

# Clustering and Segmentation

Justin Solomon

6.838: Shape Analysis  
Spring 2021



# A Confusing Distinction

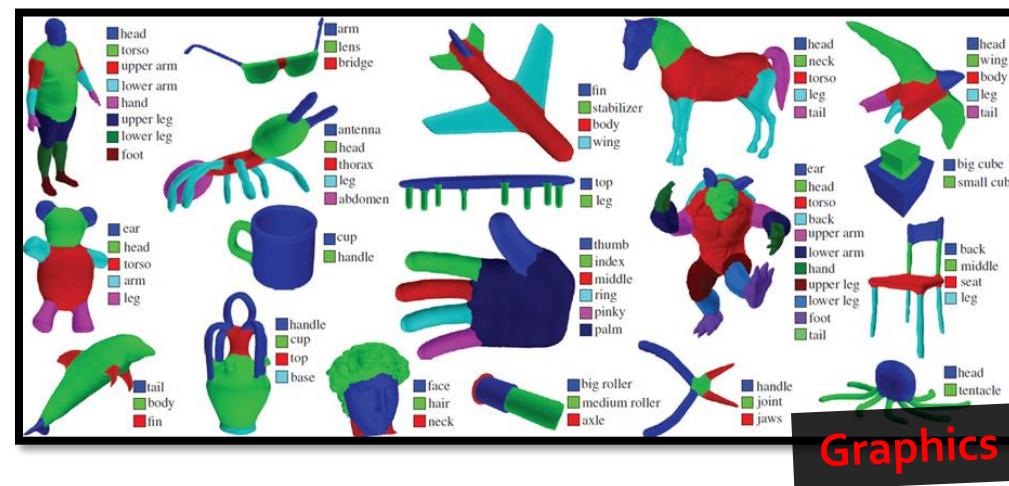
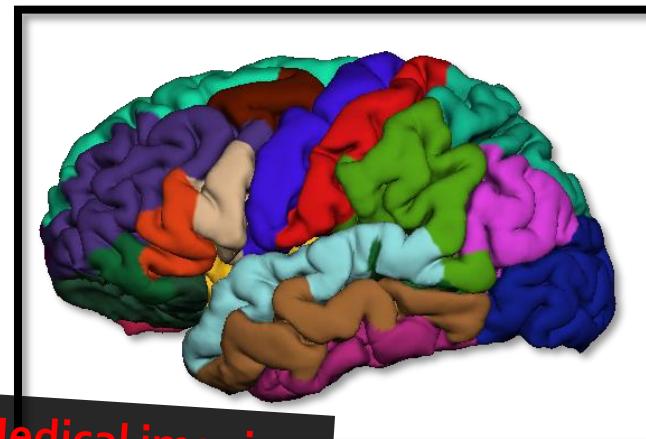
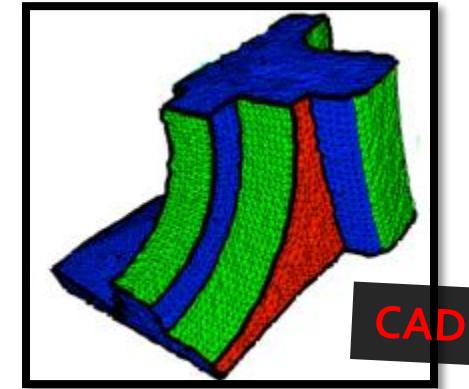
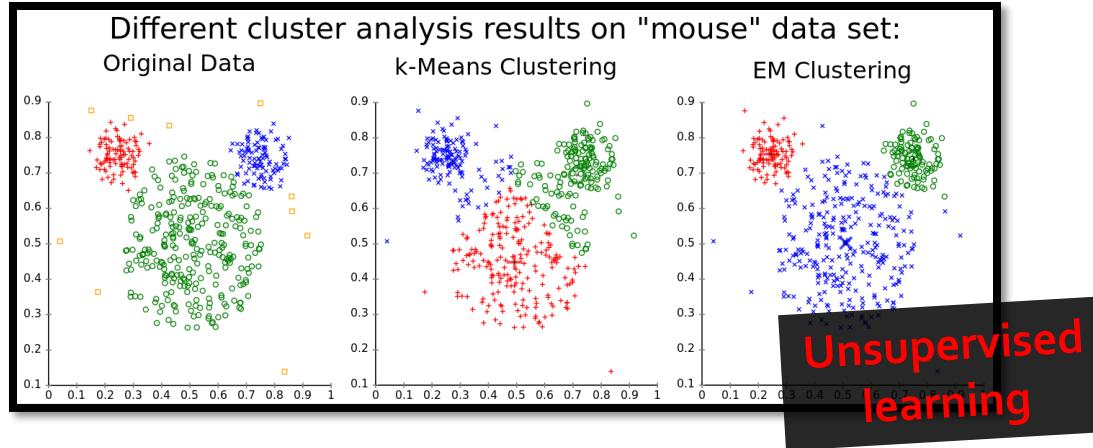
*For "Customer Data and Engagement:"*

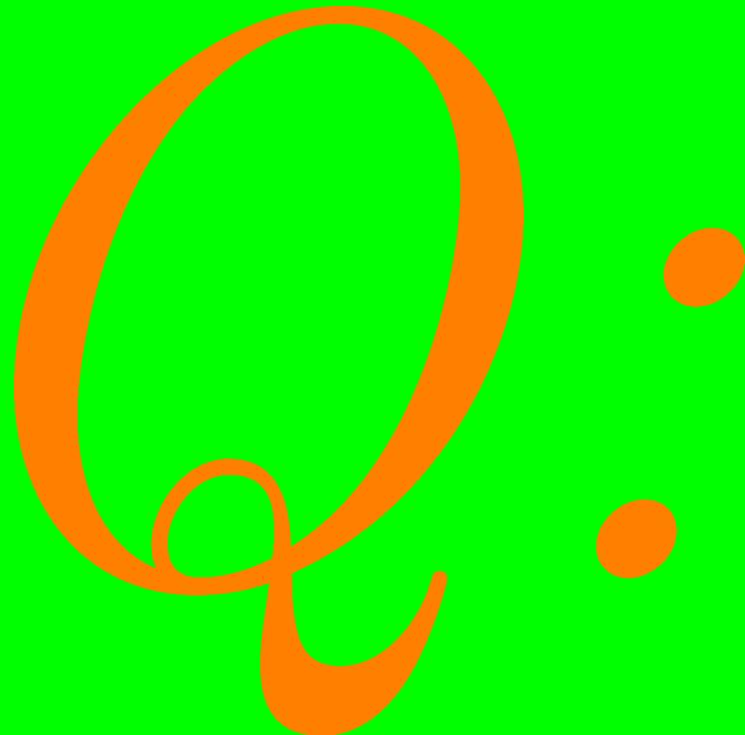
**"Segmenting is the process of putting customers into groups based on similarities, and clustering is the process of finding similarities in customers so that they can be grouped, and therefore segmented."**

# Our Objective

Divide a geometric domain  
into useful pieces.

# Many Applications



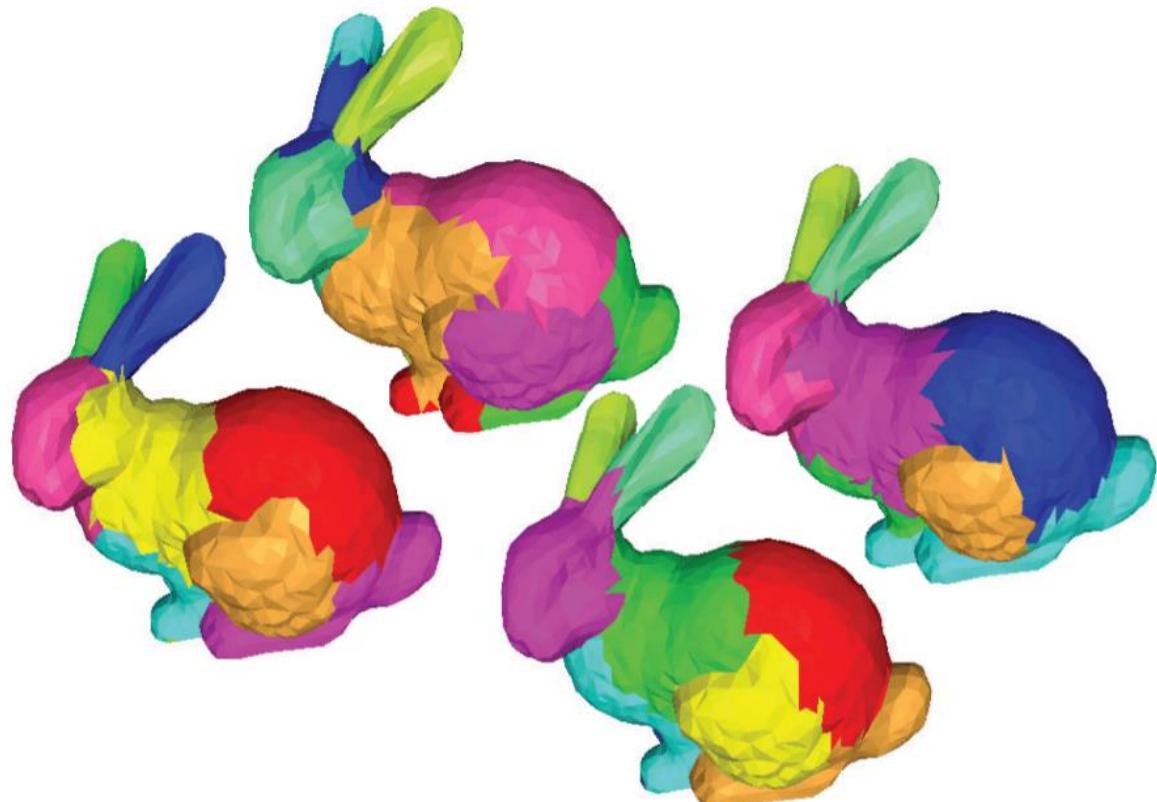


What is a good  
segmentation?

# What is a Good Segmentation?

Application dependent!

- Not an end in itself
- Unsolicited advice:  
**Be suspicious of general methods!**



# According to Facebook



Aaron Hertzmann

October 9, 2018 ·

...

One bit of sloppy writing that has permeated the computer graphics and vision literature is the use of the word "semantic." Here's why I think that you should avoid using it, or, at least, use it very carefully.

"Semantic" is a pretentious weasel-word. The word "semantic" is used in a way that means almost nothing, which is ironic. However, it sounds like it's implying some sort of insight about AI or human intelligence. I think that researchers use it when they want to indicate that there's some high-level knowledge or context involved, but they're too lazy to be concrete about it.

Instead of using the word "semantic," I suggest thinking more concretely about what you really mean, and saying that instead. You will probably find that your paper is clearer. It's a bit of extra work, but clear writing takes work.

As an example, our SIGGRAPH 2010 paper was the first paper to apply learned "semantic labeling" to 3D surfaces. I insisted that we avoid using the word "semantic" as much as possible. Instead, we wrote that our method learns to label object parts, such as "hand" or "wheel", and that the labels can be chosen by a user. Saying that we learn to apply these labels is much clearer than saying that our labeling is "semantic" or that we label "semantic parts", whatever that means.

Other typical uses (I am making these examples up) is to say "We let the user group regions based on semantic concerns" or "The video can be broken into parts based on semantics." What do these sentences add?

Doug DeCarlo first pointed this issue out to me about a decade ago. He pointed out that "semantics" is the study of meaning, like dictionary definitions; how the phrase "I like it" means something different from "It likes me." Objects in images do not have meanings in the same way. A hand or wheel does not have a meaning. He said that reading this usage of "semantic" was like "nails on a chalkboard," and now I feel that way too.

There's a descriptivist argument one can make: our community's language naturally evolves over time. However, this doesn't license arbitrary misuse of language; we shouldn't use "plus" to mean "minus". Misusing technical terms from other fields can cause lots of problems. Doug said that using "semantic" in this way makes you sound stupid to, say, a computational linguist who might review your grant proposal.

Whenever I see the word "semantic," I think that the author hasn't thought carefully about what they mean, and is only using this pretentious word because they think it sounds cool. Avoid being that person.

I do make one exception: for better or for worse, the term "semantic labeling" has come to mean a specific task in vision and in graphics. So I think it's fair to use the term in this case: this is the name of a task, and one must use shortcuts in names. The problem is that the word "semantic" is used all over in lots of other contexts where it means very little.

Fredo Durand, Alec Jacobson and 41 others

22 Comments



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Comment



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# Many Attempts to Standardize

A Benchmark Dataset and Evaluation Methodology for  
Video Object Segmentation

F. Perazzi

## A Benchmark for the Comparison of 3-D Motion Segmentation Algorithms

Roberto Tron René Vidal

Center for Imaging Science Johns Hopkins University



*Identification,  
Localisation, and  
Segmentation*



Over the past few years, a variety of motion segmentation methods have been proposed. However, these have only been tested on a handful of sequences, and object segmentation has often been tested on datasets with blur and artifacts. In this paper, we propose a new dataset for benchmarking algorithms for affine camera motion estimation and 3D mesh segmentation. The dataset consists of sequences of checkerboard patterns with truth segmentations, and it is used for a comprehensive analysis of state-of-the-art approaches using the spatial silhouette error metric. This work uncovers strengths and weaknesses of existing methods, opening up opportunities for future research.

### 1. Introduction

Motion segmentation is a key step for several applications such as surveillance, tracking and robotics. In the nineties, these applications mainly used several 2-D motion segmentation techniques aimed to separate the video frame into different regions. For example, a video frame can be divided into foreground and background regions.

In order to gauge the current state-of-the-art in automated whole-body image segmentation, we compare different methodological approaches. We are organizing the "VISCERAL" challenge for Identification, Localisation and Segmentation of the human body. For this purpose, we are making a dataset of clinical whole-body MR images.

### Call for participation

While a growing number of benchmarks exist to compare the performance of automated organ segmentation, there is no detection in images with restricted field of view. No efforts have been made to benchmark these and related automated identification and segmentation of bones, inner organs and relevant structures visible in an image volume of the trunk or even the whole body.

In order to gauge the current state-of-the-art in automated whole-body image segmentation, we compare different methodological approaches. We are organizing the "VISCERAL" challenge for Identification, Localisation and Segmentation of the human body. For this purpose, we are making a dataset of clinical whole-body MR images.



Figure 1: Composite image

## A Benchmark for 3D Mesh Segmentation

Xiaobai Chen, Aleksey Golovinskiy, Thomas Funkhouser  
Princeton University

IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 34, NO. 10, OCTOBER 2015

1993

## The Multimodal Brain Tumor Image Segmentation Benchmark (BraTS)

1st International Conference on Advances in Science, Engineering and Robotics Technology (ICASERT 2019)

*Performance Analysis and Benchmarking  
of Clustering Algorithms with gene datasets*

Bjoern H. Menze\*, A. Yuliya Burren, N. Marc-André Weber, Nicolas Cordier, Christopher R. D. Ben Glocker, P. Nigel M. John, Endre Doina Precup, Stephen Lawrence Schwartz,

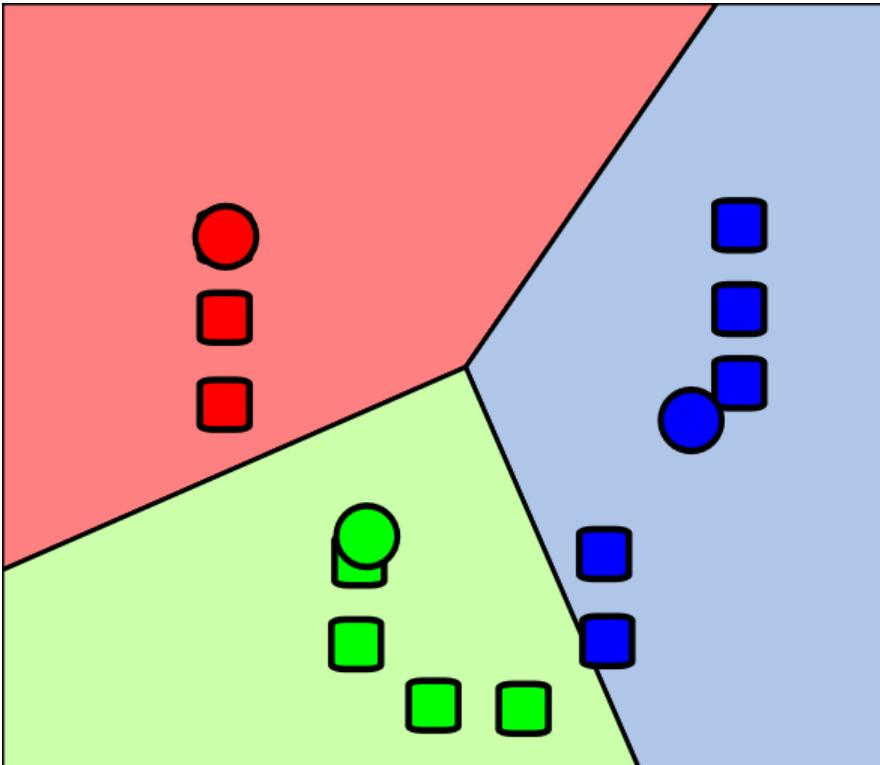
# Our Approach

A few interesting  
geometric methods.

Geometry can come from:

- Embedding of a dataset
- Structure of a surface mesh
- Metric learning

# Simplest Possible



$$\min_{S, \mu_i} \sum_{i=1}^k \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \mu_i\|^2$$

[https://upload.wikimedia.org/wikipedia/commons/d/d2/K\\_Means\\_Example\\_Step\\_4.svg](https://upload.wikimedia.org/wikipedia/commons/d/d2/K_Means_Example_Step_4.svg)

***k-means clustering***

# Alternating Algorithm

$$\min_{S, \mu_i} \sum_{i=1}^k \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \mu_i\|_2^2$$

Initialization?

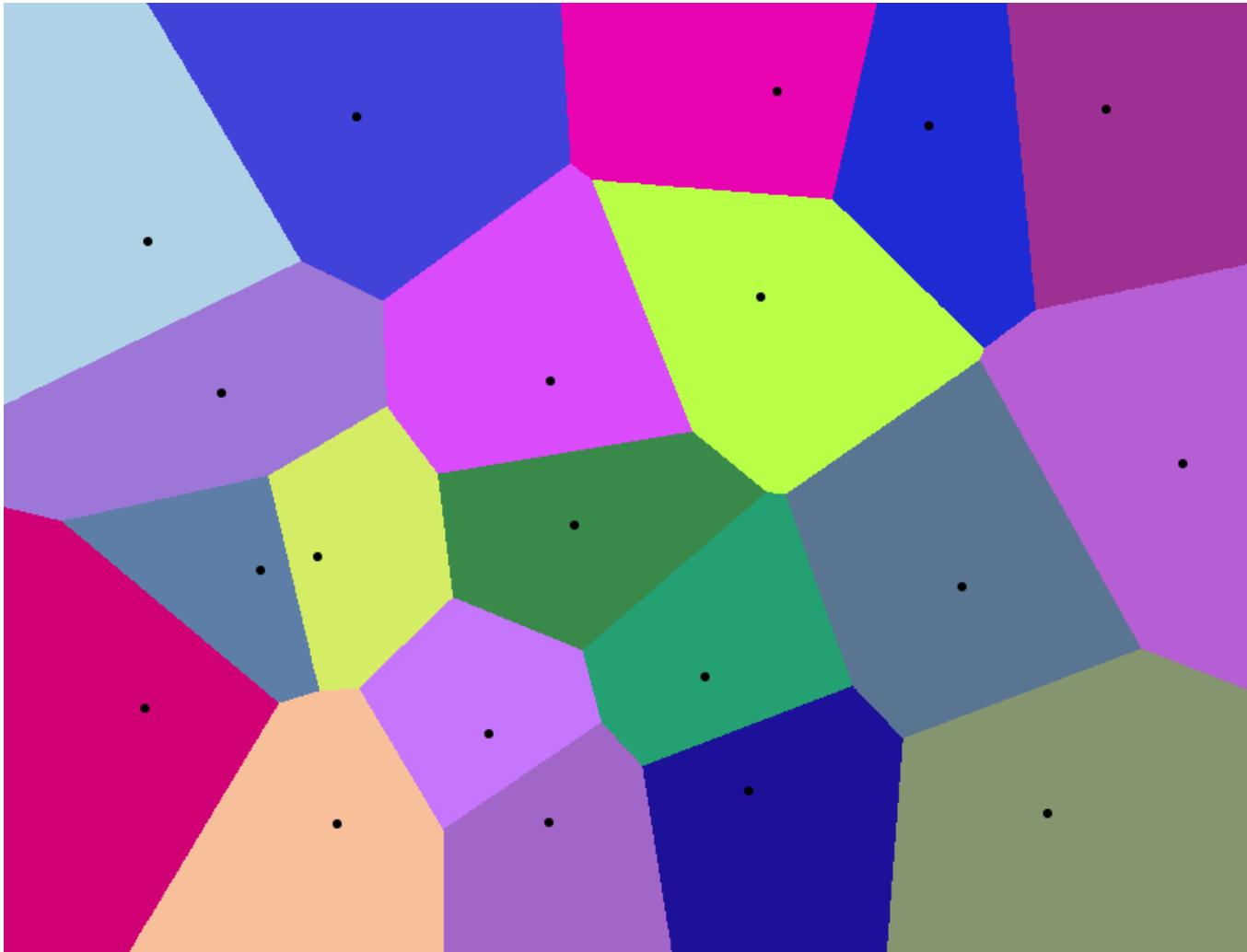
- Assignment step ( $S$ ): Voronoi cells

$$S_i \leftarrow \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x} - \mu_i\|_2 \leq \|\mathbf{x} - \mu_j\|_2 \forall j \neq i\}$$

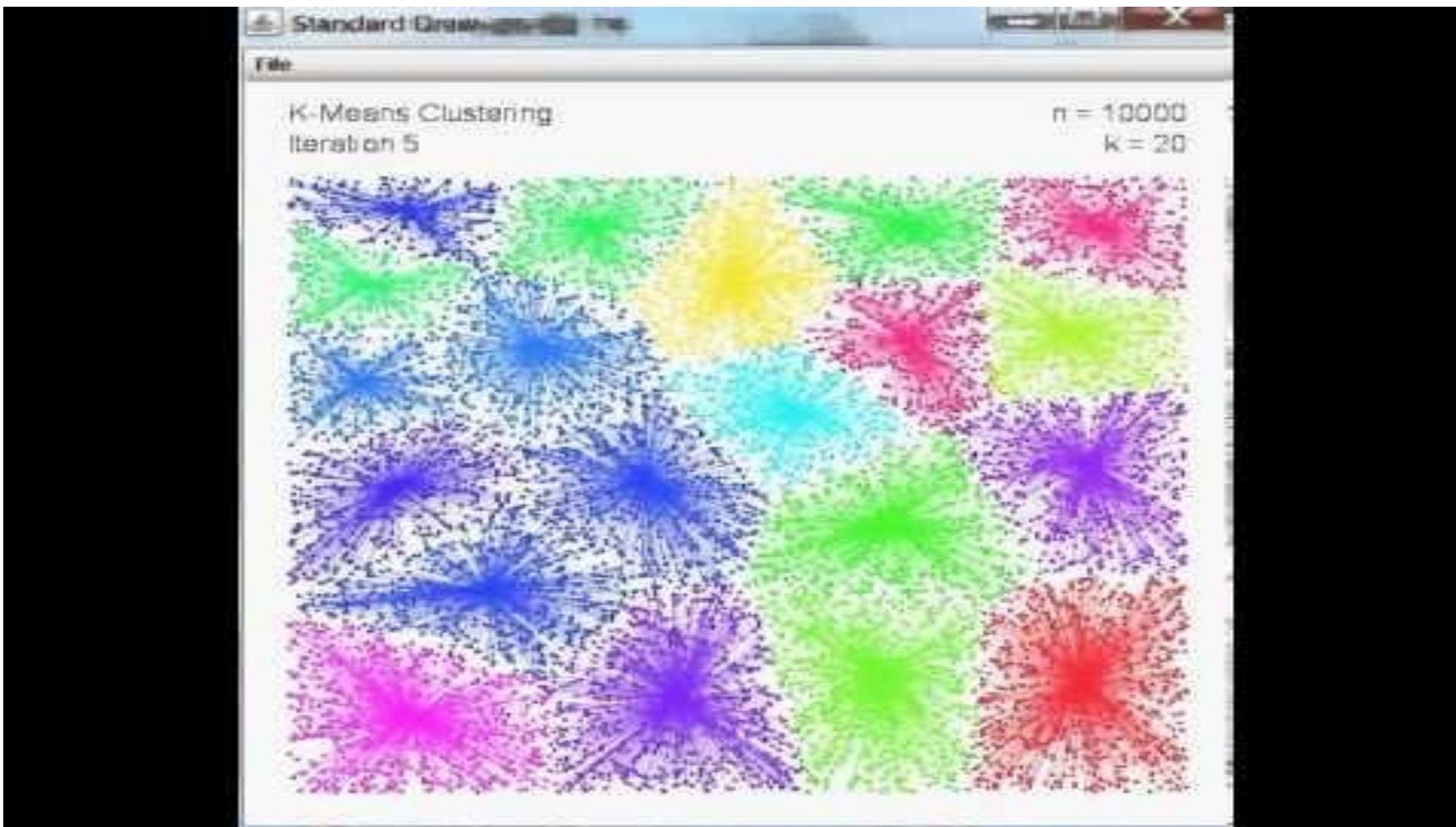
- Update step ( $\mu$ )

$$\mu_i \leftarrow \frac{1}{|S_i|} \sum_{\mathbf{x} \in S_i} \mathbf{x}$$

# Voronoi Diagram



# Example



# K-Means++

1. Choose one center uniformly at random.
2. For each data point  $x$  not yet chosen, compute  $D(x)$ , the distance between  $x$  and the nearest center that has already been chosen.
3. Choose a new center randomly, with probability proportional to  $D(x)^2$ .
4. Repeat 1-3 until  $k$  centers are chosen.
5. Proceed with  $k$ -means clustering.

**Theorem 1.1.** *For any set of data points,  $E[\phi] \leq 8(\ln k + 2)\phi_{OPT}$ .*

# Modern Seeding Algorithms: Many Options

## Scalable K-Means++

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## ABSTRACT

Over half a century old and showing no signs of aging, *k-means* remains one of the most popular data processing algorithms. As is well-known, a proper initialization of *k-means* is crucial for obtaining a good final solution. The recently proposed *k-means++* initialization algorithm achieves this, obtaining an initial set of centers that is provably close to the optimum solution. A major downside of the *k-means++* is its inherent sequential nature, which limits its applicability to massive data: one must make  $k$  passes over the data to find a good initial set of centers. In this work we show how to drastically reduce the number of passes needed to obtain, in parallel, a good initialization. This is unlike prevailing efforts on parallelizing *k-means* that have mostly focused on the post-initialization phases of *k-means*. We prove that our proposed initialization algorithm *k-means||* obtains a nearly optimal solution after a logarithmic number of passes, and then show that in practice a constant number of passes suffices. Experimental evaluation on real-world large-scale data demonstrates that *k-means||* outperforms *k-means++* in both sequential and parallel settings.

## 1. INTRODUCTION

Clustering is a central problem in data management and machine learning. It is a multi-faceted discipline that

single method — *k-means* — remains the most popular clustering method; in fact, it was identified as one of the top 10 algorithms in data mining [34]. The advantage of *k-means* is its simplicity: starting with a set of randomly chosen initial centers, one repeatedly assigns each input point to its nearest center, and then recomputes the centers given the point assignment. This local search, called *Lloyd's* iteration, continues until the solution does not change between two consecutive rounds.

The *k-means* algorithm has maintained its popularity even as datasets have grown in size. Scaling *k-means* to massive data is relatively easy due to its simple iterative nature. Given a set of cluster centers, each point can independently decide which center is closest to it and, given an assignment of points to clusters, computing the optimum center can be done by simply averaging the points. Indeed parallel implementations of *k-means* are readily available (see, for example, [cwiki.apache.org/MAHOUT/k-means-clustering.html](http://cwiki.apache.org/MAHOUT/k-means-clustering.html)).

From a theoretical standpoint, *k-means* is not a good clustering algorithm in terms of efficiency or quality: the running time can be exponential in the worst case [32, 4] and even though the final solution is locally optimal, it can be very far away from the global optimum (even under repeated random initializations). Nevertheless, in practice the speed and simplicity of *k-means* cannot be beat. Therefore, recent work has focused on improving the initialization procedure:

## Fast and Provably Good Seedings for $k$ -Means

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## Abstract

*Seeding* – the task of finding initial cluster centers – is critical in obtaining high-quality clusterings for  $k$ -Means. However,  $k$ -means++ seeding, the state of the art algorithm, does not scale well to massive datasets as it is inherently sequential and requires  $k$  full passes through the data. It was recently shown that Markov chain Monte Carlo sampling can be used to efficiently approximate the seeding step of  $k$ -means++. However, this result requires assumptions on the data generating distribution. We propose a simple yet fast seeding algorithm that produces *provably* good clusterings even *without assumptions* on the data. Our analysis shows that the algorithm allows for a favourable trade-off between solution quality and computational cost, speeding up  $k$ -means++ seeding by up to several orders of magnitude. We validate our theoretical results in extensive experiments on a

# Issue: Choice of $k$

*Informal intuition*  
“Elbow method:”  
Look at percentage of variance explained by clusters (vague!)

*J. R. Statist. Soc. B (2001)  
63, Part 2, pp. 411–423*

## Estimating the number of clusters in a data set via the gap statistic

Robert Tibshirani, Guenther Walther and Trevor Hastie

*Stanford University, USA*

[Received February 2000. Final revision November 2000]

**Summary.** We propose a method (the ‘gap statistic’) for estimating the number of clusters (groups) in a set of data. The technique uses the output of any clustering algorithm (e.g.  $K$ -means or hierarchical), comparing the change in within-cluster dispersion with that expected under an appropriate reference null distribution. Some theory is developed for the proposal and a simulation study shows that the gap statistic usually outperforms other methods that have been proposed in the literature.

**Keywords:** Clustering; Groups; Hierarchy;  $K$ -means; Uniform distribution

### 1. Introduction

Cluster analysis is an important tool for ‘unsupervised’ learning—the problem of finding groups in data without the help of a response variable. A major challenge in cluster analysis is the estimation of the optimal number of ‘clusters’. Fig. 1(b) shows a typical plot of an error measure  $W_k$  (the within-cluster dispersion defined below) for a clustering procedure *versus* the number of clusters  $k$  employed: the error measure  $W_k$  decreases monotonically as the number of clusters  $k$  increases, but from some  $k$  onwards the decrease flattens markedly. Statistical folklore has it that the location of such an ‘elbow’ indicates the appropriate number of clusters. The goal of this paper is to provide a statistical procedure to formalize that heuristic.

For recent studies of the elbow phenomenon, see Sugar (1998) and Sugar *et al.* (1999). A comprehensive survey of methods for estimating the number of clusters is given in Milligan and Cooper (1985), whereas Gordon (1999) discusses the best performers. Some of these methods are described in Sections 5 and 6, where they are compared with our method.

In this paper we propose the ‘gap’ method for estimating the number of clusters. It is designed to be applicable to virtually any clustering method. For simplicity, the theoretical

“Gap statistic”

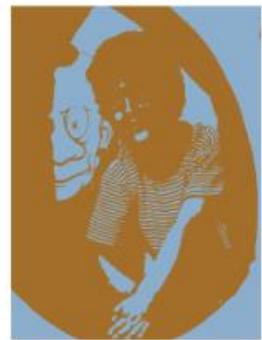
$$D_i := \sum_{\mathbf{x}, \mathbf{x}' \in S_i} \|\mathbf{x} - \mathbf{x}'\|_2^2$$

$$W_k := \sum_{i=1}^k \frac{1}{2n_i} D_i$$

$$\text{Gap}_n(k) := \mathbb{E}_n^*[\log W_k] - \log W_k$$

# Application to Color Space

K=2



K=3



K=10



Original



4%



8%



17%



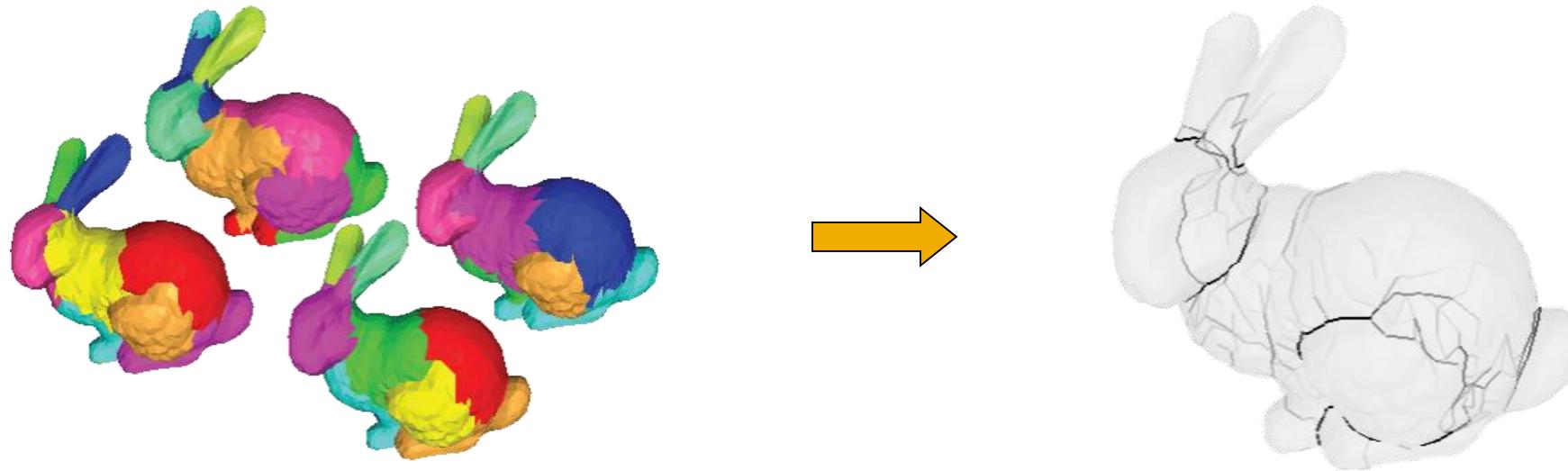
# Can Apply to Features



**Figure 1:** *The k-means clustering on the GPS coordinates results in a pose invariant segmentation.*

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

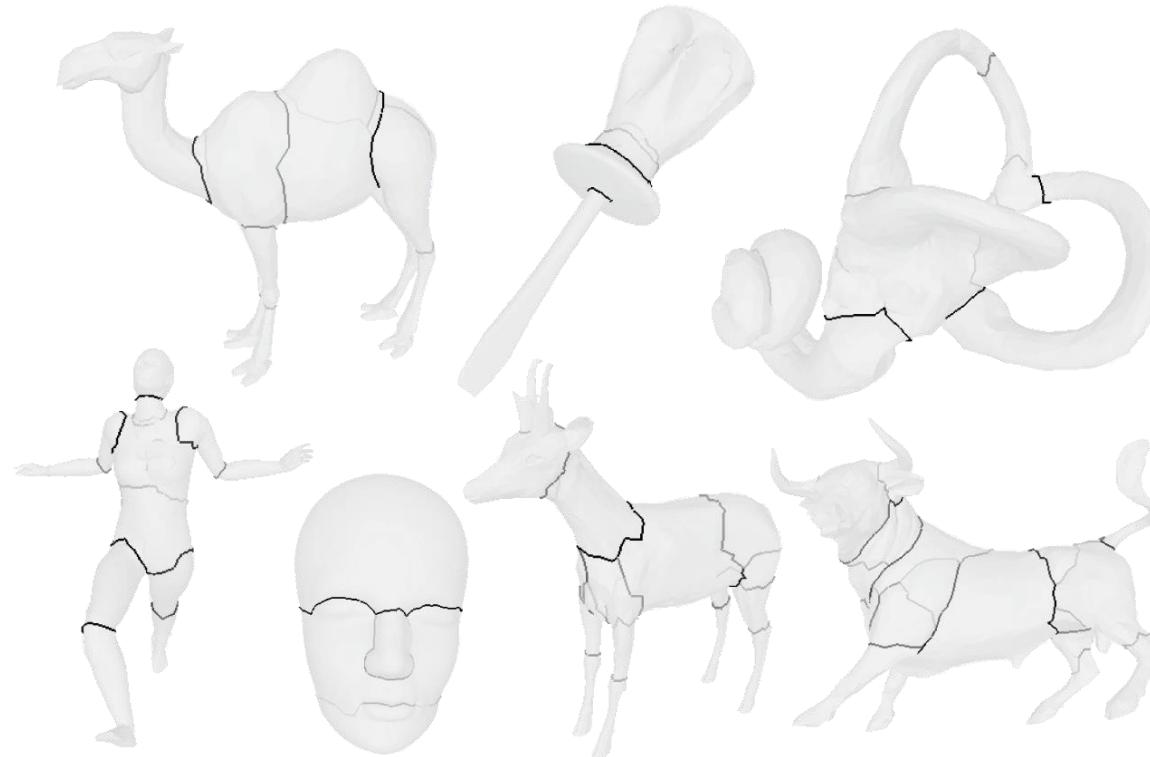
# Dependence on Initial Guess



["Randomized Cuts for 3D Mesh Analysis."](#)  
Golovinskiy and Funkhouser; SIGGRAPH Asia 2008

Bug ... or feature?

# Dependence on Initial Guess



["Randomized Cuts for 3D Mesh Analysis."](#)  
Golovinskiy and Funkhouser; SIGGRAPH Asia 2008

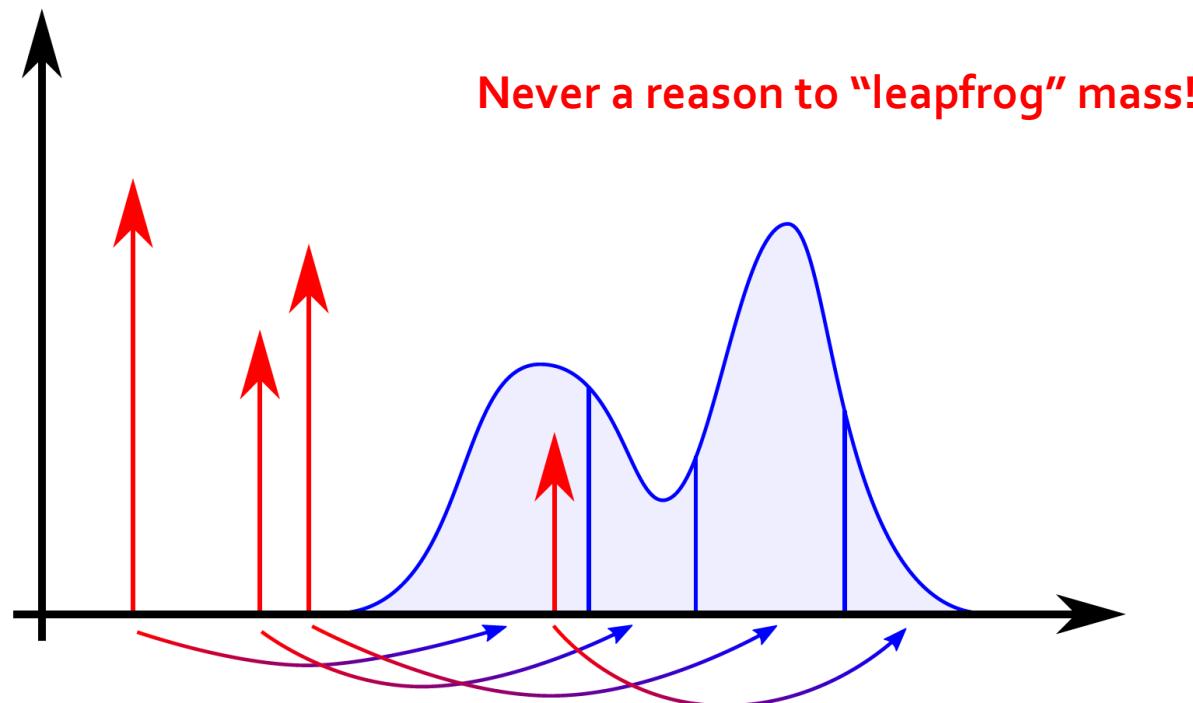
Bug ... or feature?

*Link to past lecture:*

# Semidiscrete Transport

$$\mu_0 := \sum_{i=1}^{k_0} a_{0i} \delta_{\mathbf{x}_{0i}}$$

$$\mu_1(S) := \int_S \rho_1(\mathbf{x}) d\mathbf{x}$$

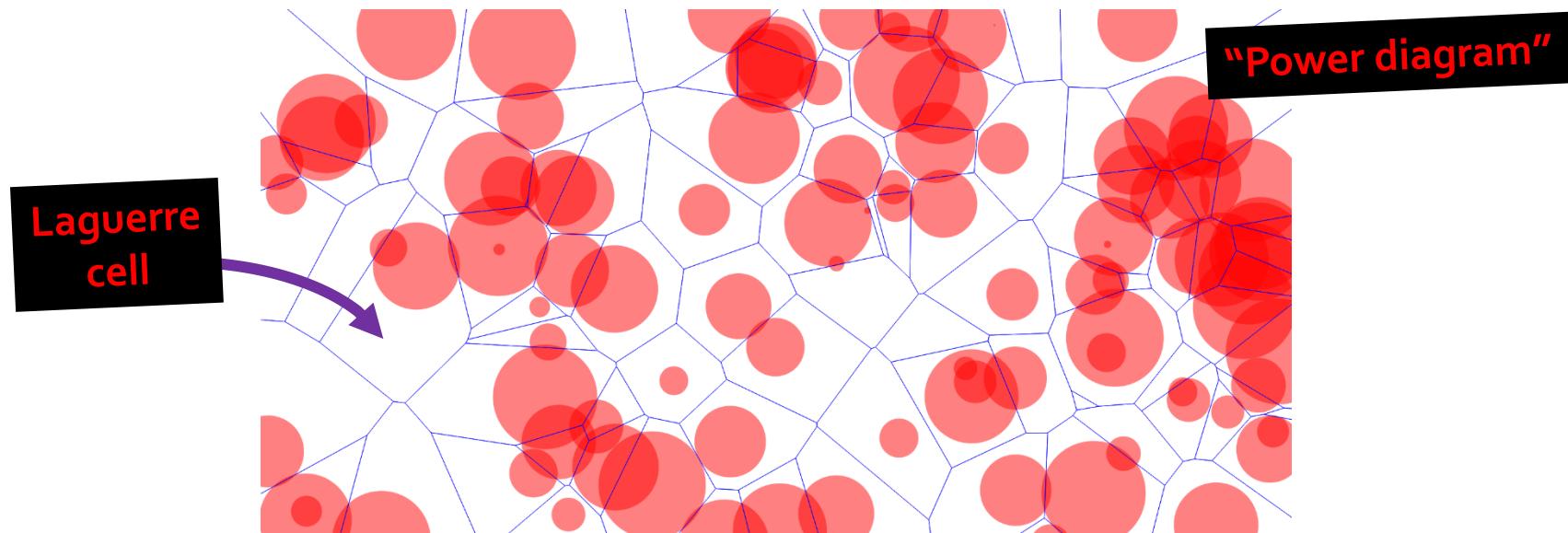


# Semidiscrete Transport

$$\mu_0 := \sum_{i=1}^k a_i \delta_{\mathbf{x}_i}$$

$$\nu(S) := \int_S \rho(\mathbf{x}) d\mathbf{x}$$

$$\mathcal{W}_2^2(\mu, \nu) = \sup_{\phi \in \mathbb{R}^k} \sum_i \left[ a_i \phi_i + \int_{\text{Lag}_{\phi}^c(\mathbf{x}_i)} \rho(\mathbf{y}) [c(\mathbf{x}_i, \mathbf{y}) - \phi_i] dA(\mathbf{y}) \right]$$
$$\text{Lag}_{\phi}^c(\mathbf{x}_i) := \{\mathbf{y} \in \mathbb{R}^n : c(\mathbf{x}_i, \mathbf{y}) - \phi_i \leq c(\mathbf{x}_j, \mathbf{y}) - \phi_j \ \forall j \neq i\}$$



# Measure Quantization Problem (Balanced k-means)

Approximate by a **discrete measure**:

$$\frac{1}{k} \sum_{i=1}^k \delta_{\mathbf{x}_i}$$

Solve for *positions* of the points  $x_i$ .

# Kantorovich Dual Problem

$$F[f, x_1, \dots, x_m] = \frac{1}{m} \sum_{i=1}^m f_i + \sum_{i=1}^m \int_{V_{x_i}} (d(x_i, y)^2 - f_i) d\mu_2(y)$$

weights                      Power diagram regions

*Alternating algorithm:*

## 1. Update weights

Stochastic gradient descent

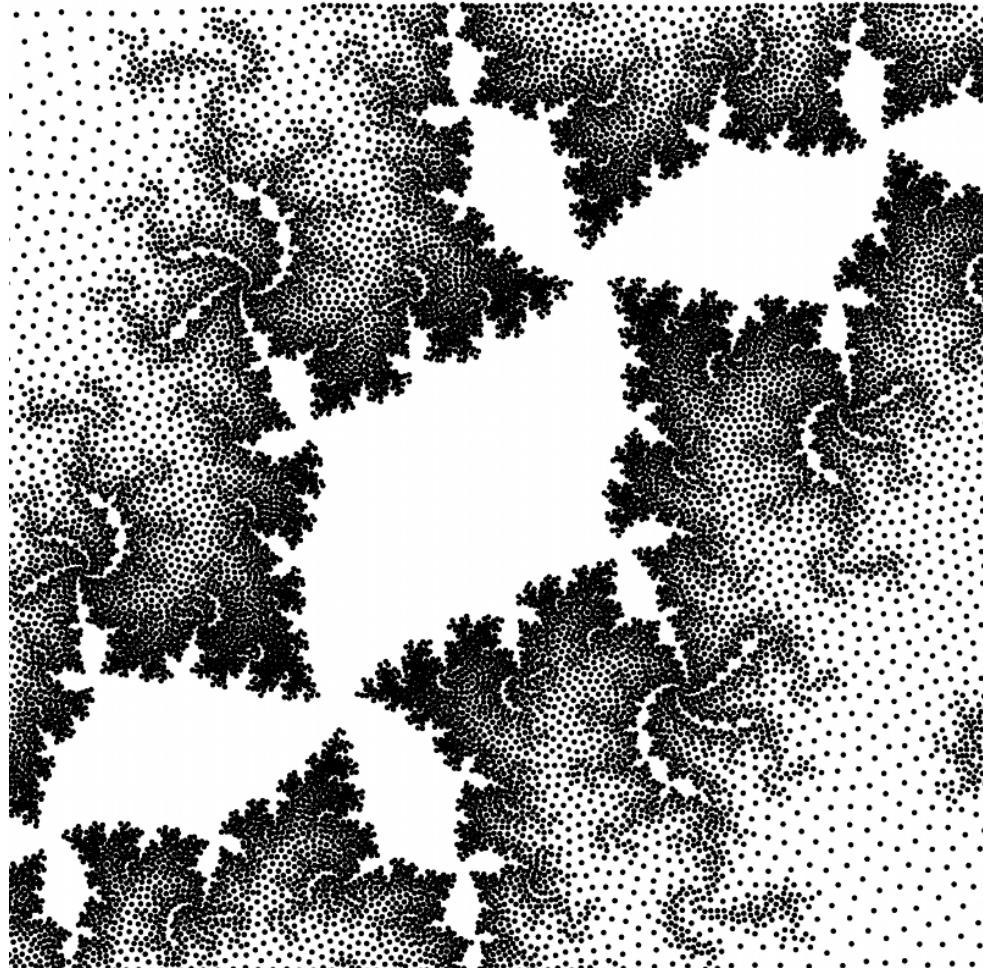
$$\frac{\partial F}{\partial f_i} = \frac{1}{m} - \int_{V_{x_i}} d\mu_2(y)$$

## 2. Update points

Fixed-point iteration

$$\frac{\partial F}{\partial x_i} = x_i \int_{V_{x_i}} d\mu_2(y) - \int_{V_{x_i}} y d\mu_2(y)$$

# Related Algorithm for Low-Dimensional Problems



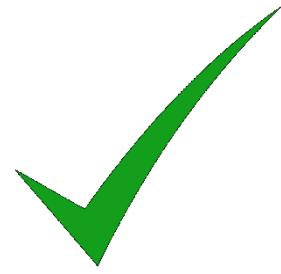
De Goes et al. "Blue Noise through Optimal Transport." SIGGRAPH Asia 2012.

# Geometry of $k$ -Means

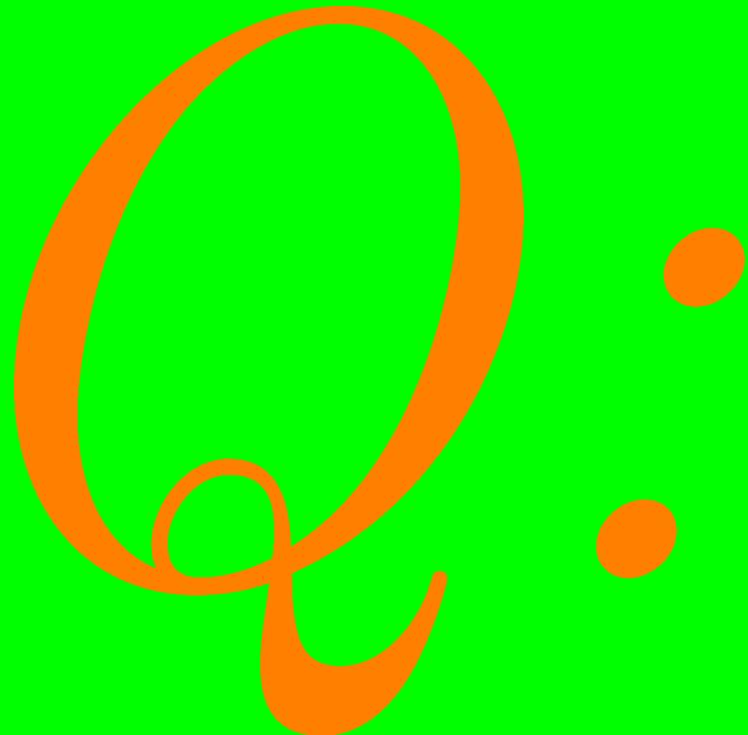
- Assignment step
  - Assign point to its **closest** cluster center
- Update step
  - **Average** all points in a cluster

Doesn't have to be Euclidean

# Geometry of $k$ -Means

- Assignment step 
  - Assign point to its **closest** cluster center
- Update step 
  - **Average** all points in a cluster

In a metric space



What does it mean to  
**average** points in a  
metric space?

# Fréchet Mean

aka  
“Karcher mean”

$$\arg \min_{p \in M} \sum_{i=1}^N d(p, x_i)^2$$

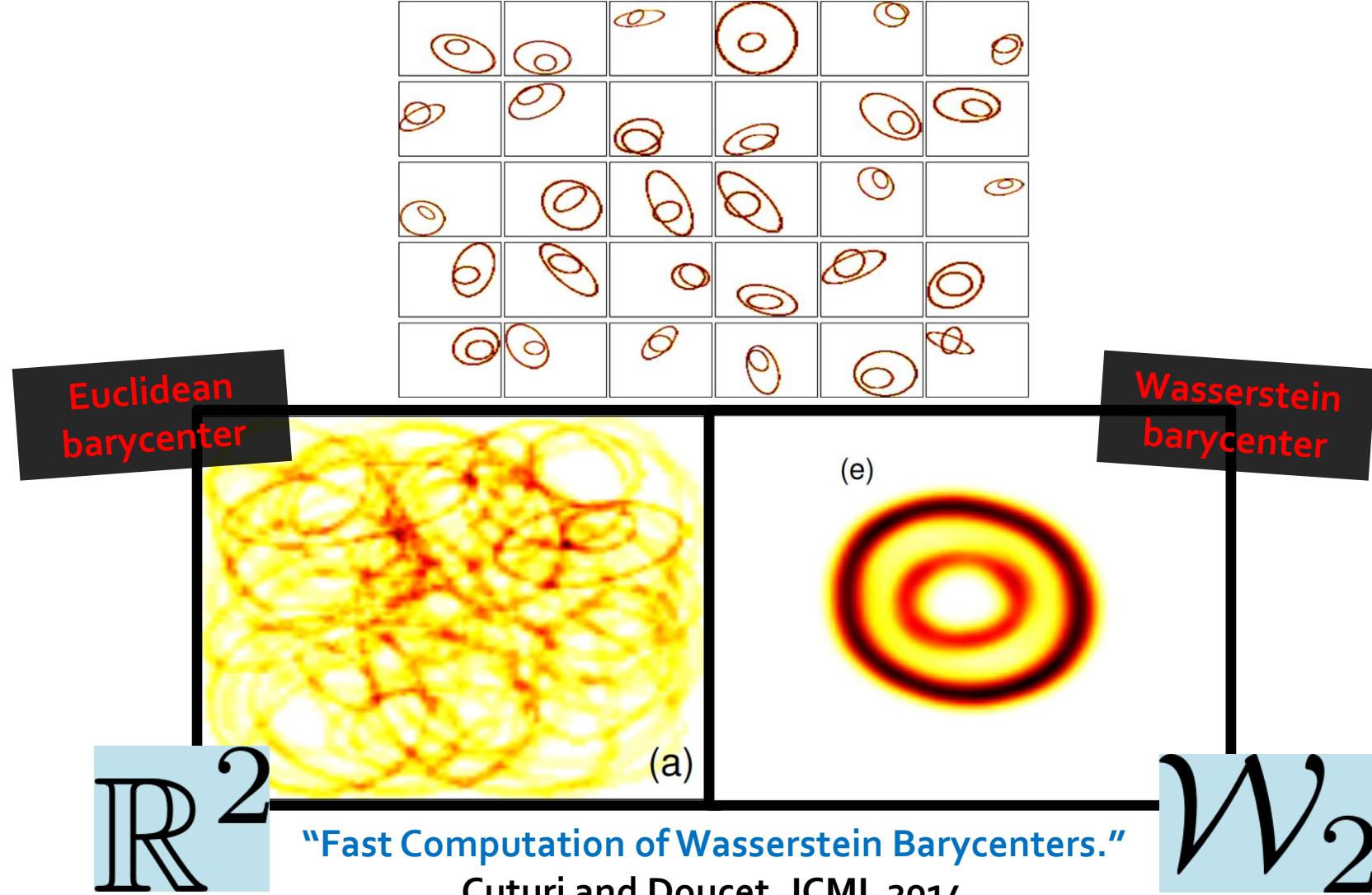
“Fréchet variance”

Generalizes Euclidean notation of “mean.”

$$\arg\min_{\mathbf{p}\in\mathbb{R}^n}\sum_{i=1}^N\|\mathbf{p}-\mathbf{x}_i\|_2^2$$



# Example from Past Lecture



# Application to Neural Networks

## Differentiating through the Fréchet Mean

Aaron Lou <sup>\*1</sup> Isay Katsman <sup>\*1</sup> Qingxuan Jiang <sup>\*1</sup> Serge Belongie <sup>1</sup> Ser-Nam Lim <sup>2</sup> Christopher De Sa <sup>1</sup>

### Abstract

Recent advances in deep representation learning on Riemannian manifolds extend classical deep learning operations to better capture the geometry of the manifold. One possible extension is the Fréchet mean, the generalization of the Euclidean mean; however, it has been difficult to apply because it lacks a closed form with an easily computable derivative. In this paper, we show how to differentiate through the Fréchet mean for arbitrary Riemannian manifolds. Then, focusing on hyperbolic space, we derive explicit gradient expressions and a fast, accurate, and hyperparameter-free Fréchet mean solver. This fully integrates the Fréchet mean into the hyperbolic neural network pipeline. To demonstrate this integration, we present two case studies. First, we apply our Fréchet mean to the existing Hyperbolic Graph Convolutional Network, replacing its projected aggregation to obtain state-of-the-art results on datasets with high hyperbolicity. Second, to demonstrate the Fréchet mean's capacity to generalize Euclidean neural network operations, we develop a hyperbolic batch normalization method that gives an improvement parallel to the one observed in the Euclidean setting<sup>1</sup>.

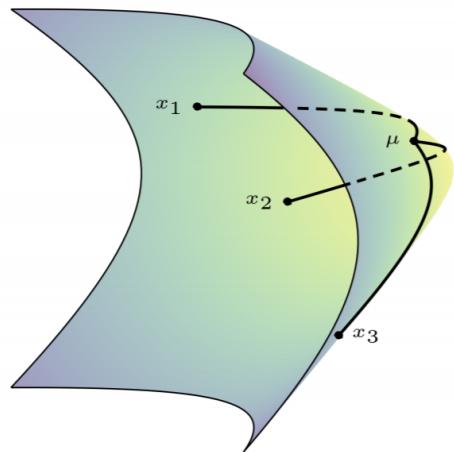


Figure 1. Depicted above is the Fréchet mean,  $\mu$ , of three points  $x_1, x_2, x_3$  in the Lorentz model of hyperbolic space. As we can see, the Fréchet mean conforms with the geometry of the hyperboloid and is vastly different from the standard Euclidean mean.

space, in which distances grow exponentially as one moves away from the origin. Such a geometry is naturally equipped to embed trees, since if we embed the root of the tree at the origin and layers at successive radii, the geometry of hyperbolic space admits a natural hierarchical structure. More

Table 1. Summary of operations in the Poincaré ball model and the hyperboloid model ( $K < 0$ )

Manifold	Poincaré Ball	Hyperboloid
Metric	$\mathbb{D}_K^n = \{x \in \mathbb{R}^n : \langle x, x \rangle_2 < -\frac{1}{K}\}$	$\mathbb{H}_K^n = \{x \in \mathbb{R}^{n+1} : \langle x, x \rangle_{\mathcal{L}} = \frac{1}{K}\}$
Distance	$d_{\mathbb{D}}^K(x, y) = \frac{1}{\sqrt{ K }} \cosh^{-1} \left( 1 - \frac{2K\ x-y\ _2^2}{(1+K\ x\ _2^2)(1+K\ y\ _2^2)} \right)$	$d_{\mathbb{H}}^K(x, y) = \frac{1}{\sqrt{ K }} \cosh^{-1}(K\langle x, y \rangle_{\mathcal{L}})$
Exp map	$\exp_x^K(v) = x \oplus_K \left( \tanh \left( \sqrt{ K } \frac{\lambda_x^K \ v\ _2}{2} \right) \frac{v}{\sqrt{ K } \ v\ _2} \right)$	$\exp_x^K(v) = \cosh(\sqrt{ K } \ v\ _{\mathcal{L}}) x + v \frac{\sinh(\sqrt{ K } \ v\ _{\mathcal{L}})}{\sqrt{ K } \ v\ _{\mathcal{L}}}$
Log map	$\log_x^K(y) = \frac{2}{\sqrt{ K } \lambda_x^K} \tanh^{-1} \left( \sqrt{ K } \  -x \oplus_K y \ _2 \right) \frac{-x \oplus_K y}{\  -x \oplus_K y \ _2}$	$\log_x^K(y) = \frac{\cosh^{-1}(K\langle x, y \rangle_{\mathcal{L}})}{\sinh(\cosh^{-1}(K\langle x, y \rangle_{\mathcal{L}}))} (y - K\langle x, y \rangle_{\mathcal{L}} x)$
Transport	$PT_{x \rightarrow y}^K(v) = \frac{\lambda_x^K}{\lambda_y^K} \text{gyr}[y, -x]v$	$PT_{x \rightarrow y}^K(v) = v - \frac{K\langle y, v \rangle_{\mathcal{L}}}{1+K\langle x, y \rangle_{\mathcal{L}}} (x + y)$

Table 2. Summary of hyperbolic counterparts of Euclidean operations in neural networks

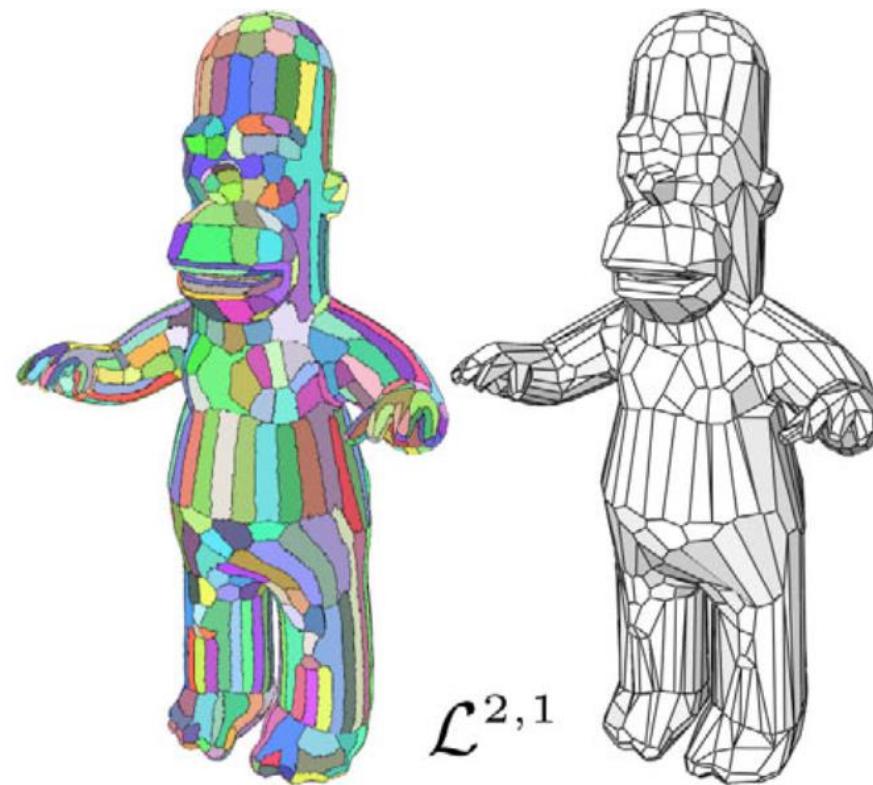
Operation	Formula
Matrix-vector multiplication	$A \otimes^K x = \exp_0^K(A \log_0^K(x))$
Bias translation	$x \oplus^K b = \exp_x^K(PT_{0 \rightarrow x}^K(b))$
Activation function	$\sigma^{K_1, K_2}(x) = \exp_0^{K_1}(\sigma(\log_0^{K_2}(x)))$

# Finding Nicely-Shaped Regions on a Surface

## Lloyd's Algorithm

*Alternate between*

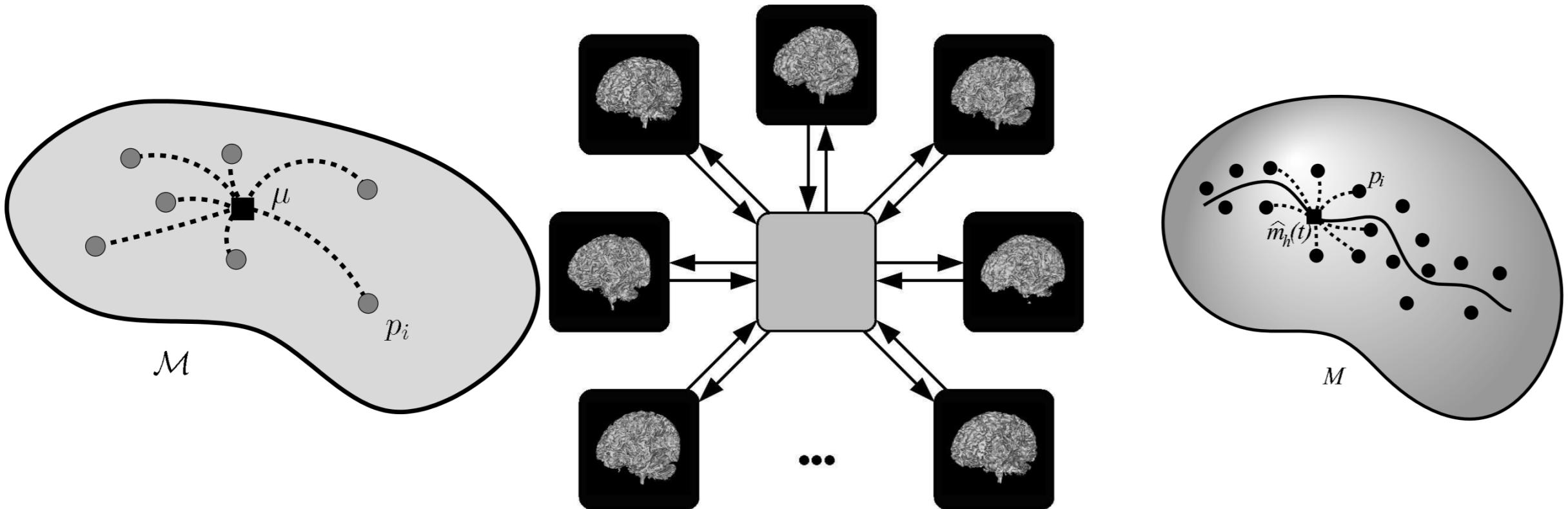
- 1. Fitting primitive parameters**
- 2. Assign points to patches**



“Variational Shape Approximation.”

Cohen-Steiner, Alliez, and Desbrun; SIGGRAPH 2004

# Shape Collections



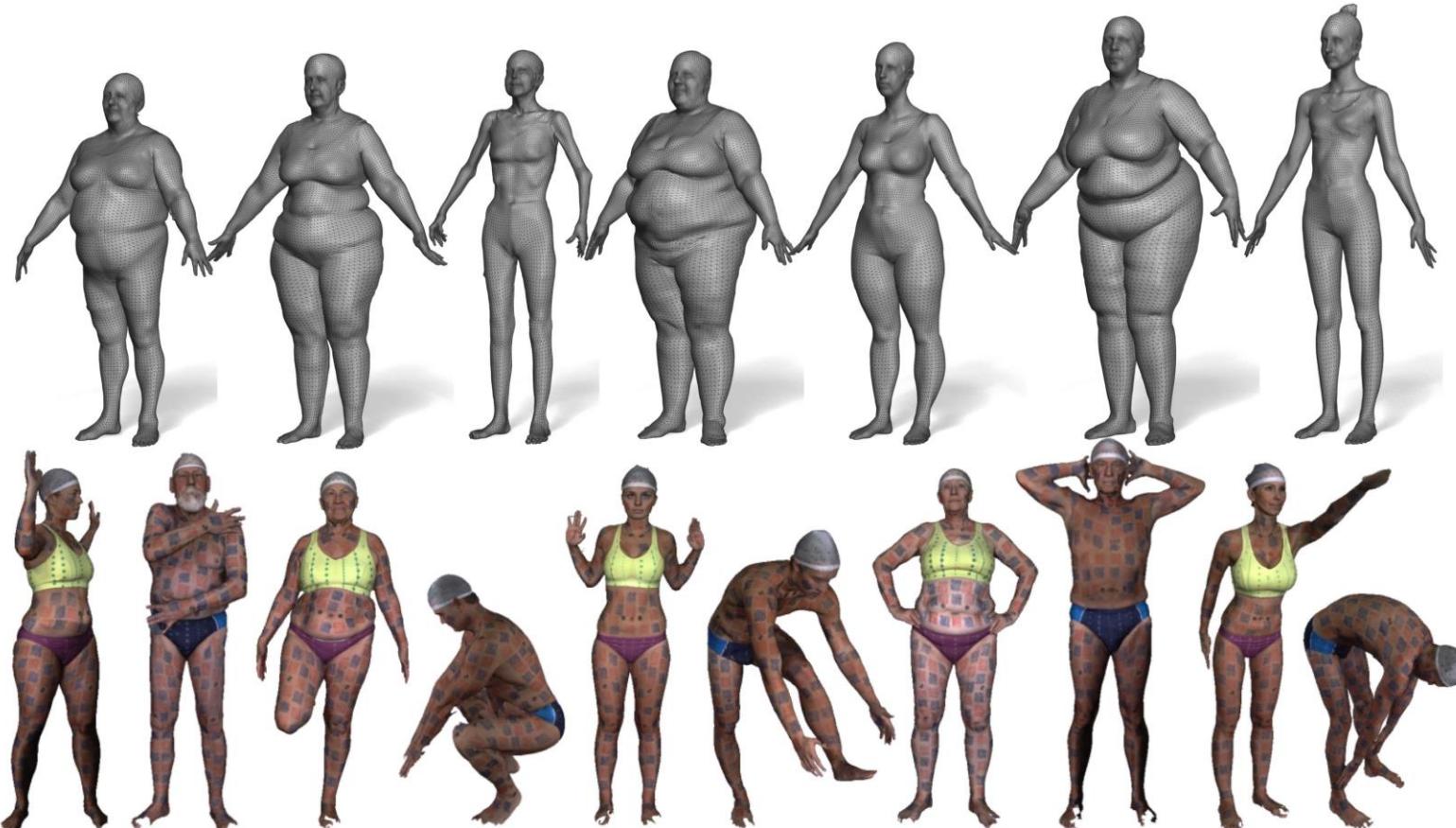
# *k*-Medoids

- Assignment step
  - Assign point to its **closest** cluster center

- Update step
  - Replace cluster center with most **central** data point

When Fréchet means won't work

# Example Task



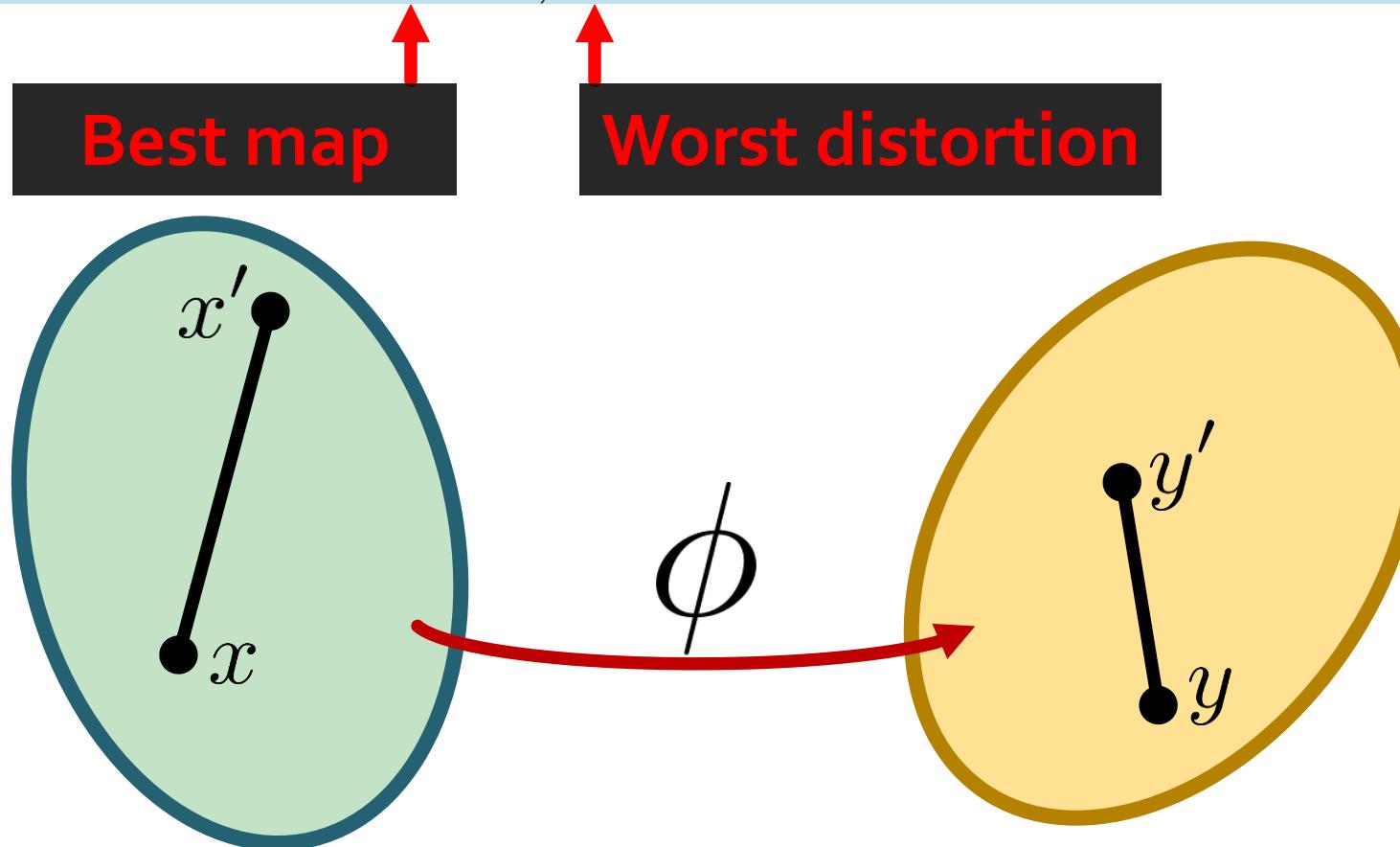
[https://ps.is.tuebingen.mpg.de/research\\_projects/3d-mesh-registration](https://ps.is.tuebingen.mpg.de/research_projects/3d-mesh-registration)

**Clustering in a shape collection**

# Gromov-Hausdorff Distance

Distance between metric spaces  $X, Y$

$$d_{\text{GH}}(X, Y) := \inf_{\phi: X \rightarrow Y} \sup_{x, x' \in X} |d_X(x, x') - d_Y(\phi(x), \phi(x'))|$$



# Gromov-Hausdorff Clustering

Eurographics Symposium on Point-Based Graphics (2007)  
M. Botsch, R. Pajarola (Editors)

## On the use of Gromov-Hausdorff Distances for Shape Comparison

Facundo Mémoli<sup>1†</sup>

<sup>1</sup>Department of Mathematics, Stanford University, California, USA.

### Abstract

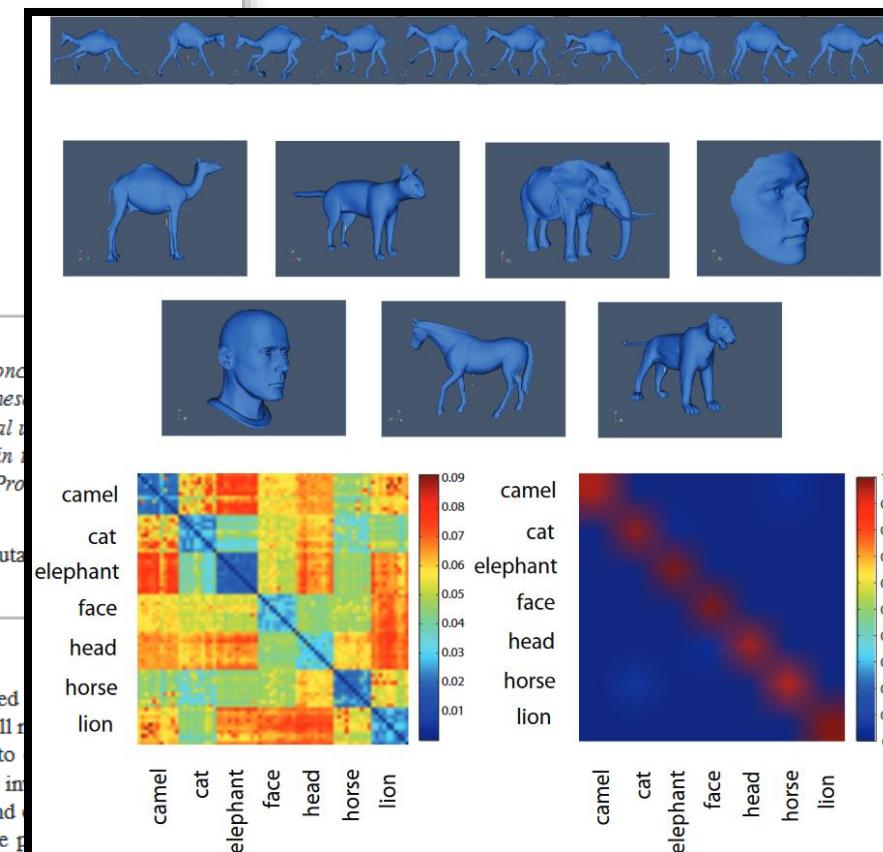
*It is the purpose of this paper to propose and discuss certain modifications of the ideas concerning Gromov-Hausdorff distances in order to tackle the problems of shape matching and comparison. These modifications render these distances more amenable to practical computations without sacrificing theoretical properties. A second goal of this paper is to establish links to several other practical methods proposed in the literature for comparing/matching shapes in precise terms. Connections with the Quadratic Assignment Problem are also established, and computational examples are presented.*

Categories and Subject Descriptors (according to ACM CCS): I.3.5 [Computer Graphics]: Computational Geometry and Object Modelling.

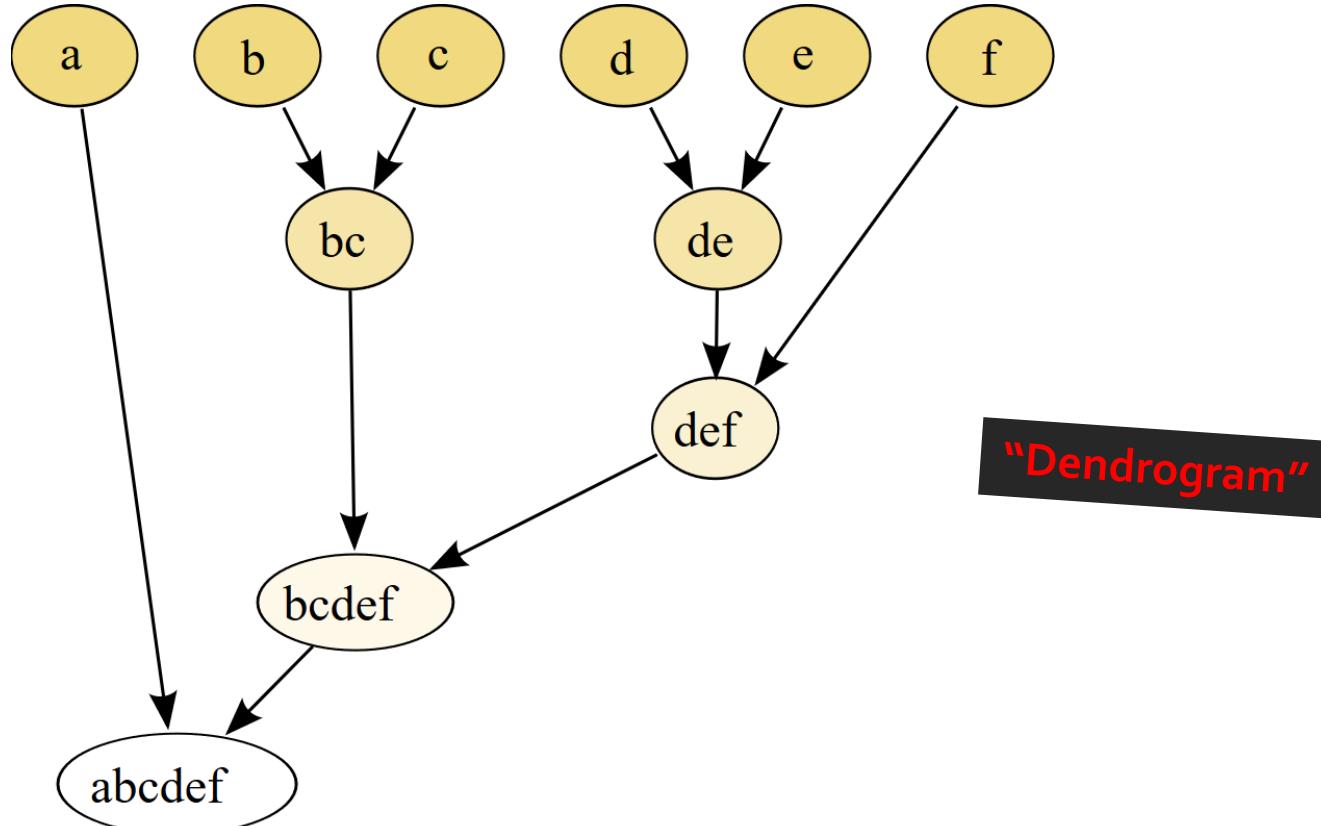
### 1. Introduction

Given the great advances in recent years in the fields of shape acquisition and modelling, and the resulting huge collections of digital models that have been obtained it is of great importance to be able to define and compute meaningful notions of similarity between shapes which exhibit invariance to different deformations and or poses of the objects represented

structure, that is, shapes are viewed as metric spaces. The notion of distance compares the full metric structure contained in the shapes, as opposed to the notion of distance that only compare simple (incomplete) information. Two shapes will be declared *equal* if and only if they are isometric. This means that the invariance properties of the shapes are encoded by the metrics one chooses to endow the shapes with.



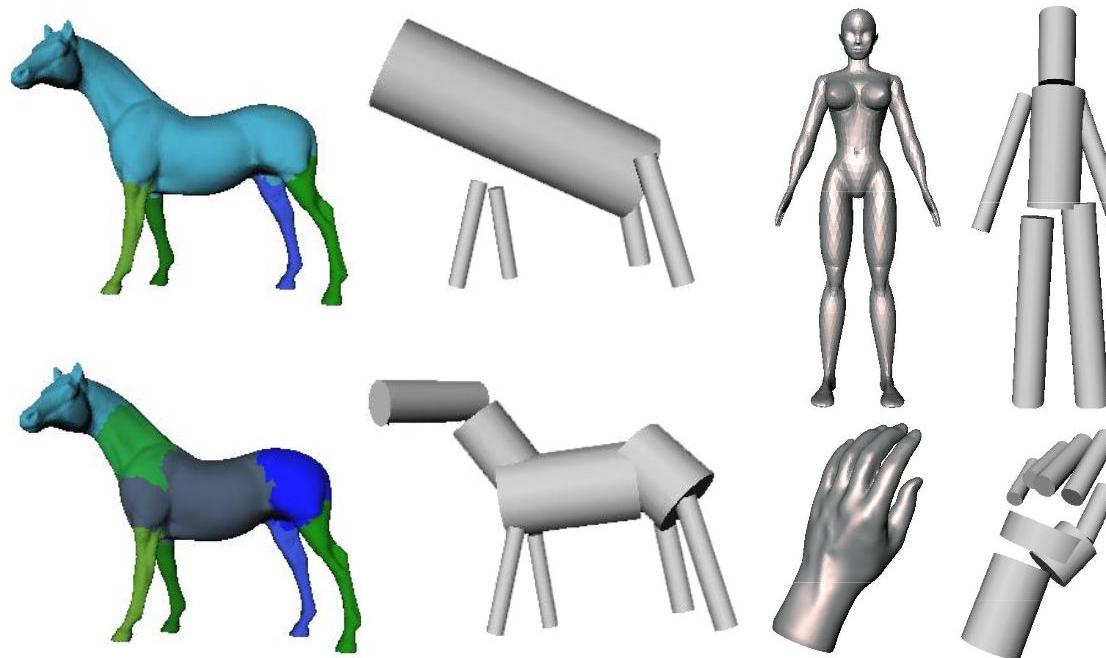
# Agglomerative Clustering



[https://upload.wikimedia.org/wikipedia/commons/a/ad/Hierarchical\\_clustering\\_simple\\_diagram.svg](https://upload.wikimedia.org/wikipedia/commons/a/ad/Hierarchical_clustering_simple_diagram.svg)

Merge from the bottom up

# Agglomerative Clustering in Geometry



[“Hierarchical mesh segmentation based on fitting primitives.”](#)  
Attene, Falcidieno, and Spagnuolo; The Visual Computer 2006

Fit a primitive and measure error

# Related Technique: Flood Fill

## Region Growing Algorithm

Initialize a priority queue  $Q$  of elements

Loop until all elements are clustered

    Choose a seed element and insert to  $Q$

    Create a cluster  $C$  from seed

    Loop until  $Q$  is empty

        Get the next element  $s$  from  $Q$

        If  $s$  can be clustered into  $C$

            Cluster  $s$  into  $C$

            Insert  $s$  neighbors to  $Q$

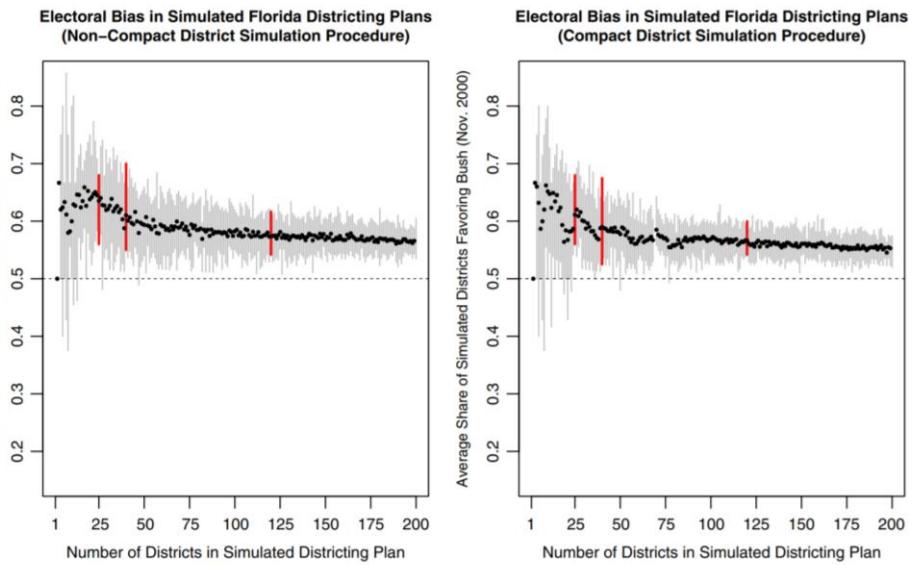
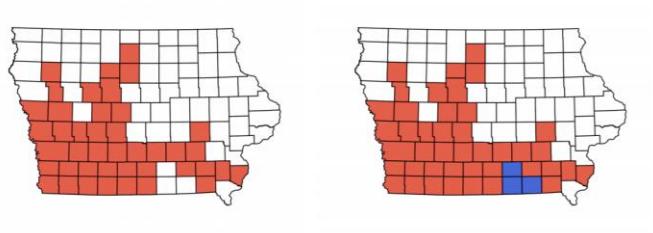
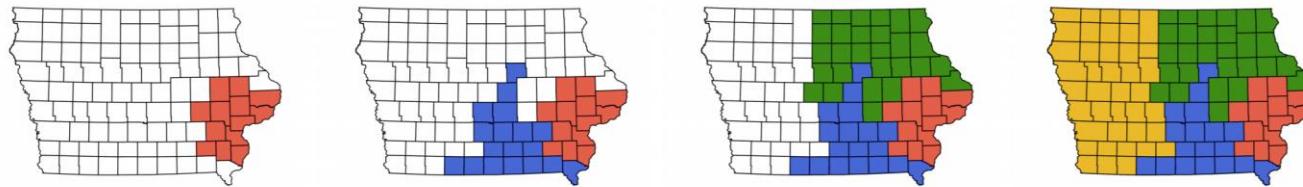
    Merge small clusters into neighboring ones

“Segmentation and Shape Extraction of 3D Boundary Meshes.”

Shamir; EG STAR 2006.

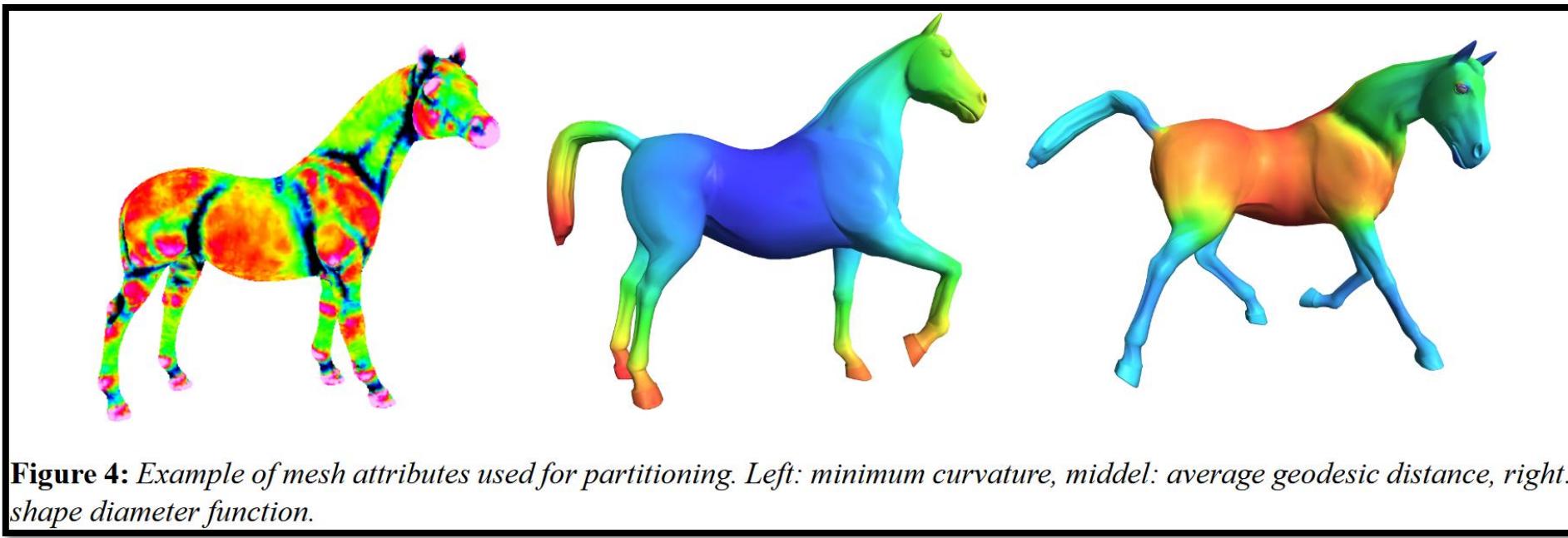
# Region growing algorithm

# Flood Fill and Agglomerative Clustering in Redistricting



**Figure 4.** Republican electoral bias in simulated Florida districting plans.  
*Note:* Black dots indicate the average share of simulated districts that have pro-Bush majorities in the simulated plans. Gray bars depict the entire range of pro-Bush district shares that were observed across all simulations for each given legislature size. Red bars depict the range of simulated outcomes for legislatures of 25 districts (Florida's Congressional Delegation), 40 districts (the Florida State Senate), and 120 districts (the Florida State House).

# Clustering in Feature Space

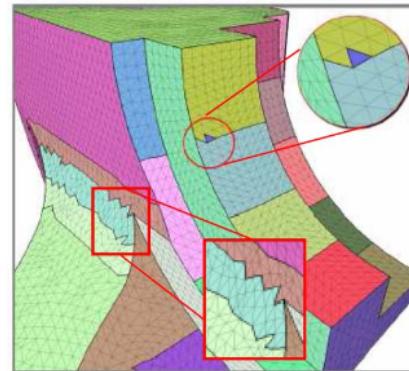


**Figure 4:** Example of mesh attributes used for partitioning. Left: minimum curvature, middle: average geodesic distance, right: shape diameter function.

“Segmentation and Shape Extraction of 3D Boundary Meshes.”  
Shamir; EG STAR 2006.

# Additional Desirable Properties

- Cardinality
  - Not too small and not too large or a given number (of segment or elements)
  - Overall balanced partition
- Geometry
  - Size: area, diameter, radius
  - Convexity, Roundness
  - Boundary smoothness
- Topology
  - Connectivity (single component)
  - Disk topology
  - a given number (of segment or elements)



“Segmentation and Shape Extraction of 3D Boundary Meshes.”

Shamir; EG STAR 2006.

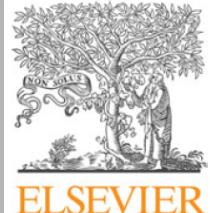
*via Q. Huang, Stanford CS 468, 2012*

# Issue So Far

No notion of optimality.

No use of  
local relationships.

# Global Optimality Unlikely



Contents lists available at SciVerse ScienceDirect

## Theoretical Computer Science

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



## The planar $k$ -means problem is NP-hard<sup>☆</sup>

Meena Mahajan <sup>a,\*</sup>, Prajakta Nimbhorkar <sup>a</sup>, Kasturi Varadarajan <sup>b</sup>

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<sup>b</sup> The University of Iowa, Iowa City, IA 52242-1419, USA

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### ARTICLE INFO

**Keywords:**

Clustering  
 $k$ -means  
Planar graphs  
NP-hardness

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### ABSTRACT

In the  $k$ -means problem, we are given a finite set  $S$  of points in  $\Re^m$ , and integer  $k \geq 1$ , and we want to find  $k$  points (centers) so as to minimize the sum of the square of the Euclidean distance of each point in  $S$  to its nearest center. We show that this well-known problem is NP-hard even for instances in the plane, answering an open question posed by Dasgupta (2007) [7].

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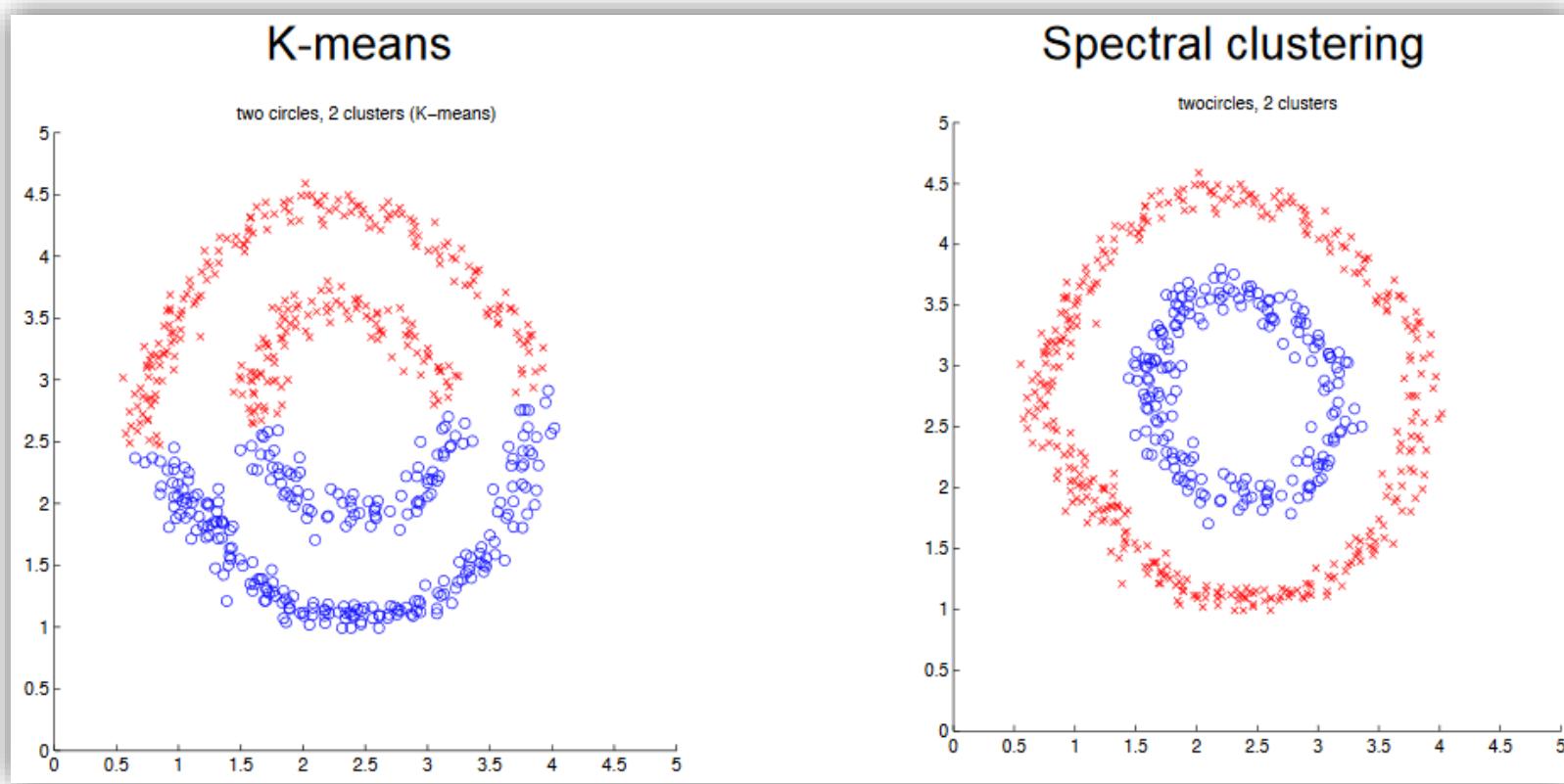
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### 1. Introduction

In the  $k$ -means problem, we are given a finite set  $S$  of points in  $\Re^m$ , and integer  $k \geq 1$ , and we want to find  $k$  points (centers) so as to minimize the sum of the square of the Euclidean distance of each point in  $S$  to its nearest center. This is a well-known and popular clustering problem that has also received a lot of attention from the algorithms community.

# Spectral Clustering

<http://cs.nyu.edu/~dsontag/courses/ml13/slides/lecture16.pdf>



- Rough notion of optimality
- Assembles local relationships

# Normalized Cuts for Two Cuts

Symmetric similarity matrix  $W$

$$\text{Cut score } C(A, B) := \sum_{\substack{i \in A \\ j \in B}} w_{ij}$$

$$\text{Volume } V(A) := \sum_{i \in A} \sum_j w_{ij}$$

Normalized cut score

$$N(A, B) := C(A, B)(V(A)^{-1} + V(B)^{-1})$$

“Normalized Cuts and Image Segmentation.”

Shi and Malik; PAMI 2000

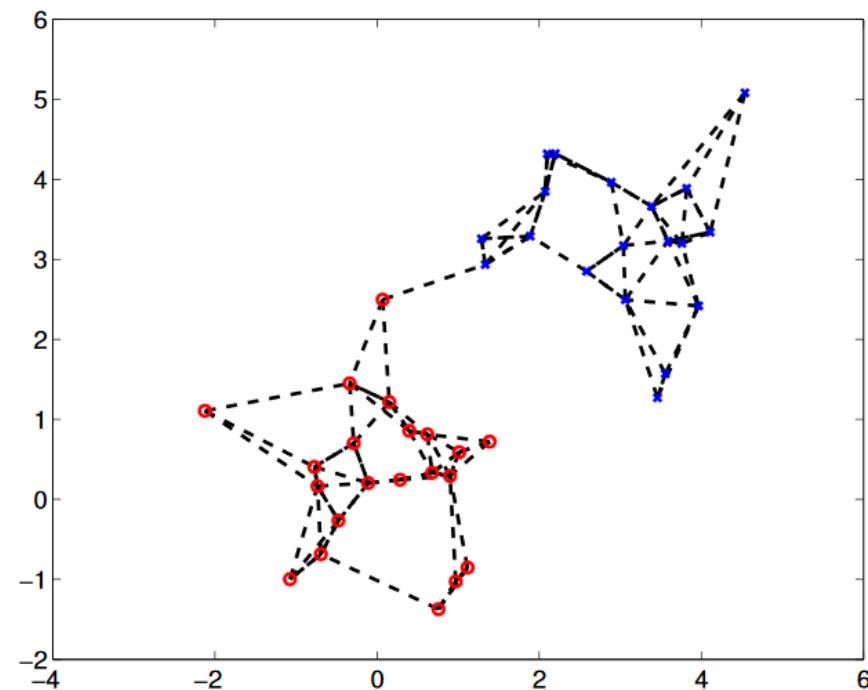
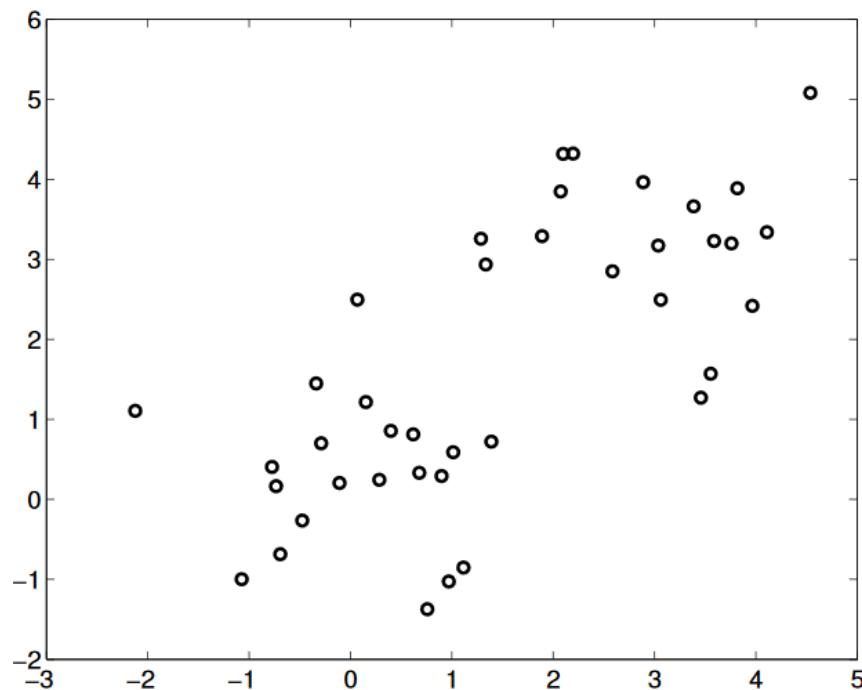


# Eigenvalue Problem

$$\begin{aligned} \min_{\mathbf{x}} \quad & \frac{\mathbf{x}^\top L \mathbf{x}}{\mathbf{x}^\top D \mathbf{x}} \\ \text{s.t. } & \mathbf{x}^\top D \mathbf{1} = 0 \end{aligned}$$

$$L\mathbf{x} = \lambda D\mathbf{x}$$

# Example on kNN Graph

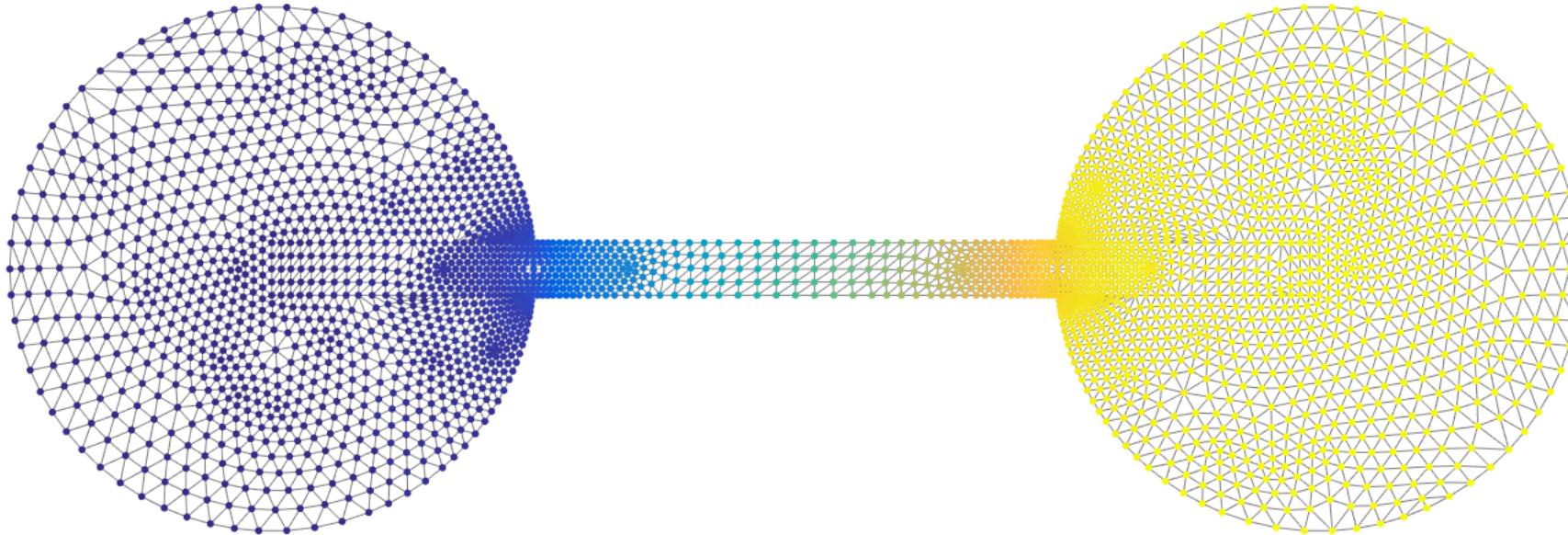


# For $\geq 2$ Clusters

- **Recursive bi-partitioning (Hagen et al. 1991)**
  - Analogy: Agglomerative clustering
  - Potentially slow/unstable
- **Cluster multiple eigenvectors**
  - Analogy:  $k$ -means after dimension reduction
  - More popular approach

*Recall:*

# Second-Smallest Eigenvector



$$L\mathbf{x} = \lambda\mathbf{x}$$

Used for graph  
partitioning

Fiedler vector (“algebraic connectivity”)

# Back to the Laplacian

Computers & Graphics 33 (2009) 381–390

Contents lists available at ScienceDirect

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

ELSEVIER

Technical Section

Discrete Laplace–Beltrami operators for shape analysis and segmentation

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<sup>a</sup> Massachusetts Institute of Technology, Cambridge, MA, USA  
<sup>b</sup> A.A. Martinos Center for Biomedical Imaging, Massachusetts General Hospital, Harvard Medical School, Boston, MA, USA  
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Nodal sets

Nodal domains

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Shape segmentation

ABSTRACT

Shape analysis plays a pivotal role in a large number of applications, ranging from traditional geometry processing to more recent 3D content management. In this scenario, spectral methods are extremely promising as they provide a natural library of tools for shape analysis, intrinsically defined by the shape itself. In particular, the eigenfunctions of the Laplace–Beltrami operator yield a set of real-valued functions that provide interesting insights in the structure and morphology of the shape. In this paper, we first analyze different discretizations of the Laplace–Beltrami operator (geometric Laplacians, linear and cubic FEM operators) in terms of the correctness of their eigenfunctions with respect to the continuous case. We then present the family of segmentations induced by the nodal sets of the

1. Introduction

Shape analysis is a discipline that deals with reasoning on geometric shapes. It has been applied to a large number of applications, ranging from traditional geometry processing to more recent 3D content management.

In the recent years, there has been a growing interest in the need to automatically analyze and process 3D objects, in order to facilitate the sharing and management of 3D content in many emerging web-based applications. A semantic

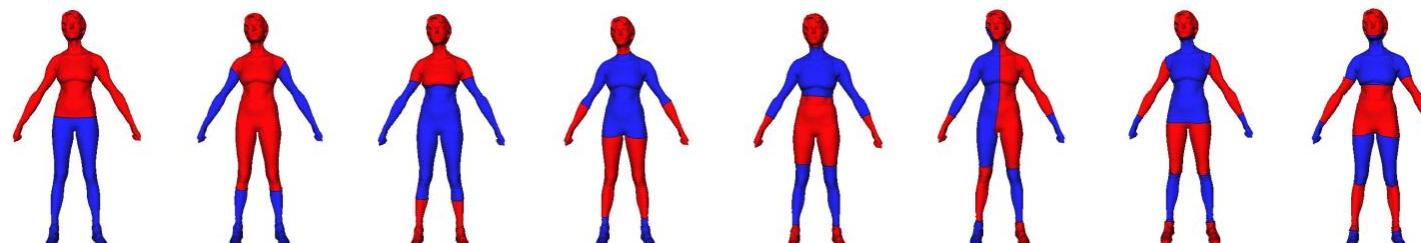


Figure 7: Segmentations induced by the nodal domains of some eigenfunctions selected among the first 15 eigenfunctions (in order of increasing eigenvalues). Blue regions correspond to regions where the eigenfunctions have negative values, while red regions correspond to positive values.

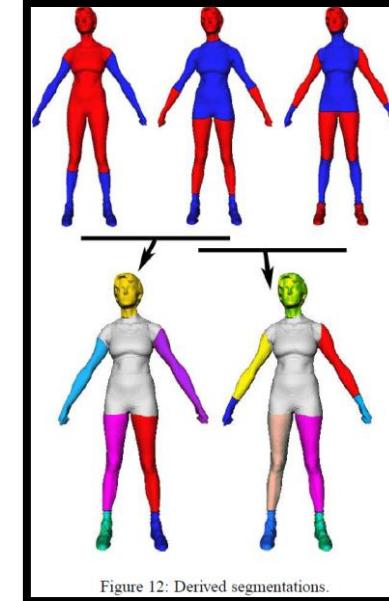


Figure 12: Derived segmentations.

# Nodal domain

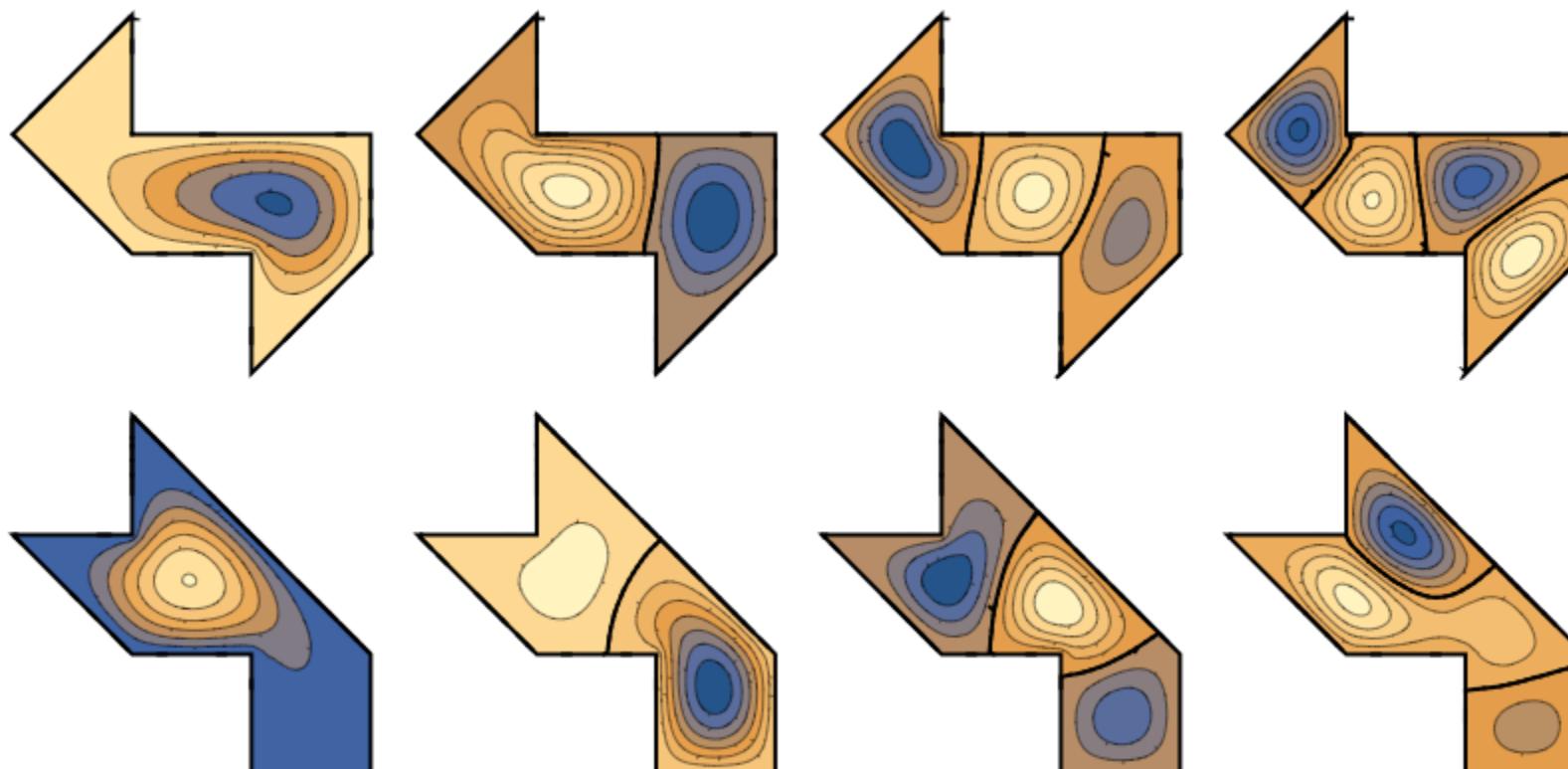
[nohd-l doh-meyn]:

A connected region where  
a Laplacian eigenfunction  
has constant sign



# Courant's Theorem

The  $k$ -th Laplacian eigenfunction has  
at most  $k$  nodal domains.



# Issue

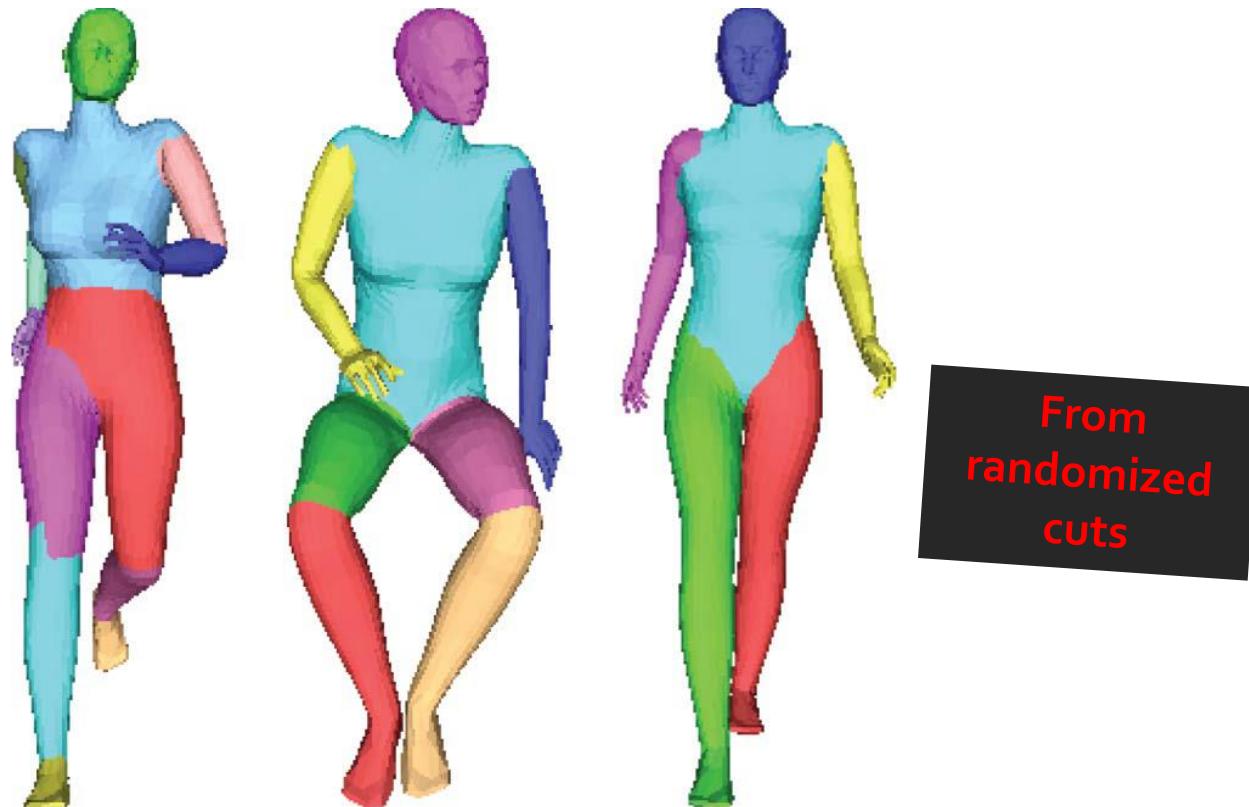
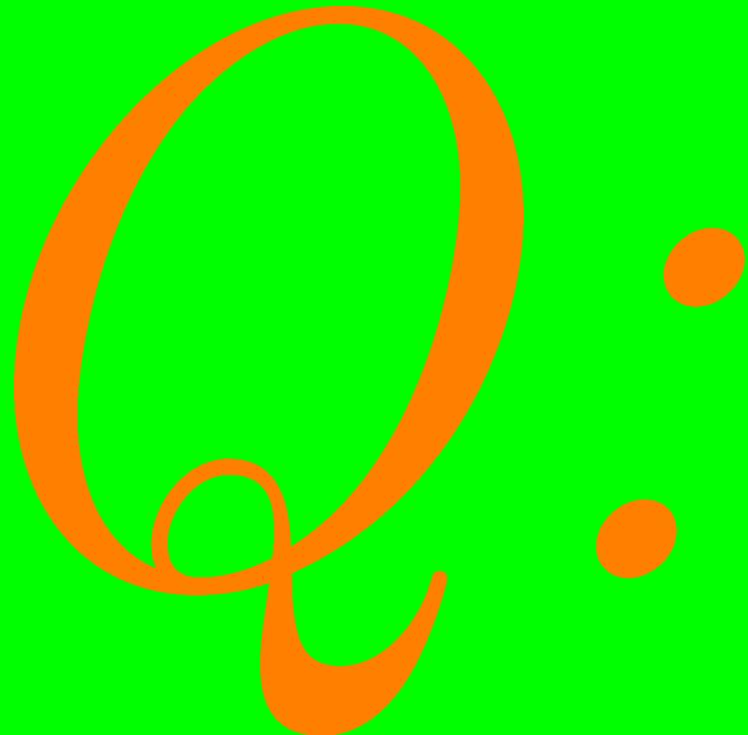


Image courtesy Q. Huang

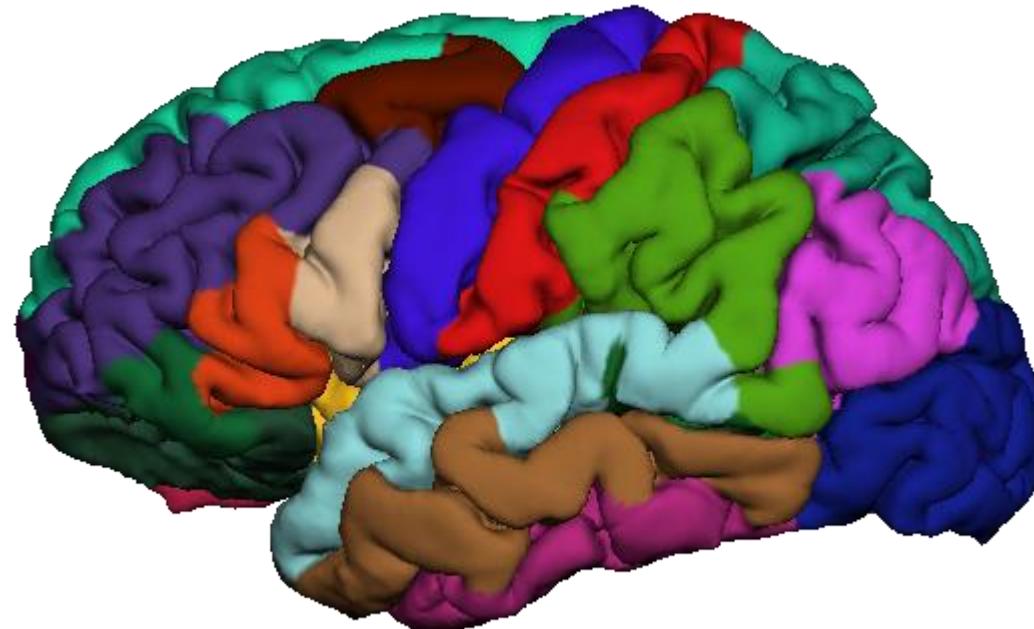
Inconsistent!



Is segmentation a  
purely geometric  
problem?

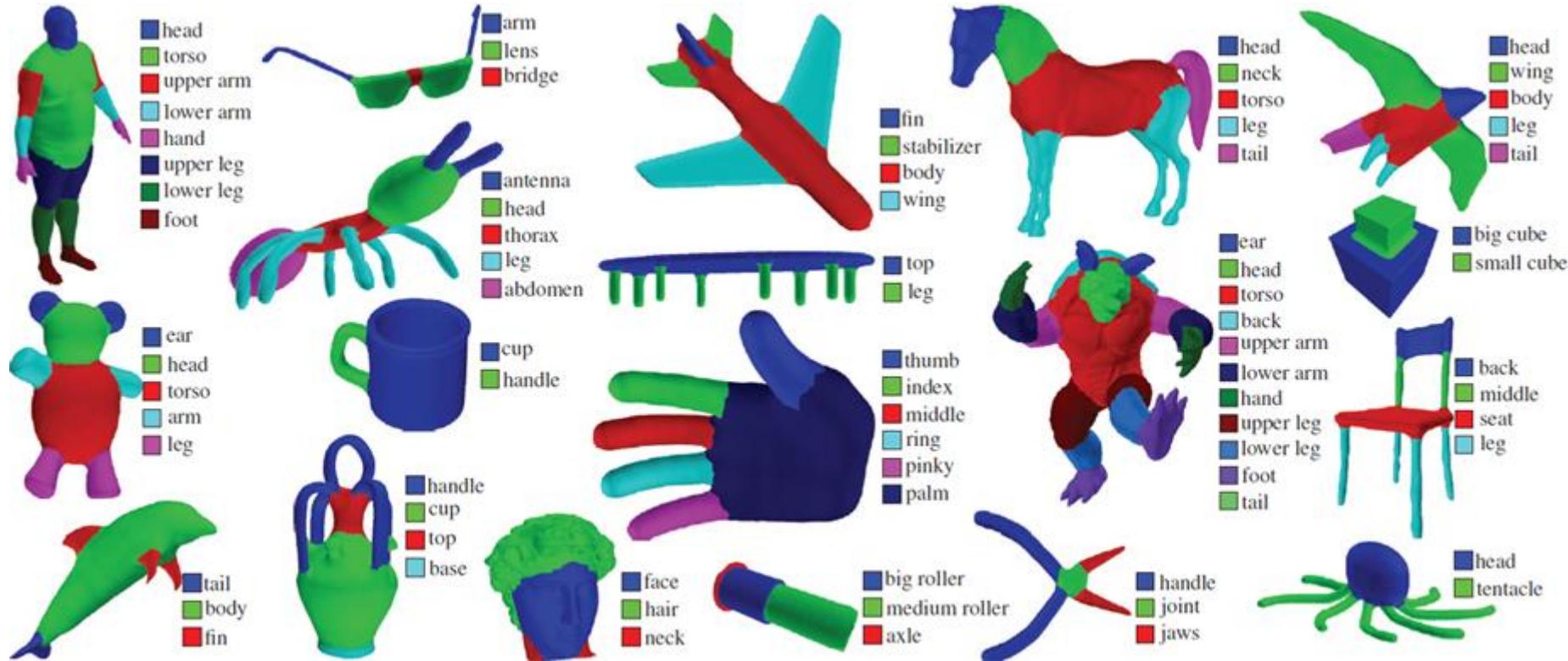
# Obvious Counterexample

<http://www.erflow.eu/brain-segmentation-science-case>



Shape provides only a clue

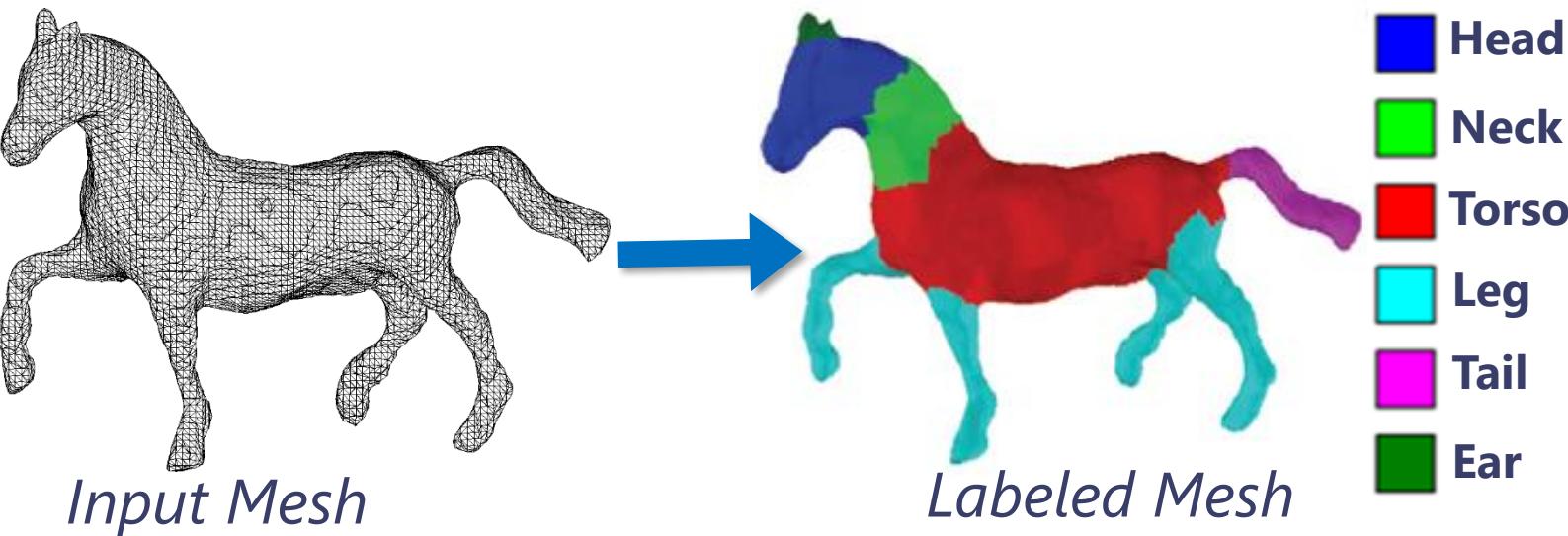
# Supervised Learning



"Learning 3D Mesh Segmentation and Labeling."  
Kalogerakis, Hertzmann, and Singh; SIGGRAPH 2010

Use example data to help

# Conditional Random Field



$$c^* := \arg \min_c \left[ \sum_i \alpha_i E_1(c_i; x_i) + \sum_{ij} \ell_{ij} E_2(c_i, c_j; y_{ij}) \right]$$

Unary  
descriptor term

Binary label  
compatibility term

# Preview: Supervised Learning

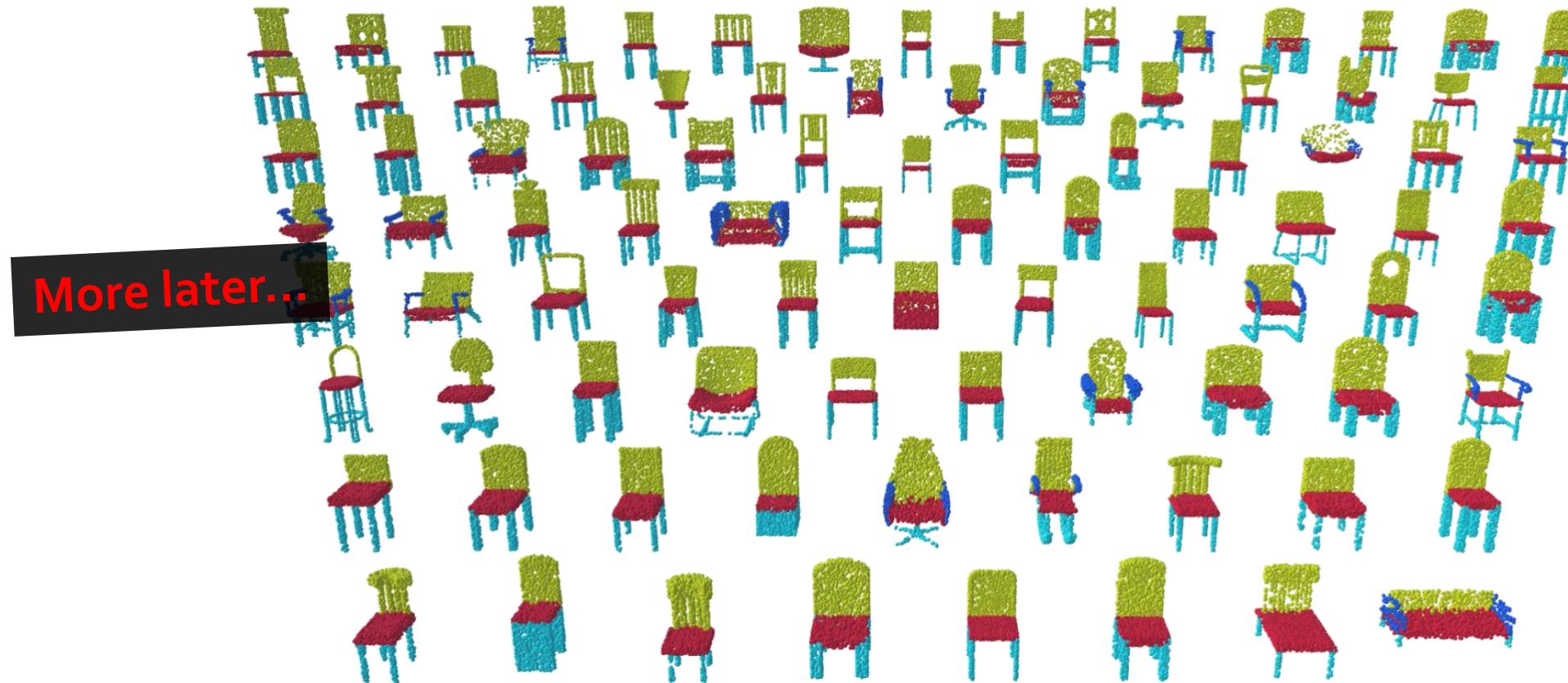
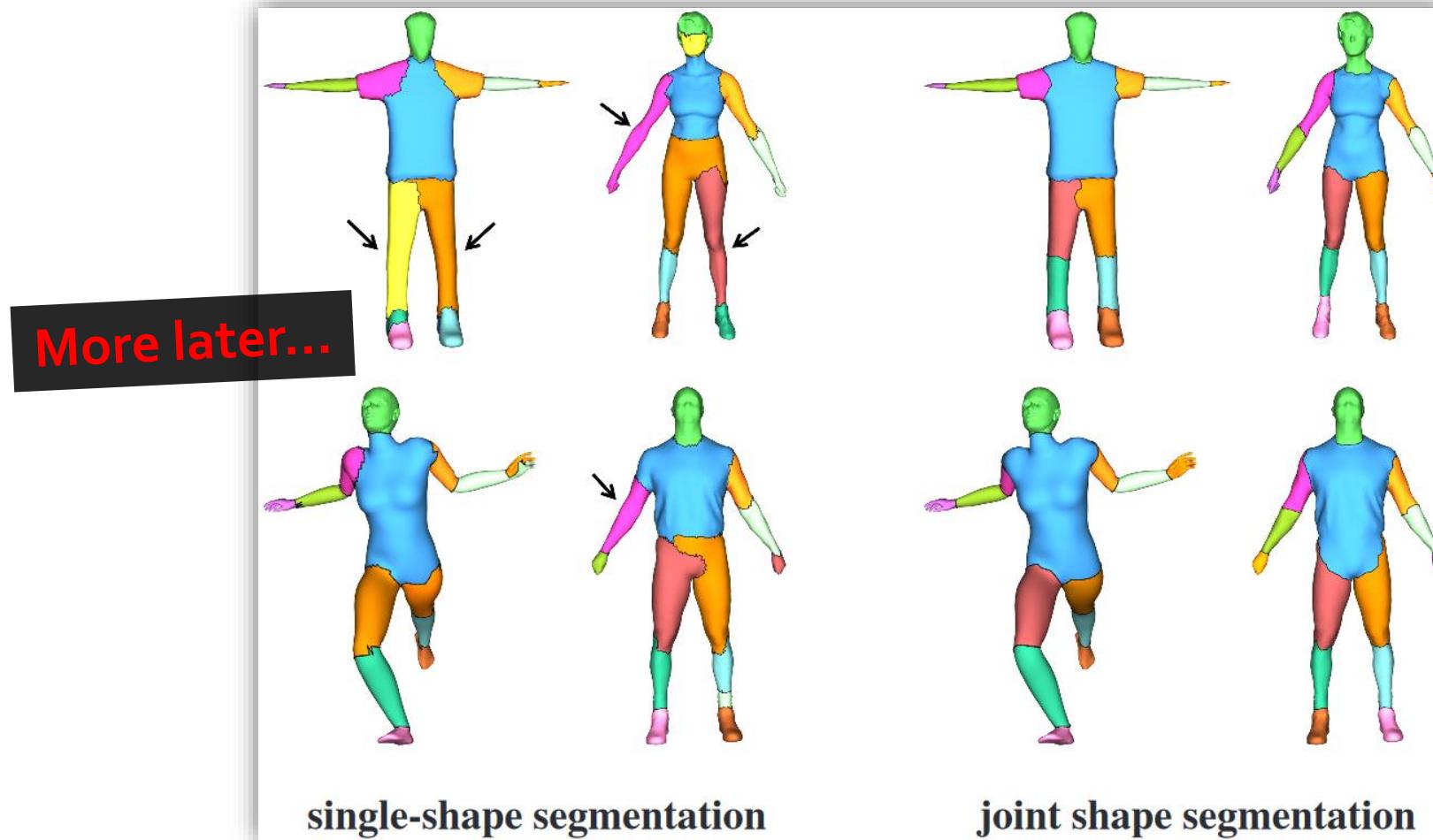


Image from "Dynamic Graph CNN for Learning on Point Clouds" (Wang et al. 2019)

# Preview: Unsupervised Learning



“Joint Shape Segmentation with Linear Programming.”

Huang, Koltun, and Guibas; SIGGRAPH Asia 2011

# Clustering and Segmentation

Justin Solomon

6.838: Shape Analysis  
Spring 2021

