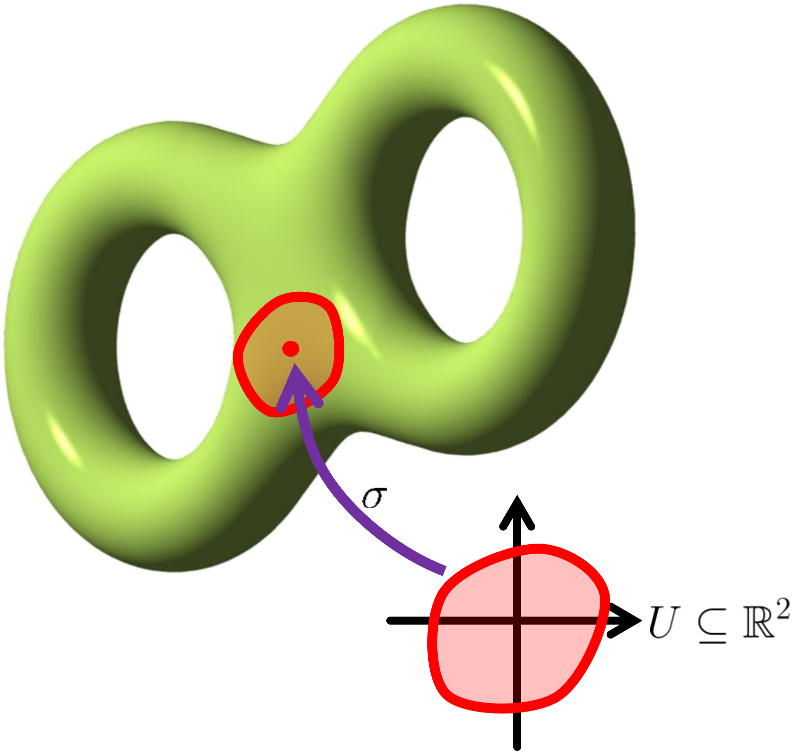
Implies
$\langle f, f \rangle \geq 0$

Laplace-Beltrami operator

Sanity Check: Local Version

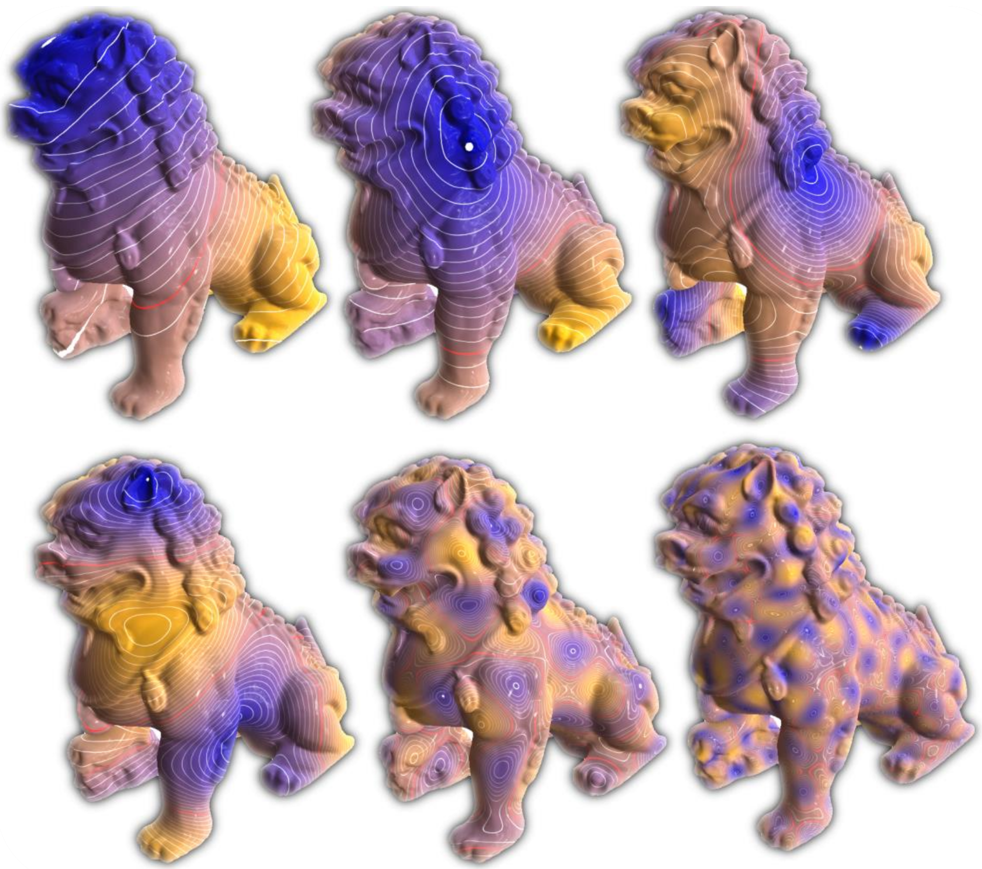
$$f : \mathcal{M} \to \mathbb{R}$$

$$\text{Pullback: } \sigma^* f := f \circ \sigma : U \to \mathbb{R}$$



Laplace-Beltrami coincides with Laplacian on $\mathbb{R}^2$ when σ takes x, y axes to orthonormal vectors.

Eigenfunctions



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

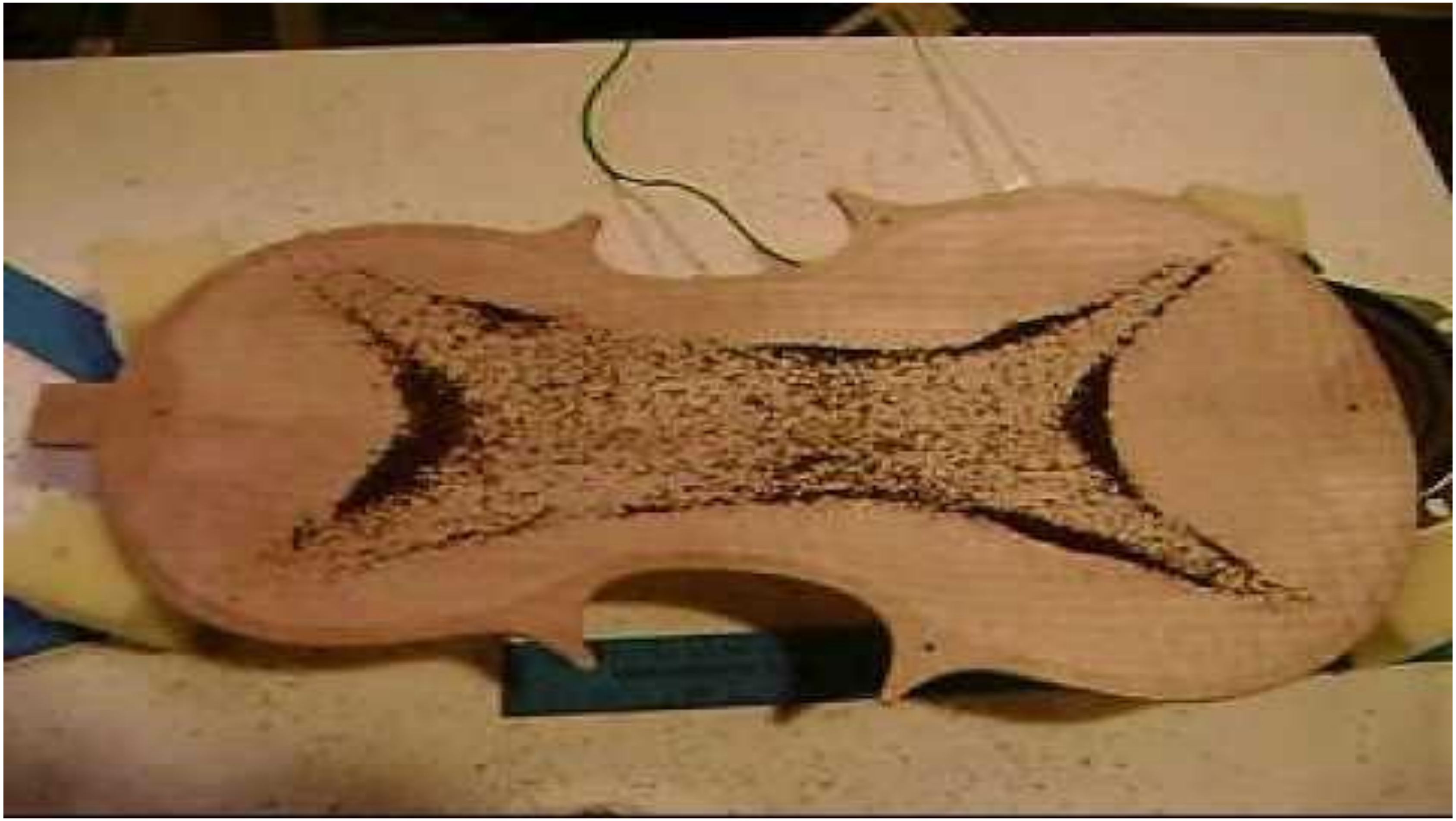
Vibration modes

http://alice.loria.fr/publications/papers/2008/ManifoldHarmonics//photo/dragon_mhb.png

Chladni Plates

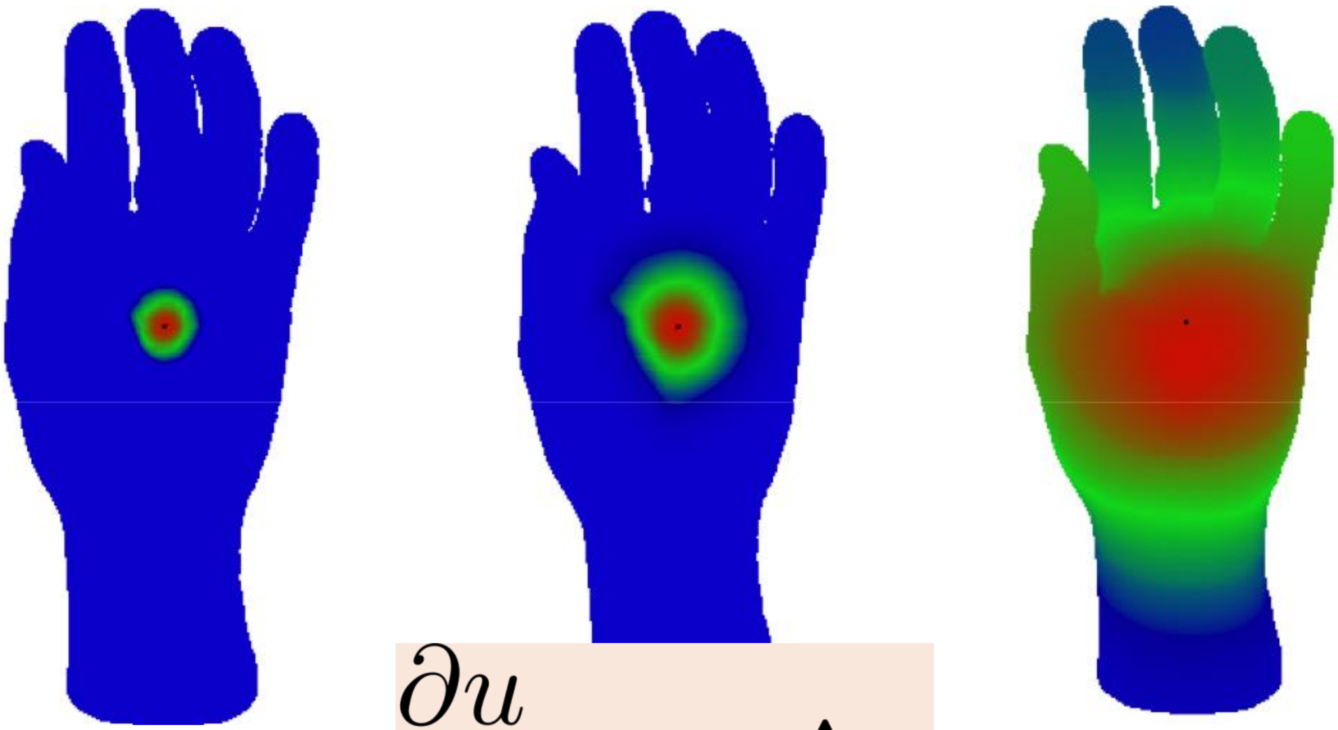
https://www.youtube.com/watch?v=CGiiSlMFFlI

Practical Application



https://www.youtube.com/watch?v=3uMZzVvnSiU

Additional Connection to Physics



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

http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf

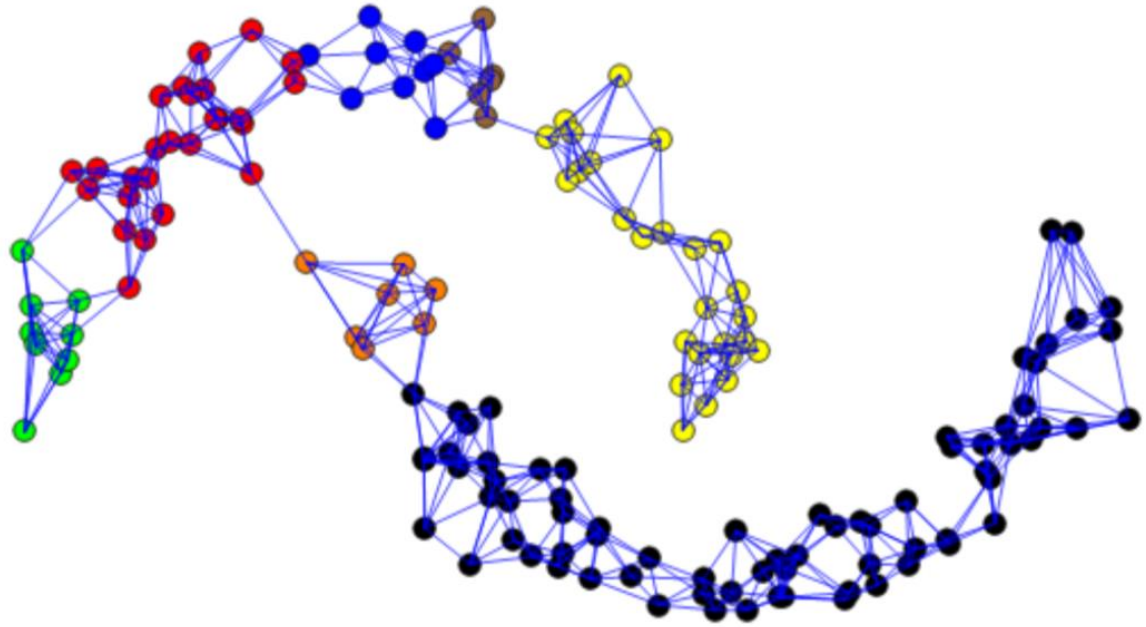
Heat equation

Q:

How can we approximate the Laplacian from data?

Option 1:

k-NN Graph Laplacian



http://math.ucdenver.edu/~sborgwardt/wiki/index.php/Spectral_clustering

Option 2:

Point Cloud Laplacian

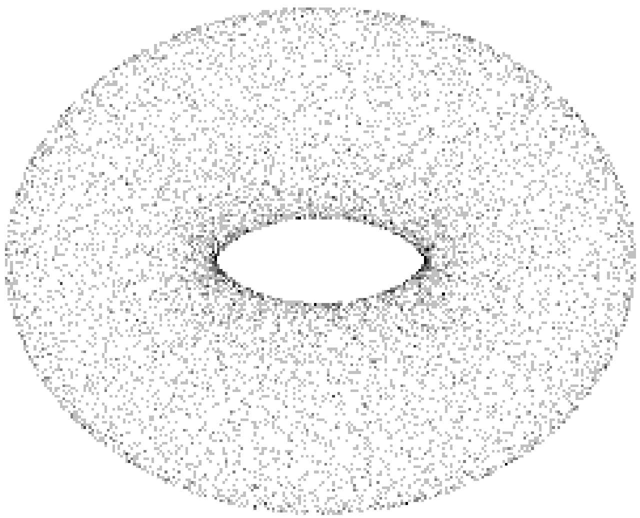
$$W_{ij} = \exp\left(-\frac{\|x_i - x_j\|^2}{t}\right)$$

Tricky parameter to choose

$$D_{ii} = \sum_j W_{ji}$$

$$L = D - W$$

$$Lf = \lambda D f$$



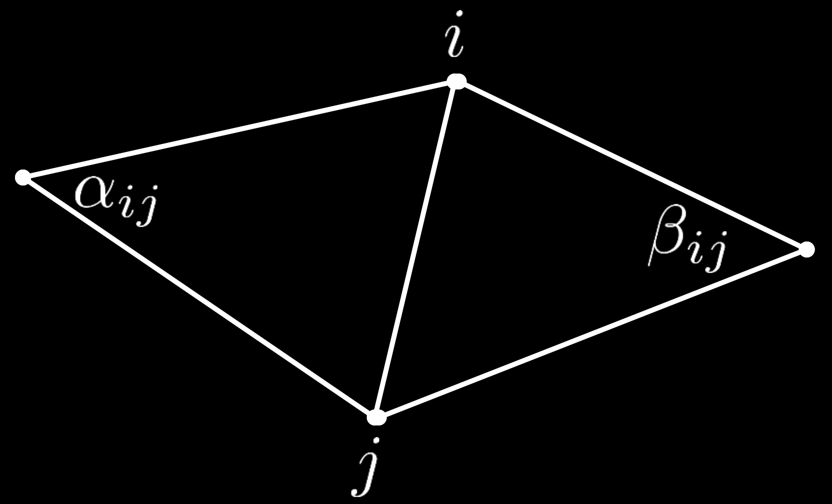
"Laplacian Eigenmaps for Dimensionality Reduction and Data Representation"

Belkin & Niyogi 2003

Aside: Preferred option on 2D meshes

The Cotangent Laplacian

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



Final Discussion

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!

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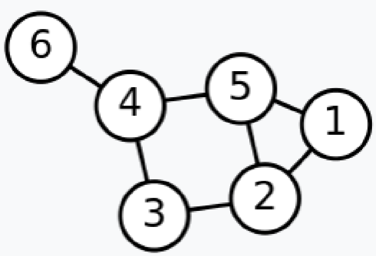
One Object, Many Interpretations

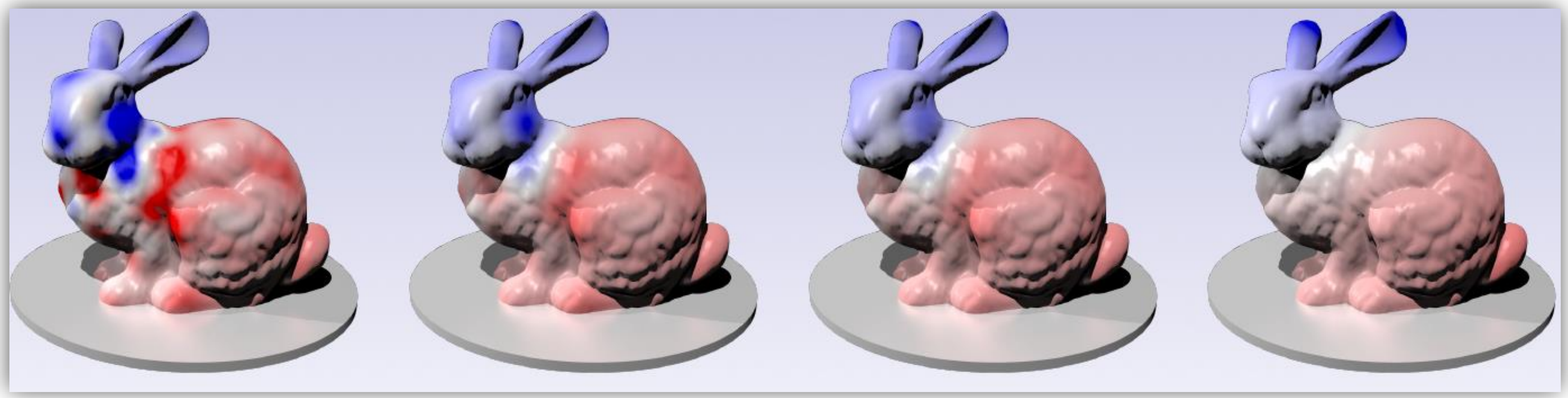
$$L_{vw} = A - D = \begin{cases} 1 & \text{if } v \sim w \\ -\text{degree}(v) & \text{if } v = w \\ 0 & \text{otherwise} \end{cases}$$

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

Deviation from neighbors

One Object, Many Interpretations



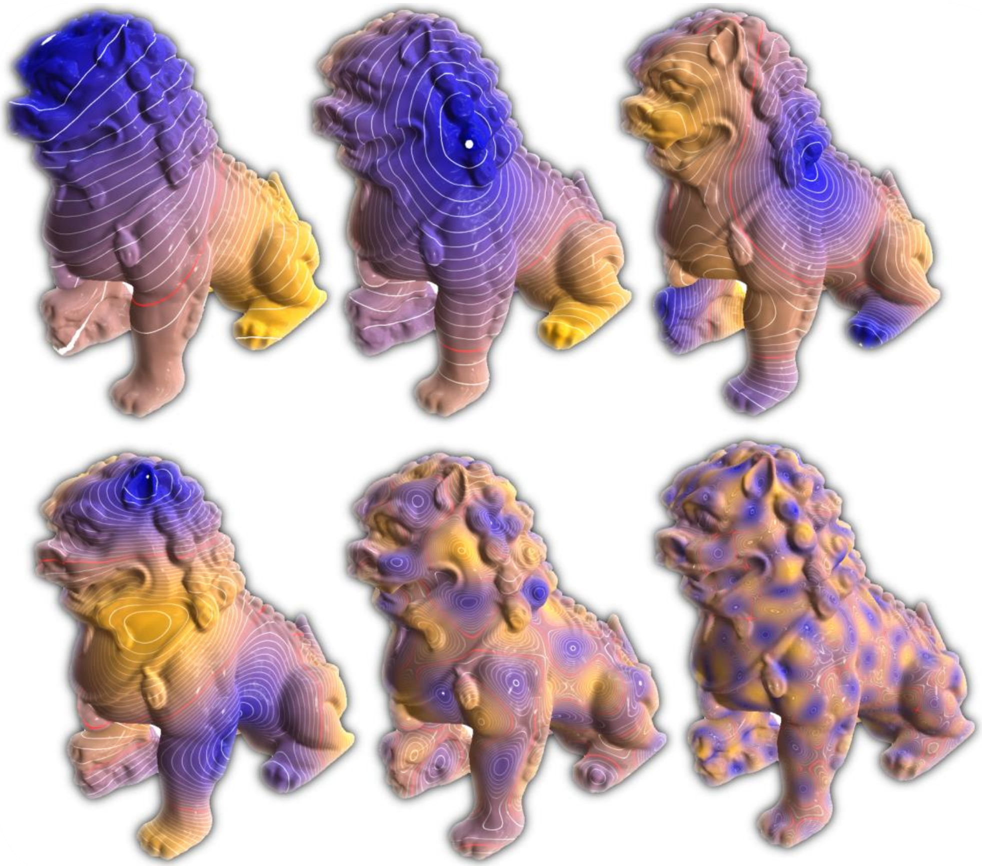
Decreasing ***E***

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

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/2008/ManifoldHarmonics//photo/dragon_mhb.png

Vibration modes

Isometry

[ahy-**som**-i-tree]:

Bending without stretching.

Intrinsic

[in-**trin**-sik]:

Invariant to isometry.

Why Study the Laplacian?

- **Encodes intrinsic geometry**
  Includes Riemannian metric on manifold
- **Multi-scale**
  Frequencies correspond to different feature sizes
- **Geometry through linear algebra**
  Linear/eigenvalue problems, sparse positive definite matrices
- **Connection to physics**
  Heat equation, wave equation, vibration, …

Final Discussion

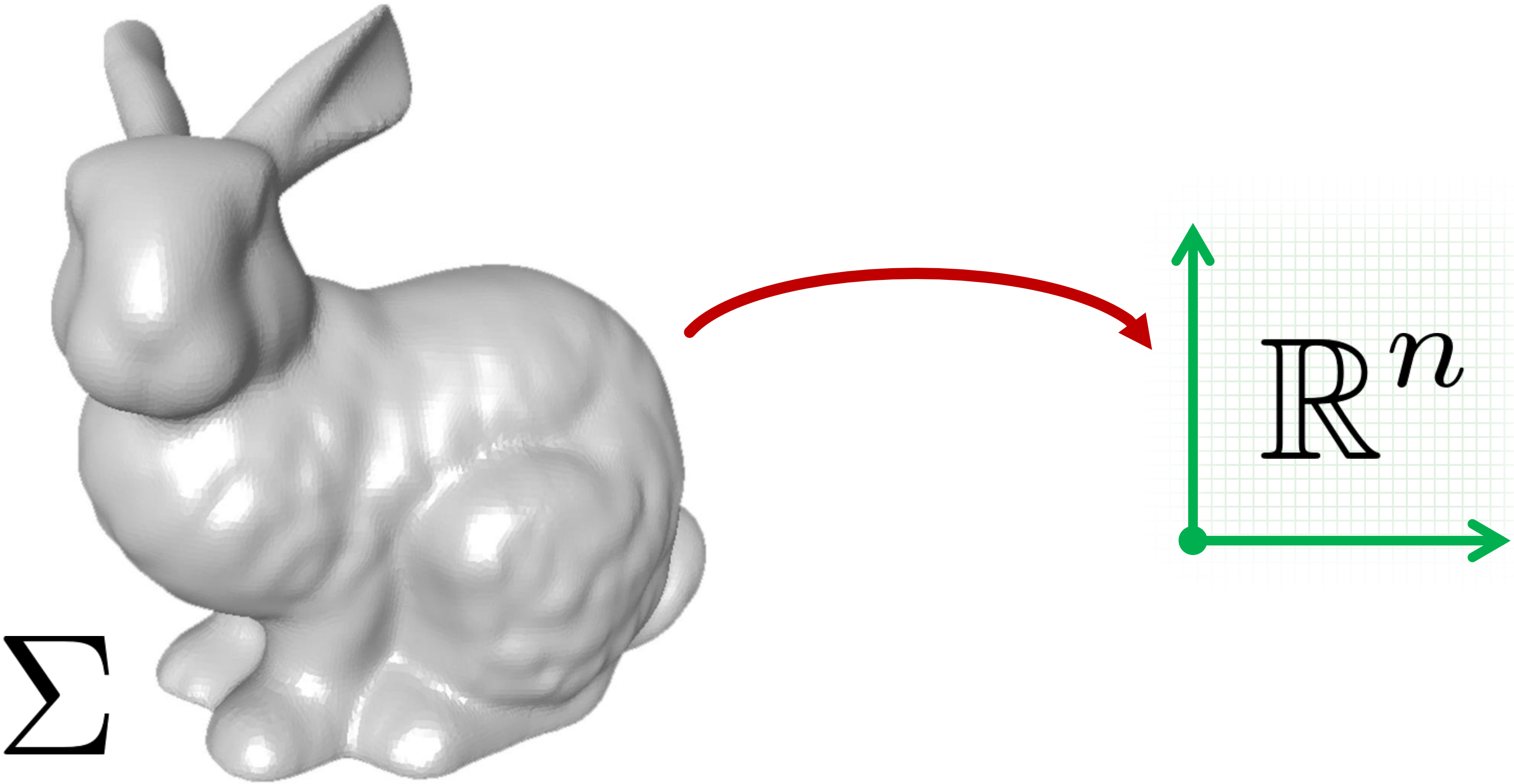
Discrete Laplacian operators:

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

Pointwise quantity

Descriptor Tasks

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

Desirable Properties

- **Distinguishing**

  Provides useful information about a point

- **Stable**

  Numerically and geometrically

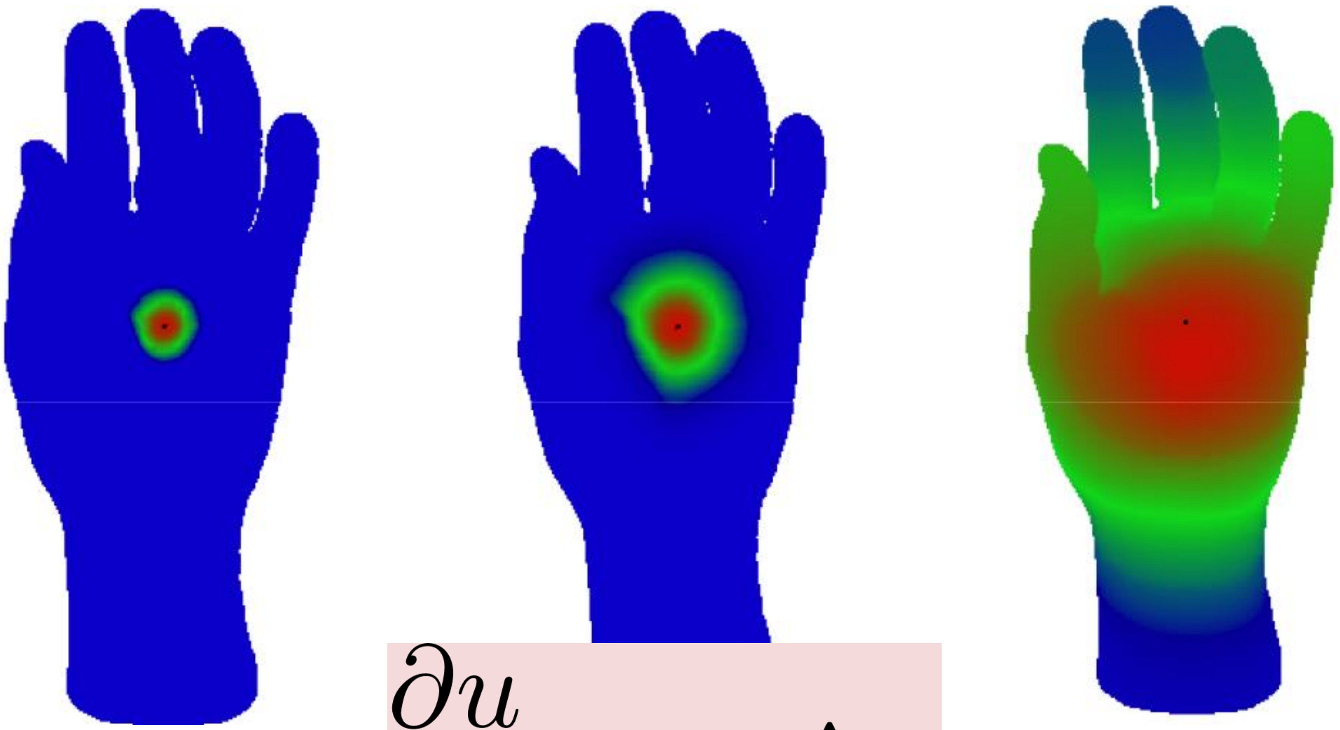
- **Intrinsic**

  No dependence on embedding

Sometimes undesirable!

Recall:

Connection to Physics



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

http://graphics.stanford.edu/courses/cs468-10-fall/LectureSlides/11_shape_matching.pdf

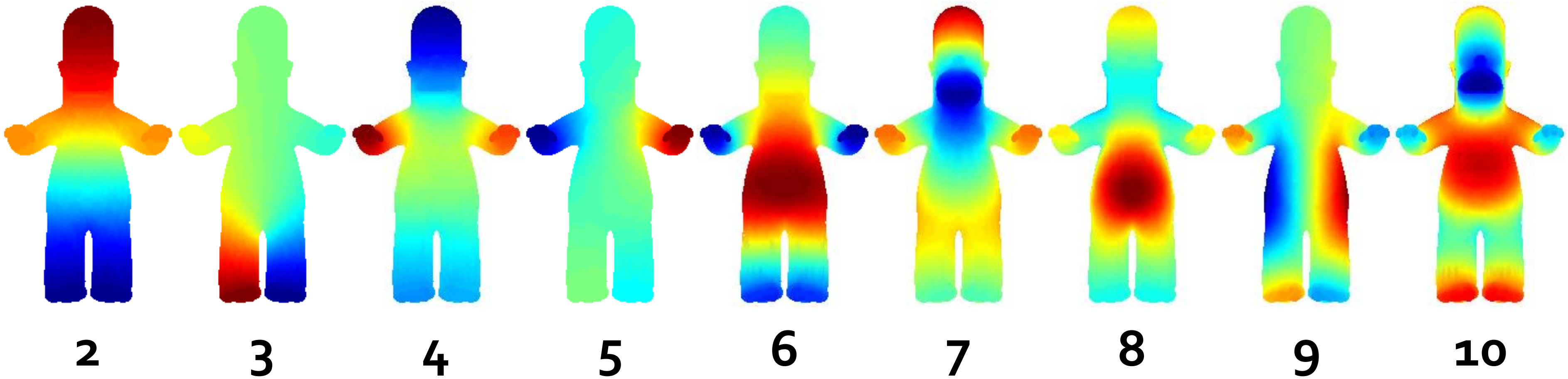
Heat equation

Intrinsic Observation

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

Example:

Global Point Signature



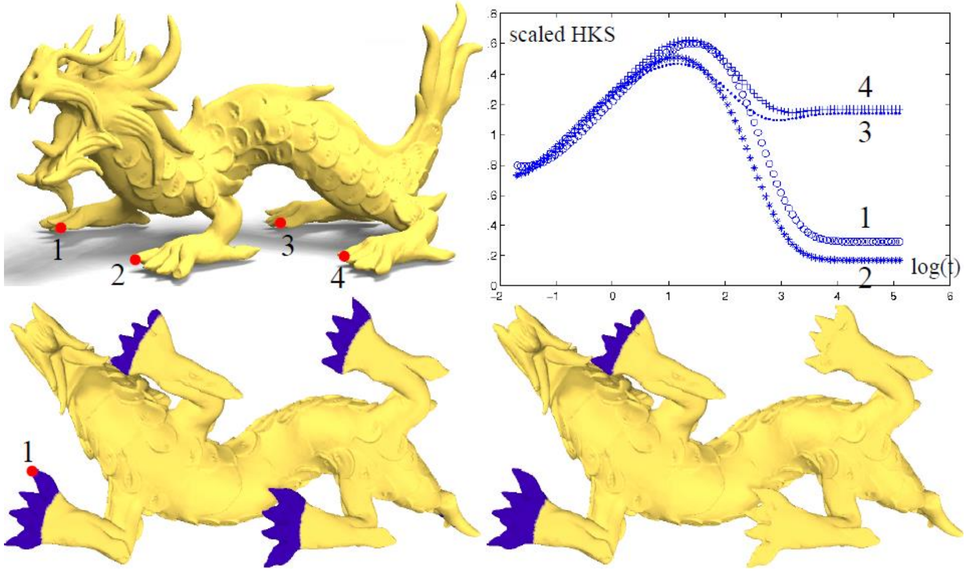
$$\mathrm{GPS}(p) := \left(-\frac{1}{\sqrt{\lambda_1}}\phi_1(p), -\frac{1}{\sqrt{\lambda_2}}\phi_2(p), -\frac{1}{\sqrt{\lambda_3}}\phi_3(p), \cdots \right)$$

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

Example:

Heat Kernel Signature (HKS)

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



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

Example:

Wave Kernel Signature (WKS)

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

HKS

WKS

vision.in.tum.de/_media/spezial/bib/aubry-et-al-4dmod11.pdf

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

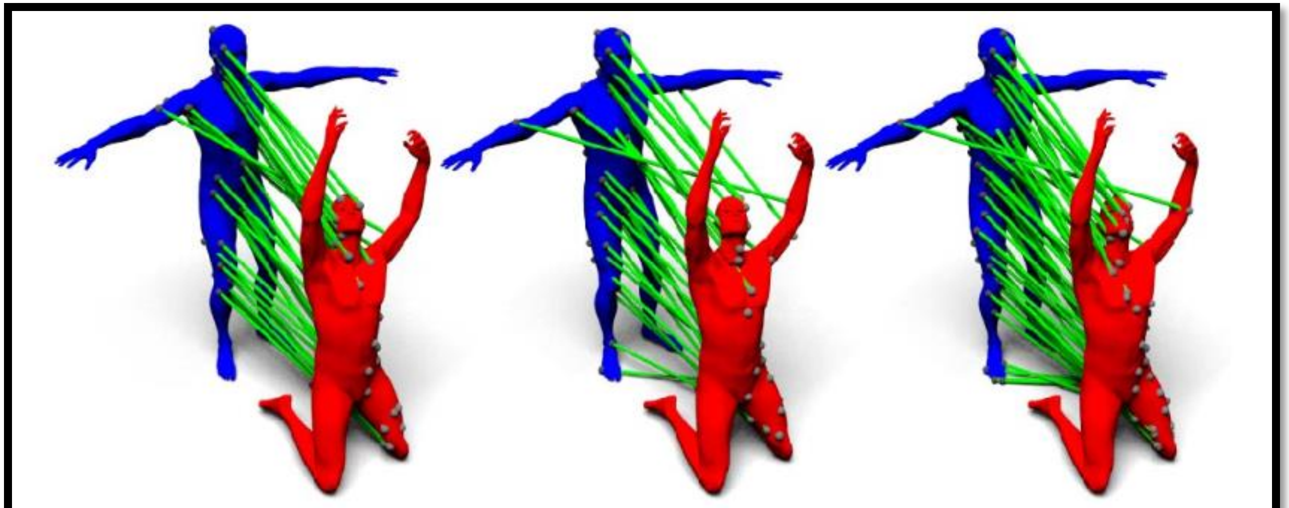


Fig. 3. Correspondences computed on TOSCA shapes using the spectral matching algorithm [30]. Shown are the matches with geodesic distance distortion below 10 percent of the shape diameter, from left to right: HKS (34 matches), WKS (30 matches), and trained descriptor (54 matches).

Learning Spectral Descriptors for Deformable Shape Correspondence

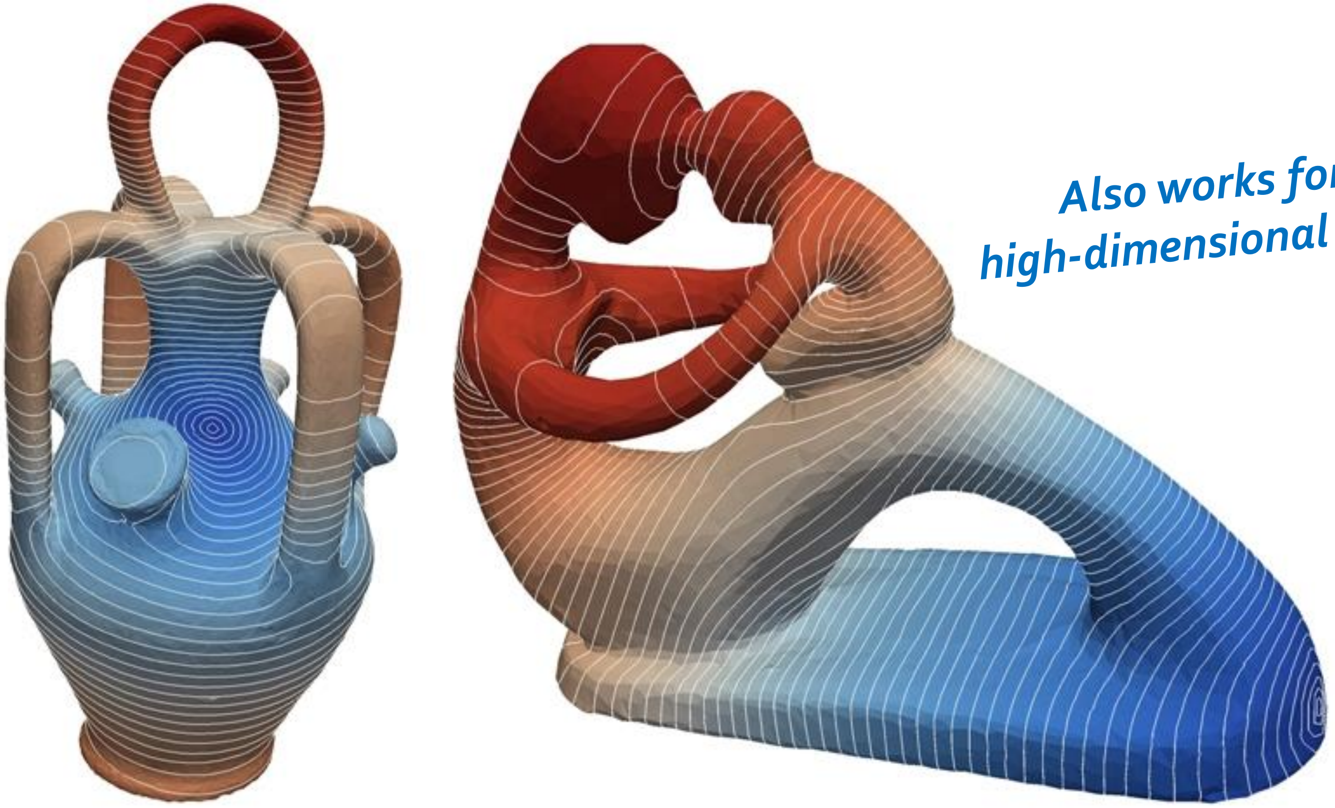
Litman and Bronstein; PAMI 2014

All Over the Place

Laplacians appear everywhere in shape analysis and machine learning.

Biharmonic Distances

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



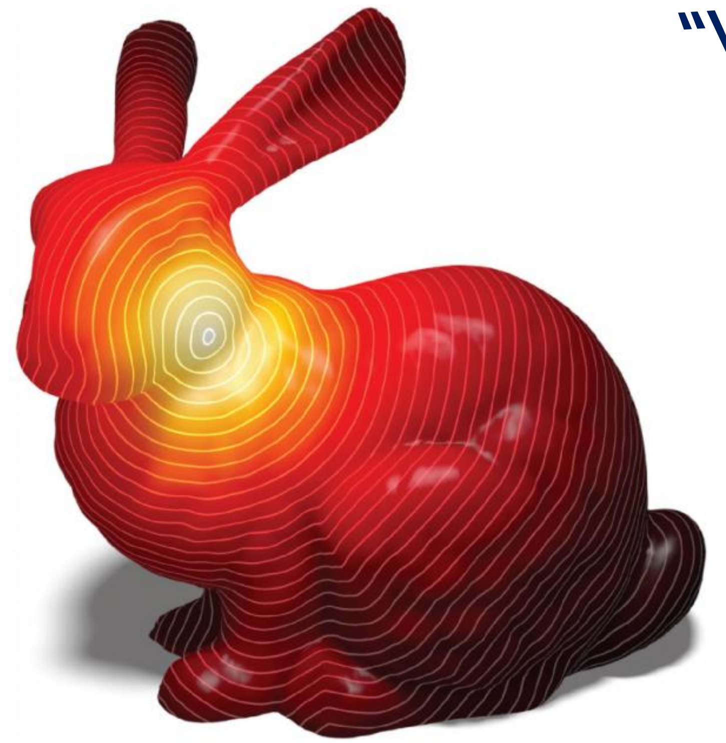
Also works for high-dimensional data!

"Biharmonic distance"
Lipman, Rustamov & Funkhouser, 2010

Geodesic Distances

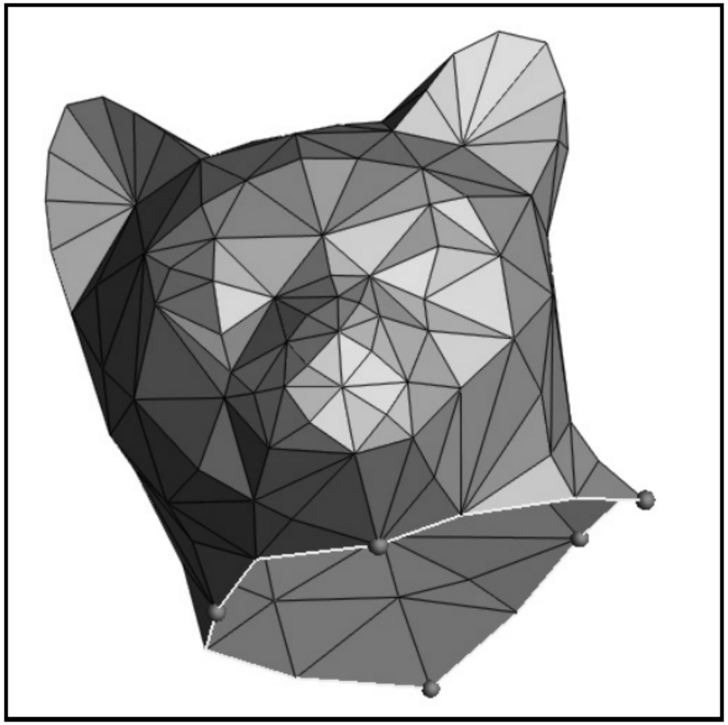
$$d_g(p,q) = \lim_{t \to 0} \sqrt{-4t \log k_{t,p}(q)}$$

"Varadhan's Theorem"

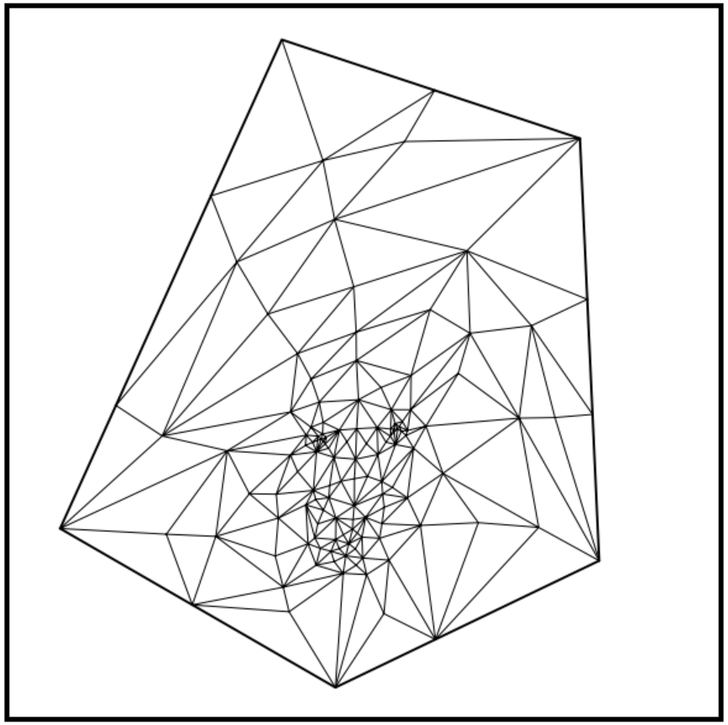


e.g. "Geodesics in heat"
Crane, Weischedel, and Wardetzky; TOG 2013

Parameterization: Harmonic Map



(a) Original mesh tile



(b) Harmonic embedding

Also works for high-dimensional data!

"Multiresolution analysis of arbitrary meshes"
Eck et al., 1995 (and many others!)

Final Discussion

Discrete Laplacian operators:

What are they good for?

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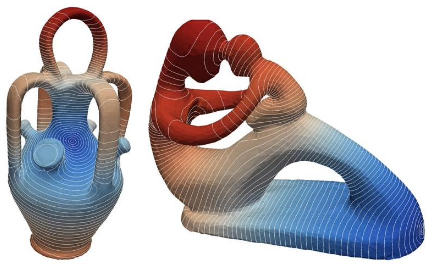
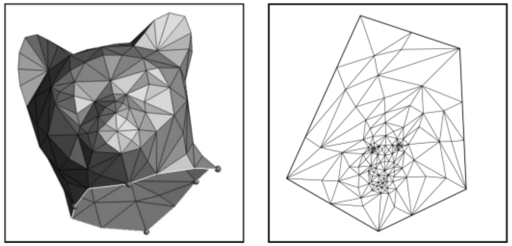
A popular field!

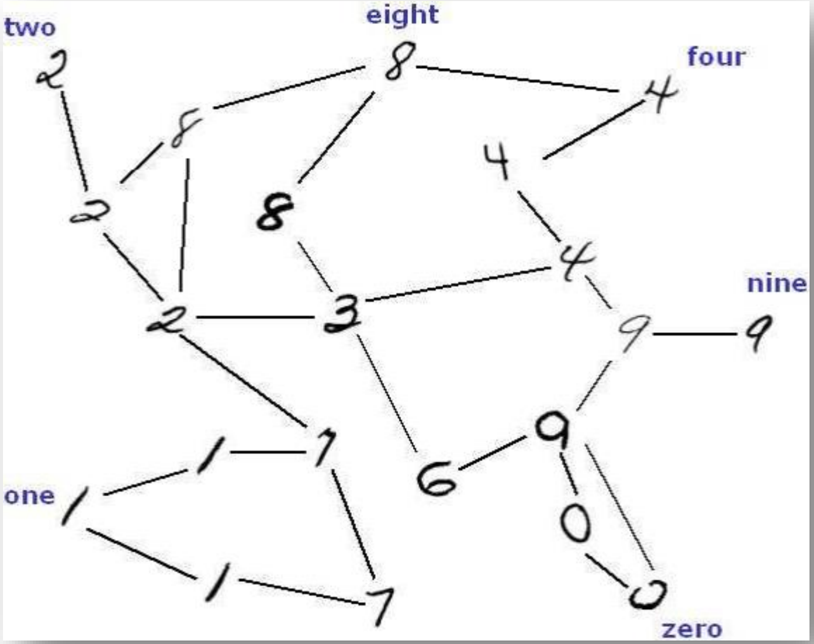
Observation

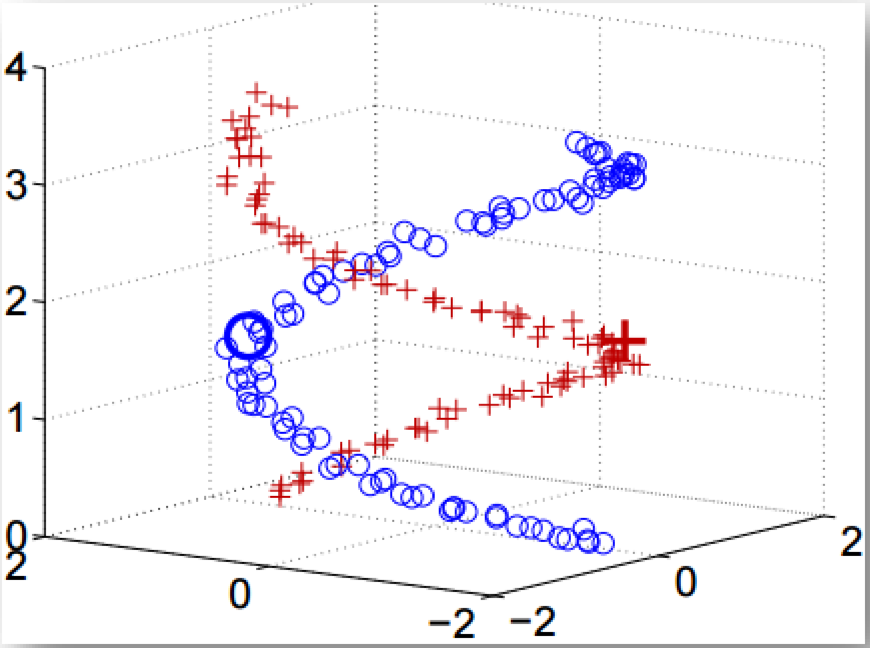
Most techniques we have already discussed apply in the high-dimensional case!





Semi-Supervised Learning





"Semi-supervised learning using Gaussian fields and harmonic functions"
Zhu, Ghahramani, & Lafferty 2003

Semi-Supervised Technique

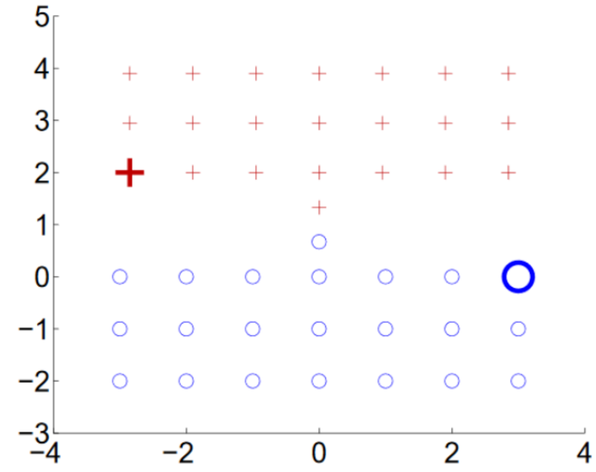
Given: ℓ labeled points $(x_1, y_1), \ldots, (x_\ell, y_\ell); y_i \in \{0, 1\}$

u unlabeled points $x_{\ell+1}, \ldots, x_{\ell+u}; \ell \ll u$

$$\min \frac{1}{2} \sum_{ij} w_{ij} (f(i) - f(j))^2$$

$$\text{s.t. } f(k) \text{ fixed } \forall k \leq \ell$$

Dirichlet energy → 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

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

$$\|f\|_I^2 := \int \underbrace{\|\nabla f(x)\|^2}_{\text{Dirichlet energy}} \, dx \approx f^\top L f$$

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

Examples of Manifold Regularization

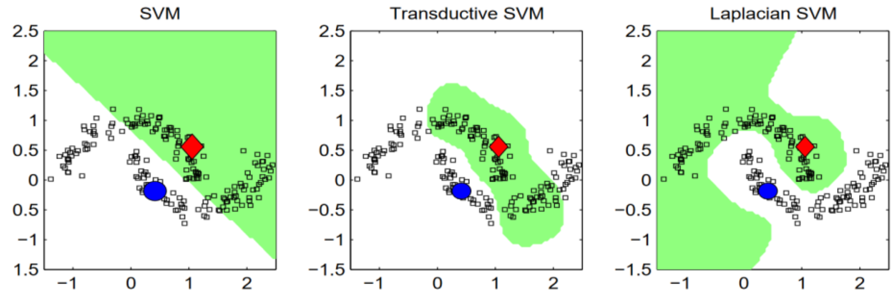
- **Laplacian-regularized least squares (LapRLS)**

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

- **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



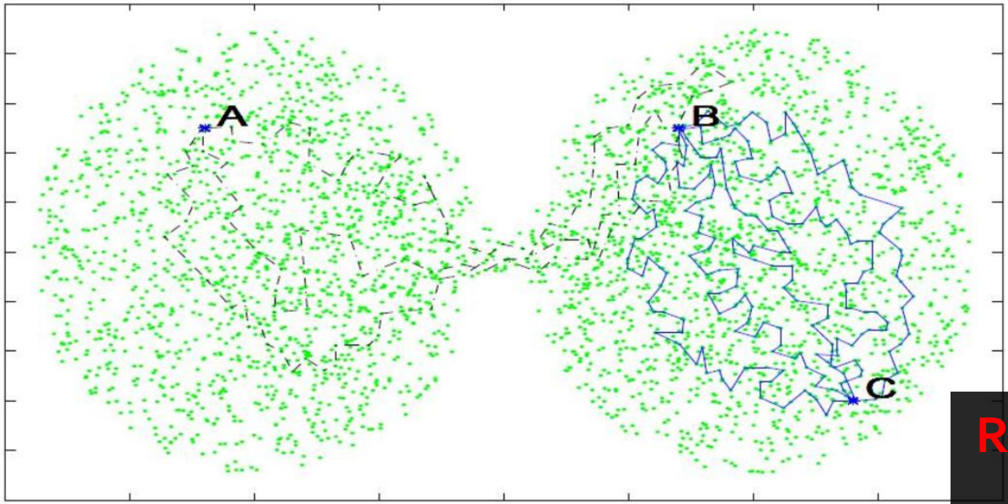
Diffusion Maps

Embedding from first *k* eigenvalues/vectors:

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

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

Image from http://users.math.yale.edu/users/gw289/CpSc-445-545/Slides/CPSC445%20-%20Topic%2010%20-%20Diffusion%20Maps.pdf (nice slides!)

Laplacian Operators

Justin Solomon

MLSS 2019

MIT EECS