

# CS233, CME251: Geometric and Topological Data Analysis

Leonidas Guibas  
Computer Science Department  
Stanford University



Lecture 12  
4 May 2022



Last Time: Differential  
Geometry of Surfaces and the  
Laplace-Beltrami Operator

# Surface Curvatures

## • Principal curvatures

- Minimal curvature
- Maximal curvature

$$\kappa_1 = \kappa_{\min} = \min_{\varphi} \kappa_n(\varphi)$$

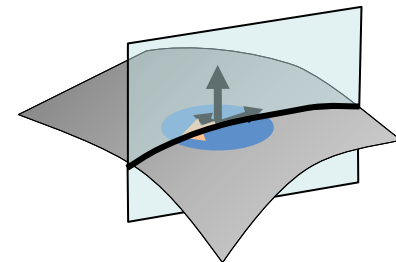
$$\kappa_2 = \kappa_{\max} = \max_{\varphi} \kappa_n(\varphi)$$

## • Mean curvature

$$H = \frac{\kappa_1 + \kappa_2}{2} = \frac{1}{2\pi} \int_0^{2\pi} \kappa_n(\varphi) d\varphi$$

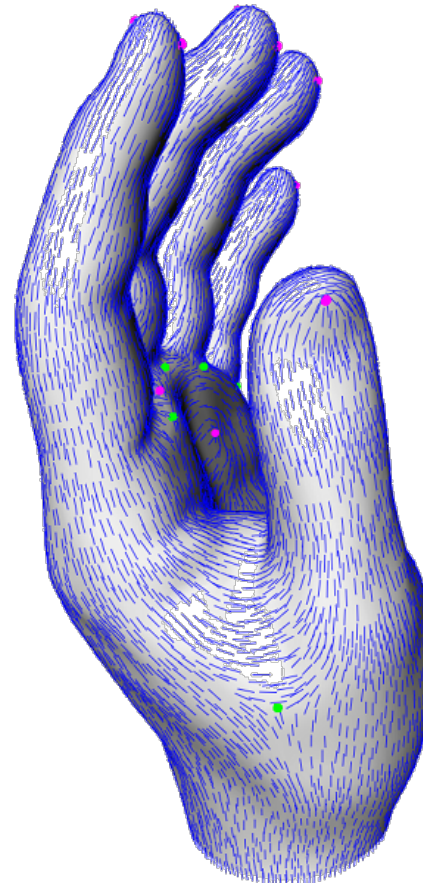
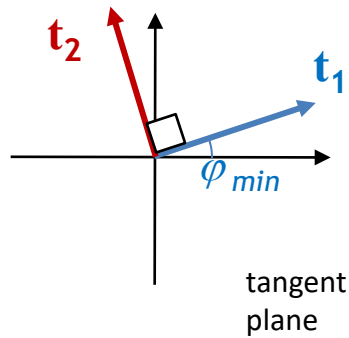
## • Gaussian curvature

$$K = \kappa_1 \cdot \kappa_2$$

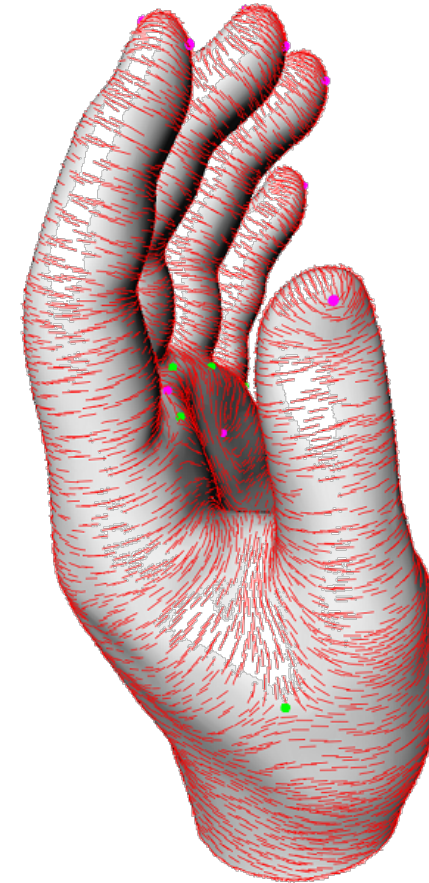


# Principal Directions

- Principal directions:  
tangent vectors  
corresponding to  
 $\varphi_{\max}$  and  $\varphi_{\min}$



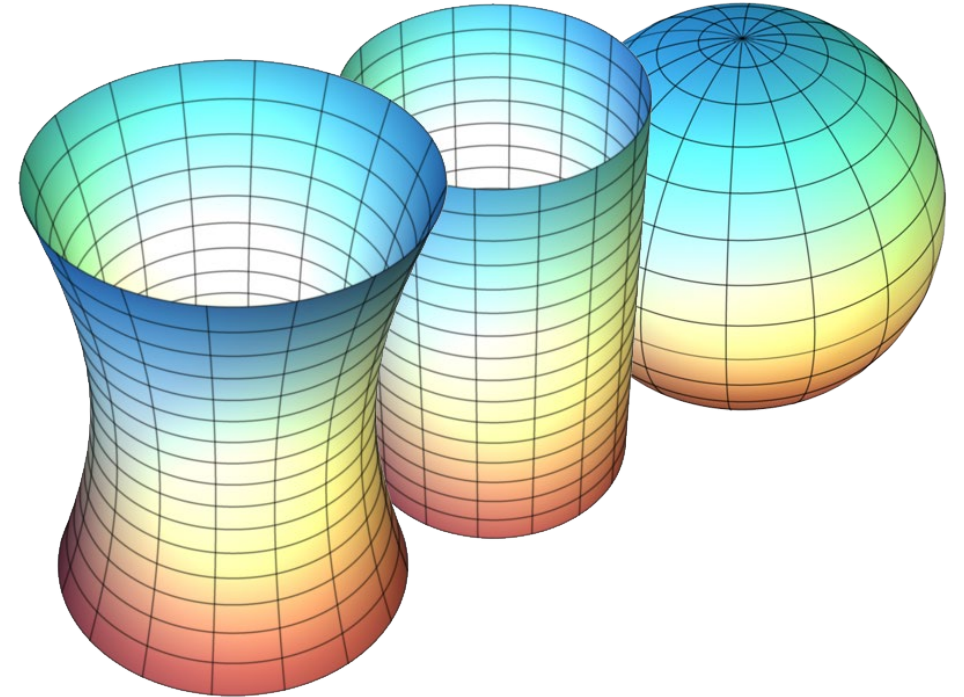
min curvature



max curvature

# Classification

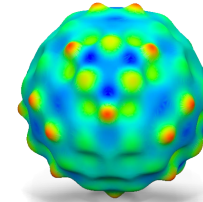
- A point  $\mathbf{p}$  on the surface is called
  - Elliptic, if  $K > 0$
  - Parabolic, if  $K = 0$
  - Hyperbolic, if  $K < 0$
- Developable surface  
iff  $K = 0$ 
  - can be mapped to the plane without distortion



# Knowledge as Functions over Data



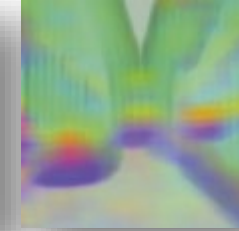
Knowledge towers over visual data: function spaces



Curvature

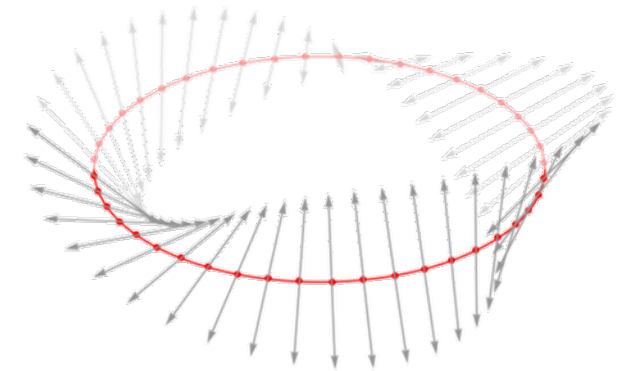


Parts



SIFT flow, C. Liu 2011

Vector bundles and sheaves



# Continuous Laplace-Beltrami Operator

- Extension of Laplace operator to functions on manifolds

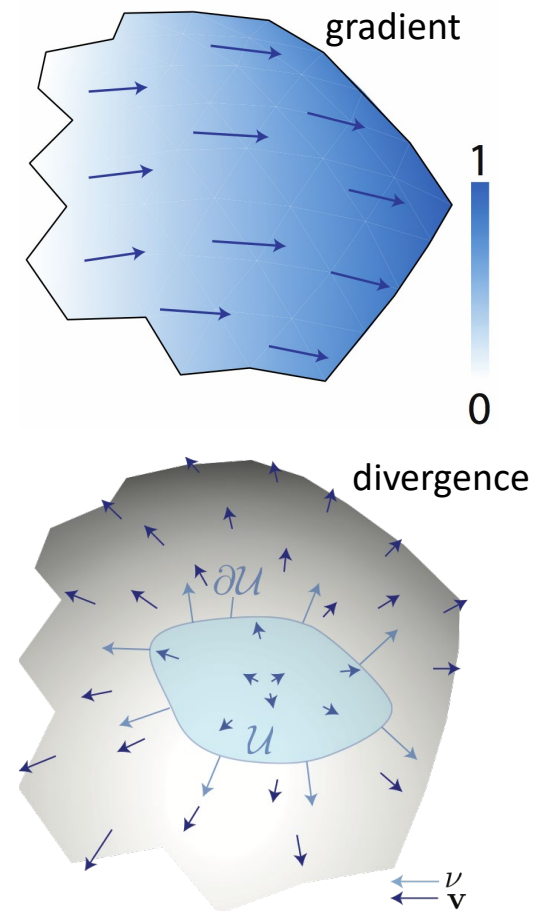
$$f : \mathcal{M} \rightarrow \mathbb{R} \quad \Delta f : \mathcal{M} \rightarrow \mathbb{R}$$

Laplace-Beltrami

function on surface  $M$

gradient operator

divergence operator

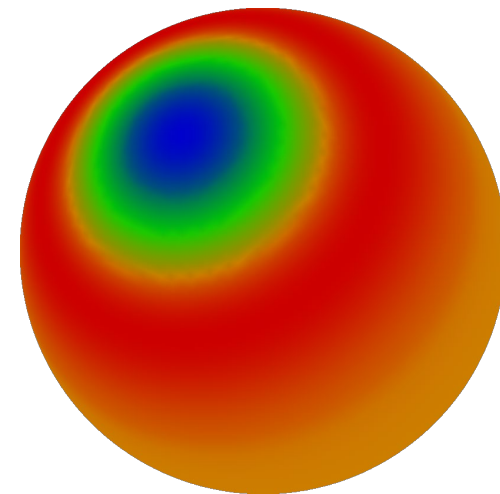
$$\Delta_{\mathcal{M}} f = \operatorname{div}_{\mathcal{M}} \nabla_{\mathcal{M}} f$$


# Laplace-Beltrami Operator

- Analog of Fourier transform on the sphere, but now on a general 2D manifold
- LB is an operator that can be applied to functions on manifolds to yield other functions

$$\Delta : C^\infty(M) \rightarrow C^\infty(M)$$

$$\Delta f = \operatorname{div} \nabla f$$



# LB Eigen-decomposition

- The Laplace-Beltrami operator  $\Delta$  has an eigendecomposition

$$\Delta \phi_i = \lambda_i \phi_i$$



$\lambda_0 = 0$

$\lambda_1 = 2.6$

$\lambda_2 = 3.4$

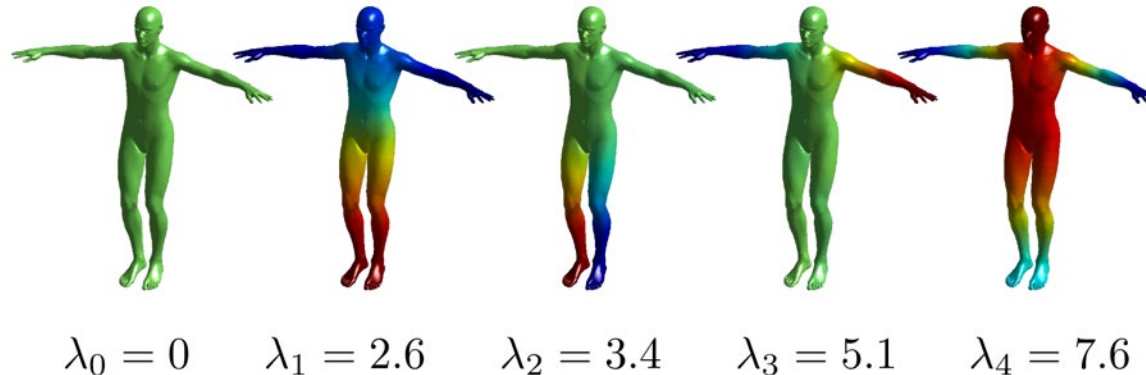
$\lambda_3 = 5.1$

$\lambda_4 = 7.6$

# Continuous Setting: Laplace-Beltrami

## Multiscale nature of the spectrum:

Intuitively, eigenfunctions corresponding to larger eigenvalues, capture *smaller details* (higher frequency) of the geometry.



- $n$ -th eigenfunction has at most  $n$  nodal domains.
- Integral of the gradient squared increases.

$$\lambda_i = \int_{\mathcal{M}} \phi_i \Delta \phi_i d\mu = \int_{\mathcal{M}} \|\nabla \phi_i\|^2 d\mu$$

# Multiscale Basis for a Function Space

$$f : M \rightarrow \mathbb{R}$$

$$= a_0 \text{ (green figure)} + a_1 \text{ (rainbow figure)} + \dots$$

$$f = \sum_{i=0}^{\infty} a_i \phi_i \quad a_i = \int_M f(x) \phi_i(x) d\mu$$

# Mesh Setting: Discrete Laplace Beltrami

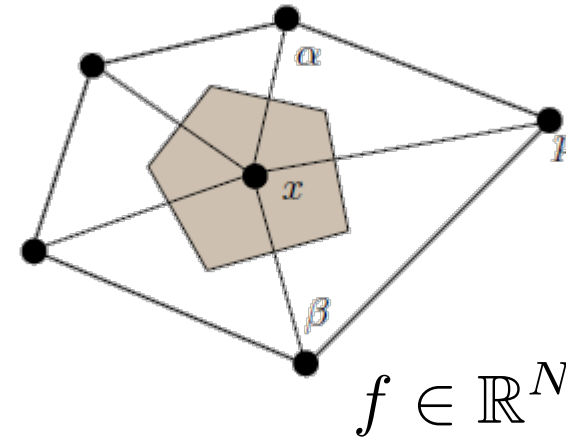
**Computing Laplace-Beltrami operator on a mesh:**

Functions are real-values defined on the triangles

Strategy: find an operator  $L$  that will satisfy

The discrete version of divergence theorem:

$$\int f L(g) dx = \int \langle \nabla f, \nabla g \rangle dx \quad \forall f, g$$

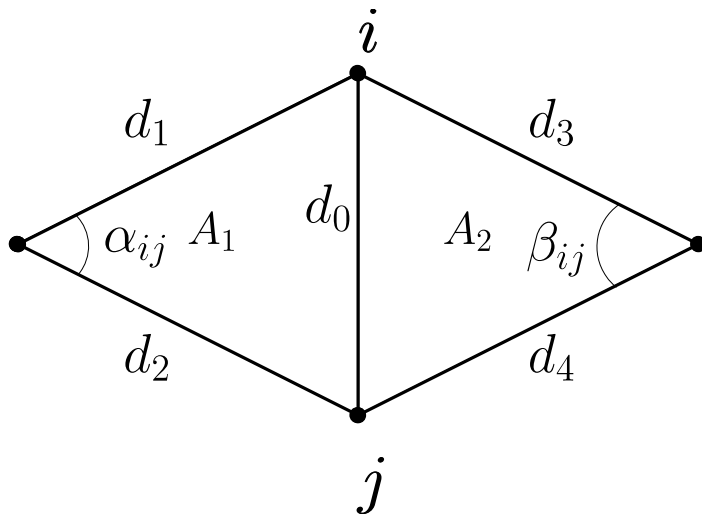


# Mesh Setting: Laplace Beltrami

In the discrete case:

$$L_{ij}A(j) = \frac{1}{2} \cot(\alpha) + \frac{1}{2} \cot(\beta)$$

In matrix notation:  $L = A^{-1}W$



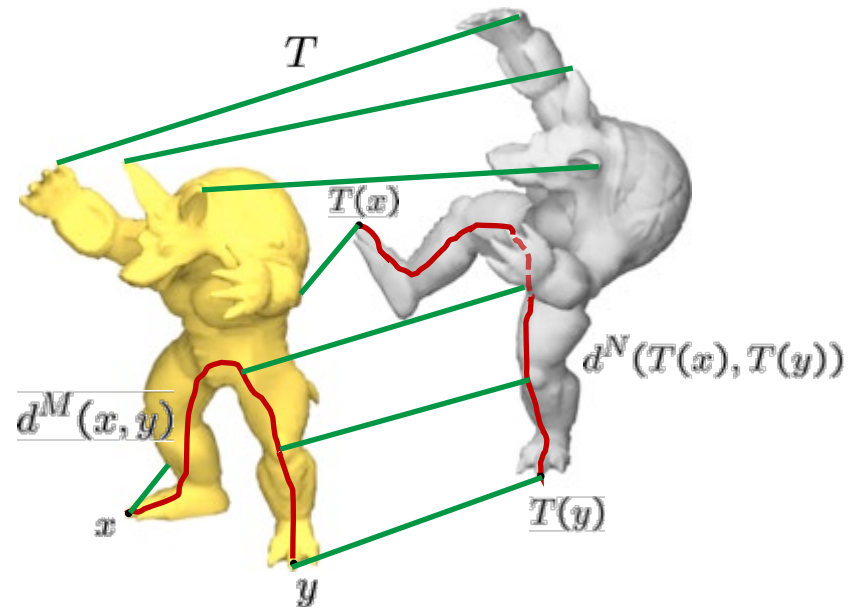
Small computational trick:

$$\begin{aligned} -W_{ij} &= \frac{1}{2} \cot(\alpha_{ij}) + \frac{1}{2} \cot(\beta_{ij}) \\ &= \frac{1}{8A_1} (d_0^2 - d_1^2 - d_2^2) \\ &\quad + \frac{1}{8A_2} (d_0^2 - d_3^2 - d_4^2) \end{aligned}$$

# Laplace-Beltrami – Isometry Invariant

## Isometry invariance (LB is intrinsic)

If two shapes are isometric then their LB operators agree.



Any quantity derived from the LB operator has to be invariant to isometries.

# Laplace-Beltrami – Some Applications

**Input:** Noisy mesh (scanned or other)

**Output:** Smooth mesh

**How:** Filter out high frequency noise

Mesh Smoothing



# Homework 3

CS233: The Shape of Data  
Geometric and Topological Data Analysis  
Stanford University

Handout # 4

Wednesday, 4 May 2022

Homework #3: Shape correspondences, shape matching, multi-way alignments. [100 points]  
Due Date: Wednesday, 18 May 2022 (11:59 PM PT)

In this homework you will experiment with two approaches for aligning the shapes in a given 3D model collection. In the first problem, you will study how to jointly align the collection of 3D shapes by formulating and solving for an appropriate Markov Random Field (MRF). In the second problem, you will build point-wise correspondences between pairs of 3D shapes based on feature matching in order to solve the alignment problem.

## Problem 1. Joint Alignment of 3D Shapes [70 points]

Aligning 3D shapes according to their orientation is an important preprocessing step for many shape analysis tasks, including finding point-to-point correspondences, performing shape comparisons and computing statistics, doing shape retrieval, etc. However, manually aligning large sets of 3D shapes is time consuming and error prone. In this problem, we study how to automatically align a set of 3D shapes in a consistent orientation (Fig. 1). To simplify the problem we make the assumption that all input models have been pre-aligned in terms of their “up” direction — their  $y$ -axis in our terminology, e.g., seats of chairs face upwards. This assumption allows us to parameterize the orientation to be estimated by only the azimuth angle, that is the rotation around the  $y$ -axis. For the coding parts of this problem we have provided you with some skeleton code located at `hmk03_code_data/code/matlab/problem1`.

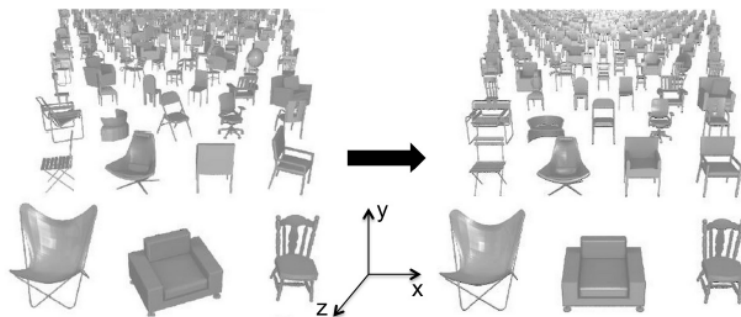


Figure 1: Joint shape alignment

# Class Midterm

- The class midterm will be in class on **Monday, May 9**, during the regular class time. It may cover material relevant to any previous lecture.
- Unlike the homeworks, the exam will consist of a number of very short problems (that also have short answers) testing basic understanding of the concepts covered in class. All problems will have the same weight and there will be some choice (do X out of Y).
- In doing the exam, you may use any of the class materials, as well as your own notes. Internet searches, however, are not allowed -- nor is any kind of human help or collaboration on the solutions.

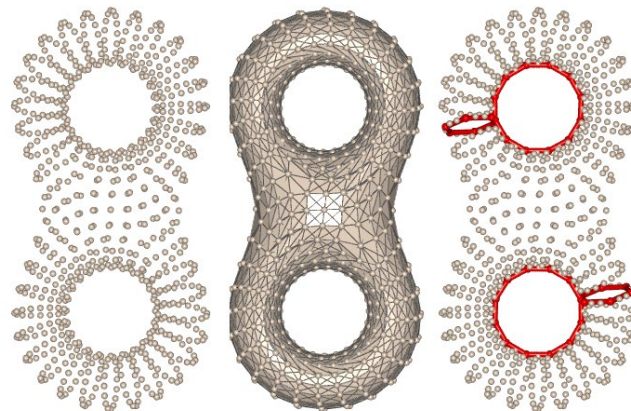
# New TDA Book

- <https://www.cs.purdue.edu/homes/tamaldey/book/CTDAbook/CTDAbook.html>

## Computational Topology for Data Analysis

Tamal Krishna Dey  
Department of Computer Science  
Purdue University  
West Lafayette, Indiana, USA 47907

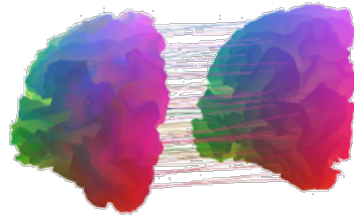
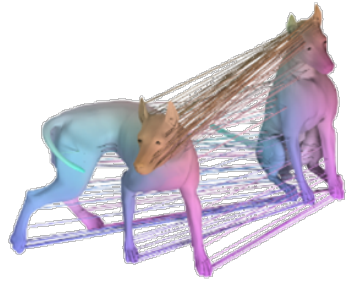
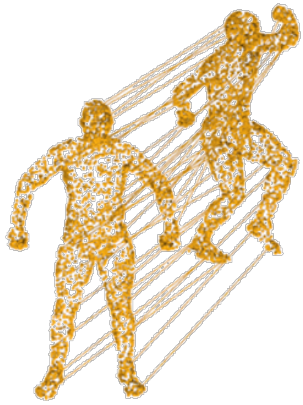
Yusu Wang  
Halıcıoğlu Data Science Institute  
University of California, San Diego  
La Jolla, California, USA 92093



# 3D Shape Features, Alignments, and Correspondences

The “wisdom of the collection” – joint data analysis

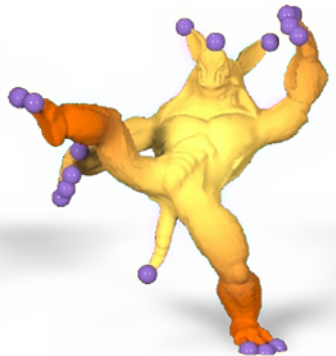
# Alignment and Correspondences, Shape Features



A



B



# Joint Learning

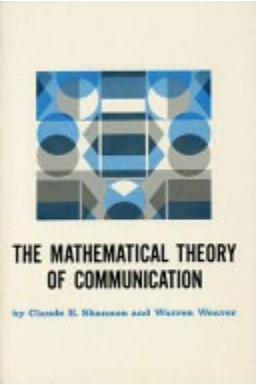
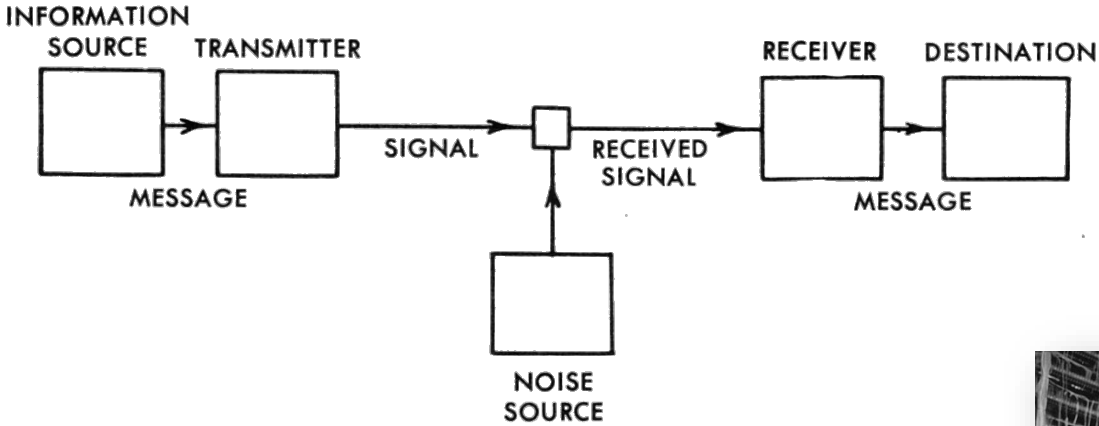


34

Similarity as a communications channel



*The Mathematical Theory of Communication*



Claude Shannon

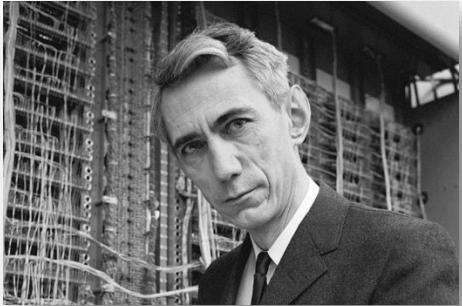
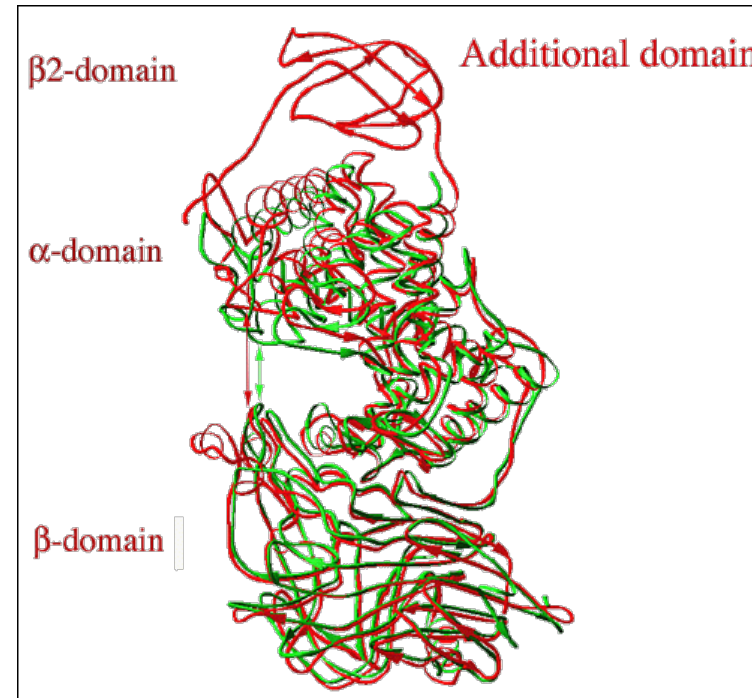
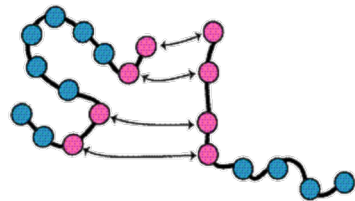


Fig. 1. — Schematic diagram of a general communication system.

# Simultaneous Estimation

- We are given two shapes  $A$  and  $B$ , each in its own coordinate system
- We must establish **correspondences** between certain parts (the **alignment supports**) of  $A$  and  $B$
- We must find an optimal **transform** that best **aligns** the supports of  $A$  and  $B$
- We must **score** this choice of supports and transform to produce a **distance measure**  $\delta$



In computing the score,

1. what distance metric do we use?
2. how do we aggregate distances?
3. how do we trade-off larger supports for larger aggregate distance?

# Rigid Alignment

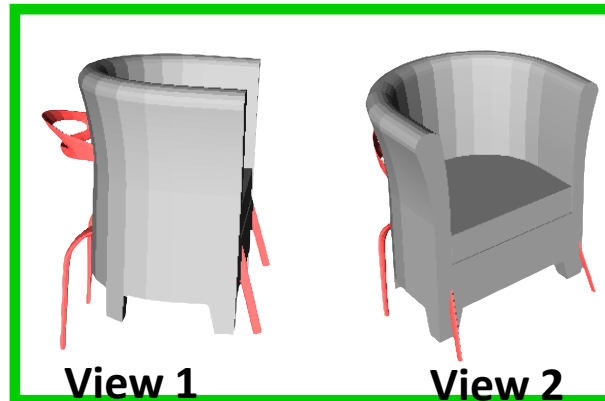
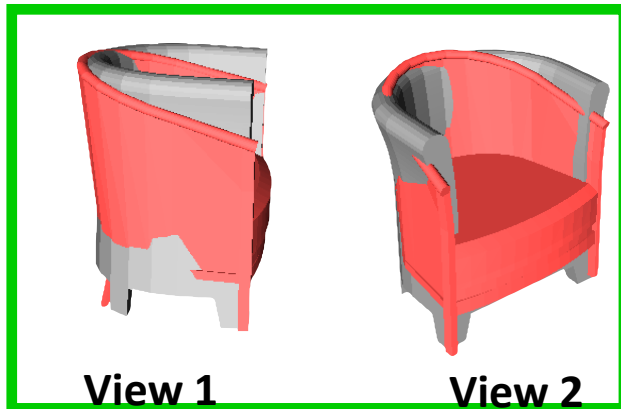
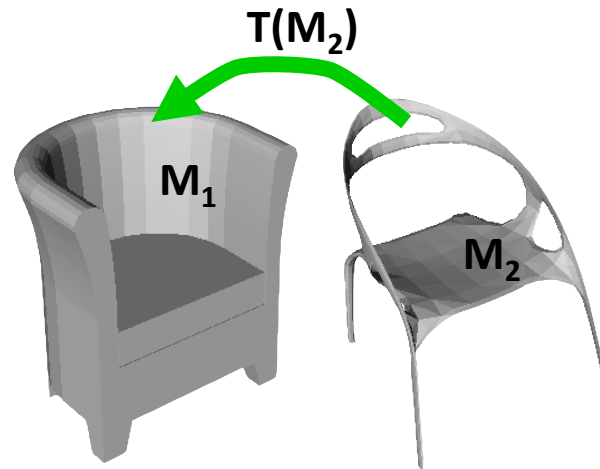
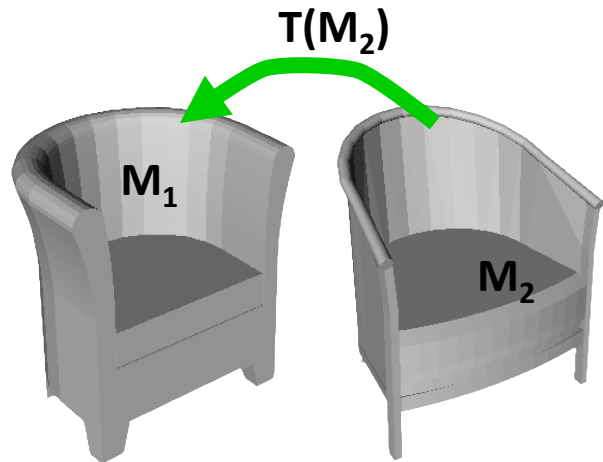
# Fundamental Registration Problem



Given two shapes with partially overlapping geometry, find an alignment between them

# General Rigid Alignment

Search for a rigid motion that best aligns the shapes, even if the shapes are different



$$M_1 \approx T(M_2)$$

$T$  : translation + rotation

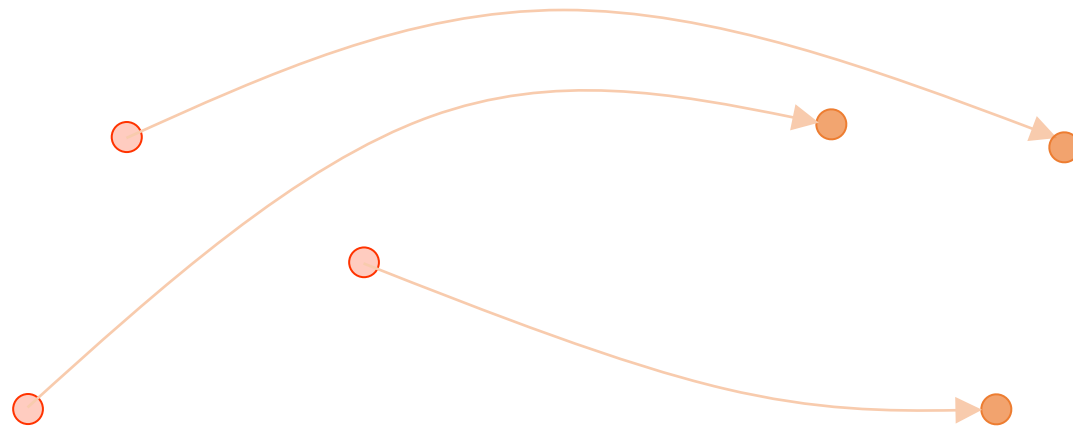
# Optimal Rigid Alignment for Points

Problem Formulation:

1. Given two sets points:  $\{x_i\}, \{y_i\}, i = 1..n$  in  $\mathbb{R}^3$  Find the rigid transform:

$\mathbf{R}, t$  that minimizes:

$$\sum_{i=1}^N \|\mathbf{R}x_i + t - y_i\|_2^2$$



# Simplest Case: Rigid Alignment, Given Correspondences

- We are given two sets of **corresponding** points  $x_1, x_2, \dots, x_n$  and  $y_1, y_2, \dots, y_n$  in  $\mathbb{R}^3$ . We wish to compute the rigid transform  $T$  that best aligns  $x_1$  to  $y_1, x_2$  to  $y_2, \dots$ , and  $x_n$  to  $y_n$ .
- We define the error to be minimized by

$$\min_T \sum_{i=1}^n \|T(x_i) - y_i\|^2$$

MSE error, RMS distance, ...



- Old Problem:
  - Known and solved as the *orthogonal Procrustes problem* in Factor Analysis (Statistics) [Shönemann, 1966]
  - Known and solved as the *absolute orientation problem* in Photogrammetry [Horn, 1986]
  - Also in robotics, graphics, medical image analysis, statistical theories of shape, etc ...



# Separability

- A rigid motion  $T$  is a combination of a translation  $a$  and a rotation  $R$ , so that  $T(x) = R(x) + a$ .
- If we place the origin of our coordinate system at the mean of the  $x_i$ 's, then the quantity to be minimized simplifies to (up to some constants):

$$\min_{a, R} \left( \sum_{i=1}^n |y_i - a|^2 - 2 \sum_{i=1}^n \langle R(x_i), y_i \rangle \right)$$

- Note that the translational and rotational parts separate. The translational part  $a$  can easily be seen to be optimized by

$$a = \frac{1}{n} \sum_{i=1}^n y_i$$

The centroids of the two point sets have to be aligned!

# The Rotation Part via SVD

- Define

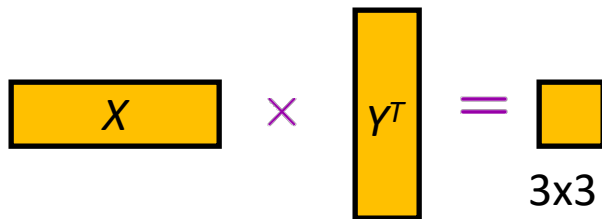
$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$$

$$X = [x_1 - \bar{x}, \dots, x_n - \bar{x}]^T$$

$$Y = [y_1 - \bar{y}, \dots, y_n - \bar{y}]^T$$

- Here  $X$  and  $Y$  are 3 by  $n$  matrices.



A diagram illustrating matrix multiplication. On the left, a yellow horizontal rectangle labeled 'X' is multiplied by a yellow vertical rectangle labeled 'Y<sup>T</sup>'. The result is a yellow square labeled '3x3'.

\*SVD = singular value decomposition

- Now compute the SVD\*

$$XY^T = UDV^T \quad (3 \times 3)$$

- $U$  and  $V$  are 3 by 3 orthogonal matrices, and  $D$  is a diagonal matrix with decreasing non-negative entries along the diagonal (the singular values).

- Define  $S$  by

$$S = \begin{cases} I, & \text{if } \det U \det V = 1 \\ \text{diag}(1, \dots, 1, -1), & \text{otherwise} \end{cases}$$

- Then

$$R = USV^T$$

**$O(n)$  algorithm!**

# Optimal Transformation Summary

Problem Formulation:

1. Given two sets points:  $\{x_i\}, \{y_i\}, i = 1..n$  in  $\mathbb{R}^3$ . Find the rigid transform:

$\mathbf{R}, t$  that minimizes: 
$$\sum_{i=1}^N \|\mathbf{R}x_i + t - y_i\|_2^2$$

2. Closed form solution:

1. Construct:  $C = \sum_{i=1}^N (y_i - \mu^Y)(x_i - \mu^X)^T$ , where  $\mu^X = \frac{1}{N} \sum_i x_i$ ,

2. Compute the SVD of C:  $C = U\Sigma V^T$   $\mu^Y = \frac{1}{N} \sum_i y_i$

1. If  $\det(UV^T) = 1, R_{\text{opt}} = UV^T$

2. Else  $R_{\text{opt}} = U\tilde{\Sigma}V^T, \tilde{\Sigma} = \text{diag}(1, 1, \dots, -1)$

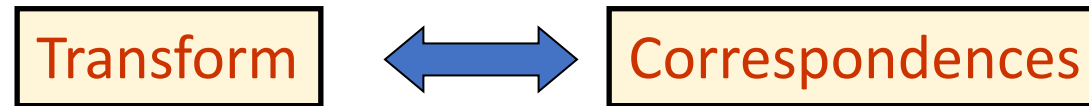
3. Set  $t_{\text{opt}} = \mu^Y - R_{\text{opt}}\mu^X$

Note that C is a 3x3 matrix. SVD is very fast.

Arun et al., Least-Squares Fitting of  
Two 3-D Point Sets

# How to Get Correspondences?

*A chicken-and-egg problem:* if we knew the optimal aligning transform, then we could get correspondences by **proximity** (possibly with the aid of some global adjustment, e.g., dynamic programming)



Guess one, estimate the other, and *iterate!*

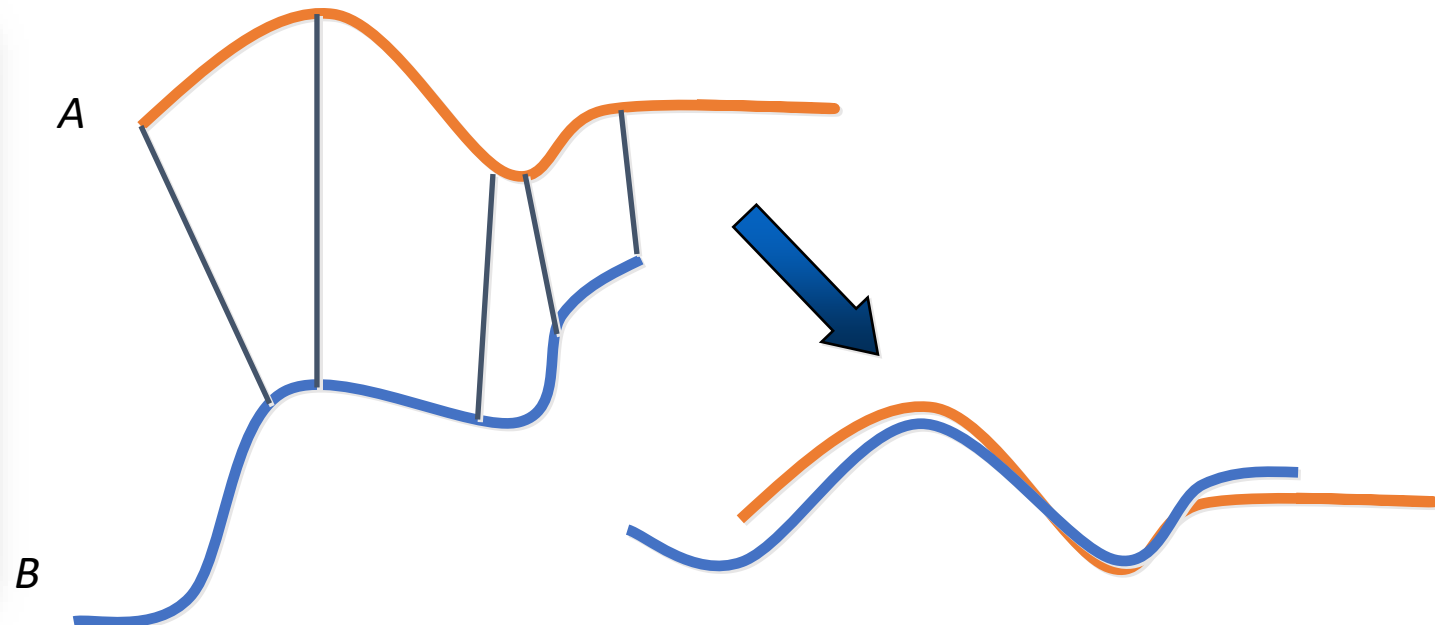
EM like

- Correspondences from proximity (**Iterated Closest Pair**)
- Correspondences from local shape descriptors (**Shape Features**)
- Transform from voting schemes (**RANSAC, Geometric Hashing**)
- Combinations

Local Methods:  
Iterated Closest Pair (ICP)  
[Besl, McKay 1992]

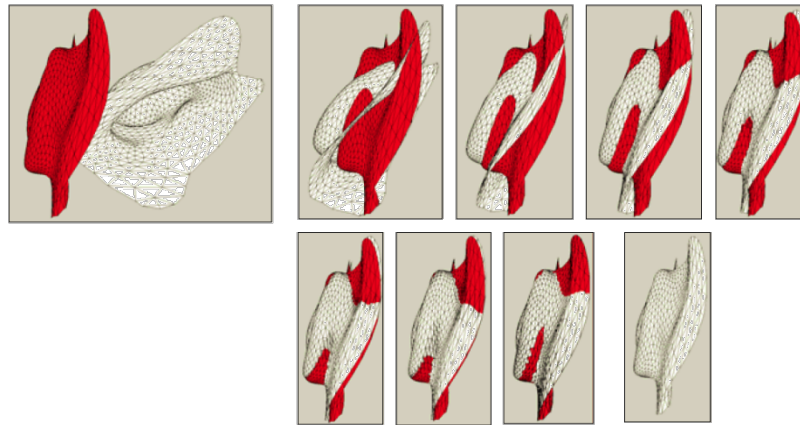
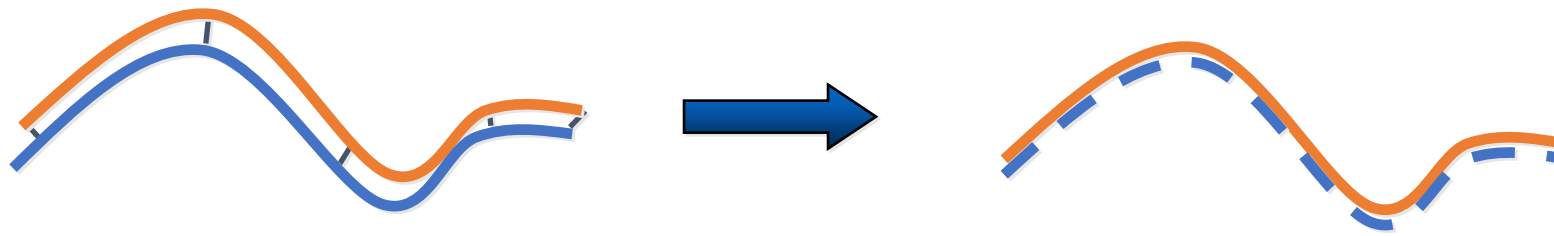
# Aligning 3D Data

- How to find correspondences: User input? Feature detection? Local shape signatures?
- When  $A$  and  $B$  are partial scans of the same stationary object captured in a consistent setting, use the simplest alternative: **assume closest points correspond**



# Aligning 3D Data

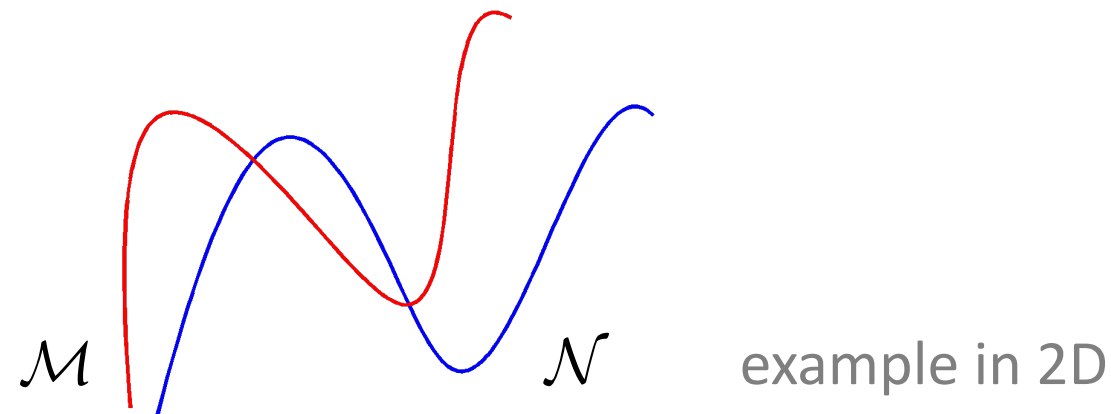
- Align the  $A$  points to their closest  $B$  neighbors, then repeat
- Converges, if starting positions are “close enough”



Successive iterations bring the objects closer together

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

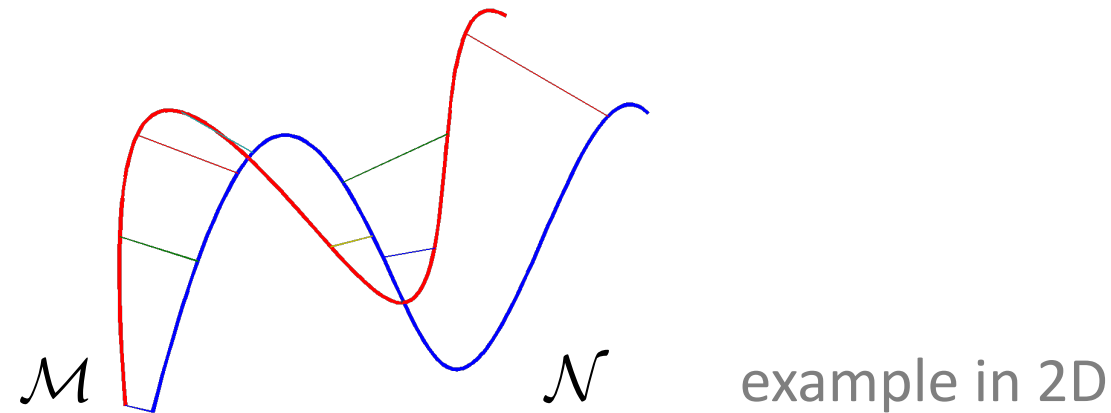
1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R, t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

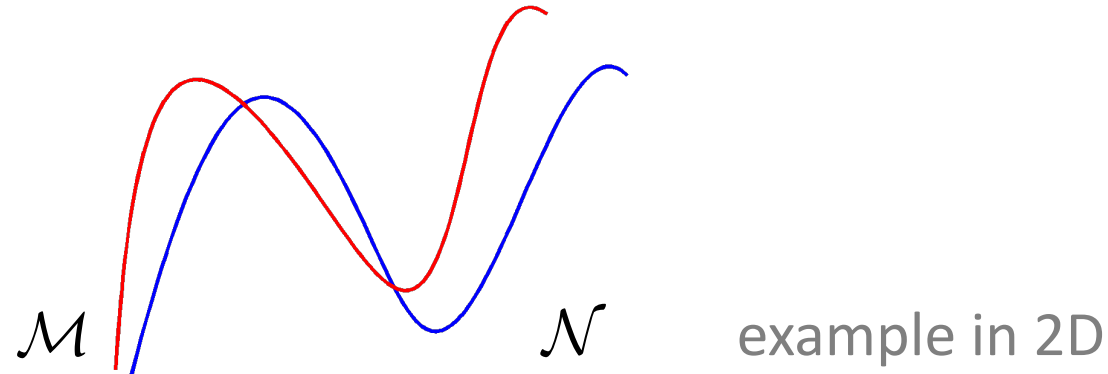
1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R,t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

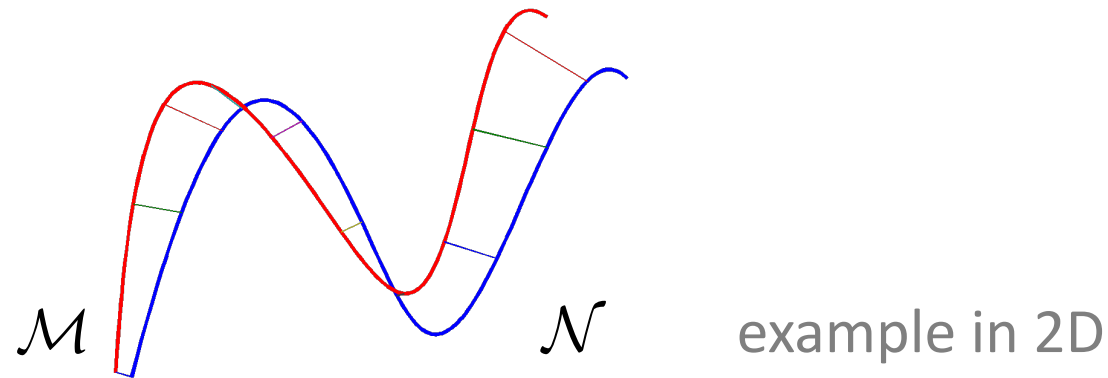
1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R, t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

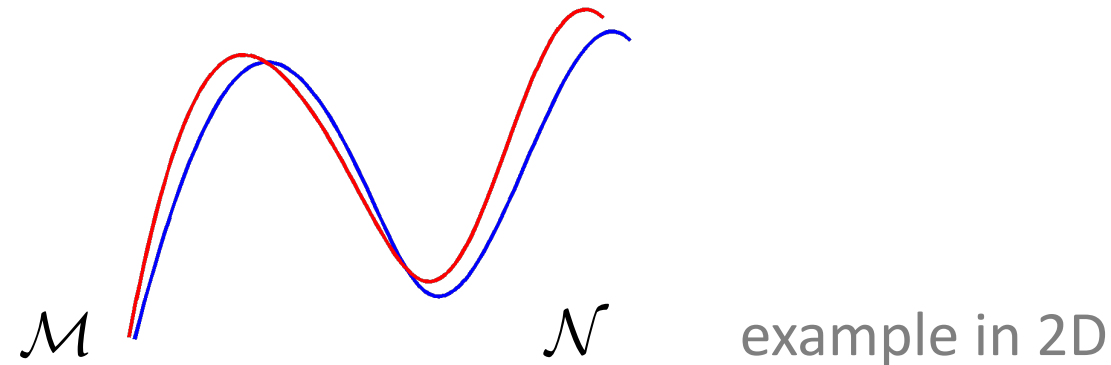
1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R,t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

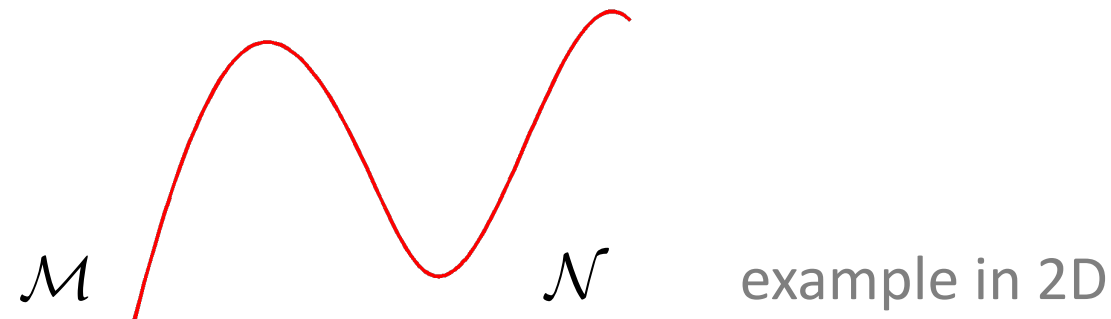
1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R,t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Iterative Closest Point (ICP)

- Classical approach: iterate between finding correspondences and finding the transformation:



Given a pair of shapes,  $\mathcal{M}$  and  $\mathcal{N}$ , iterate:

1. For each  $x_i \in \mathcal{M}$  find **nearest** neighbor  $y_i \in \mathcal{N}$
2. Find optimal transformation  $\mathbf{R}, t$  minimizing:

$$\arg \min_{R,t} \sum_i \|Rx_i + t - y_i\|_2^2$$

Classic problem,  
solvable by SVD

# Convergence Theorem

- The ICP algorithm always converges monotonically to a local minimum, with respect to the MSE distance objective function
  - Correspondence step improves error bound – because of nearest neighbor computation
  - Rotation/translation step improves error bound – because of transform optimization

# Time Analysis

Each iteration includes three main steps

A. Finding the closest points:

$O(N_M)$  per point

$O(N_M * N_S)$  total

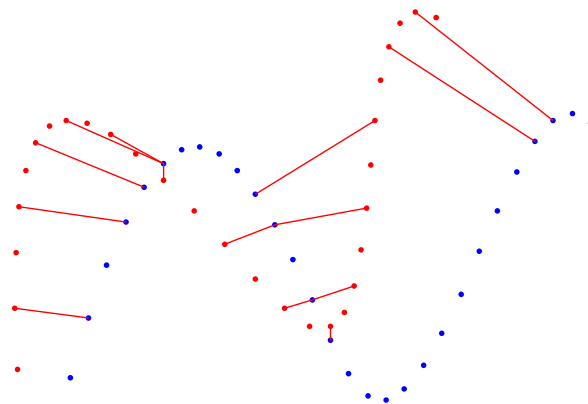
B. Calculating the optimal alignment:  $O(N_S)$

C. Updating the scene:  $O(N_S)$

Fast nearest-neighbor data structures can be very helpful here, e.g., a *k-d* tree

# Variations of ICP

1. **Selecting** source points (from one or both scans): sampling
2. **Matching** to points in the other mesh
3. **Weighting** the correspondences
4. **Rejecting** certain (outlier) point pairs
5. **Assigning** an error metric to the current transform
6. **Minimizing** the error metric w.r.t. the transformation

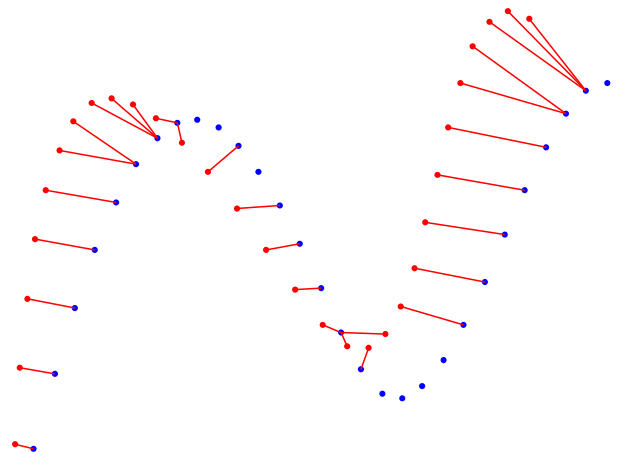


# Iterative Closest Point

Given a pair of shapes, X and Y, iterate:

1. For each  $x_i \in X$  find **nearest** neighbor  $y_i \in Y$ .
2. Find deformation  $\mathbf{R}$ ,  $t$  minimizing:

$$\sum_{i=1}^N \|\mathbf{R}x_i + t - y_i\|_2^2$$



Ideally, most correspondences are 1-1

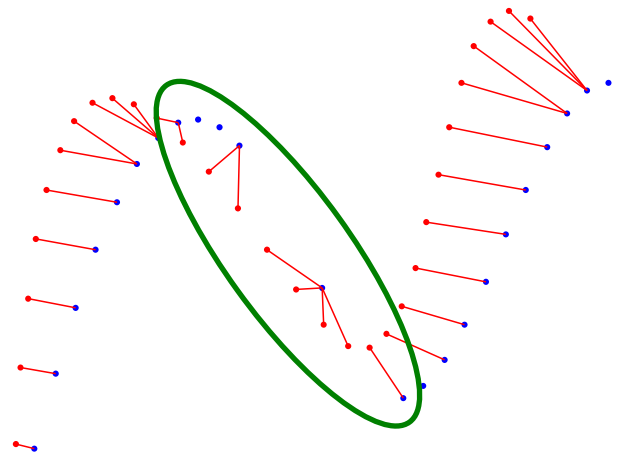
# Iterative Closest Point

Given a pair of shapes, X and Y, iterate:

1. For each  $x_i \in X$  find **nearest** neighbor  $y_i \in Y$ .
2. Find deformation  $\mathbf{R}$ ,  $t$  minimizing:

$$\sum_{i=1}^N \|\mathbf{R}x_i + t - y_i\|_2^2$$

Problem:  
uneven sampling



# Iterative Closest Point

Given a pair of shapes,  $X$  and  $Y$ , iterate:

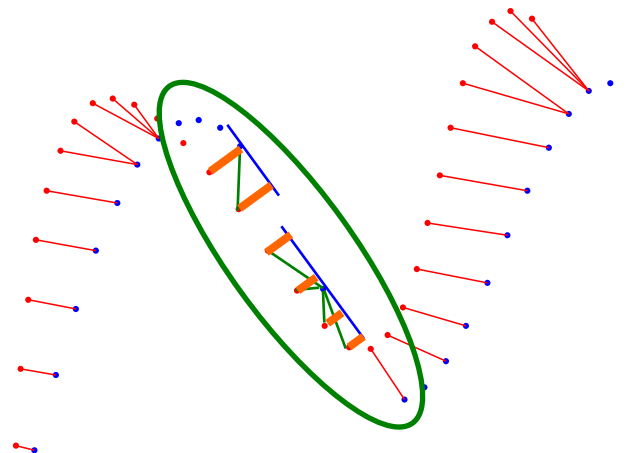
1. For each  $x_i \in X$  find **nearest** neighbor  $y_i \in Y$ .
2. Find deformation  $\mathbf{R}$ ,  $t$  minimizing:

$$\sum_{i=1}^N d(\mathbf{R}x_i + t, P(y_i))^2 = \sum_{i=1}^N ((\mathbf{R}x_i + t - y_i)^T \mathbf{n}_{y_i})$$

**Solution:**

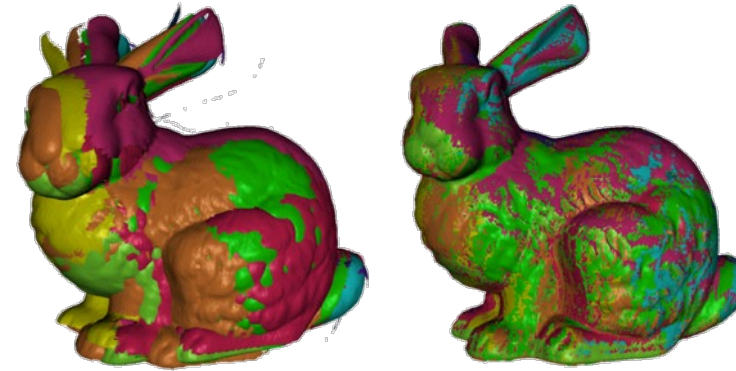
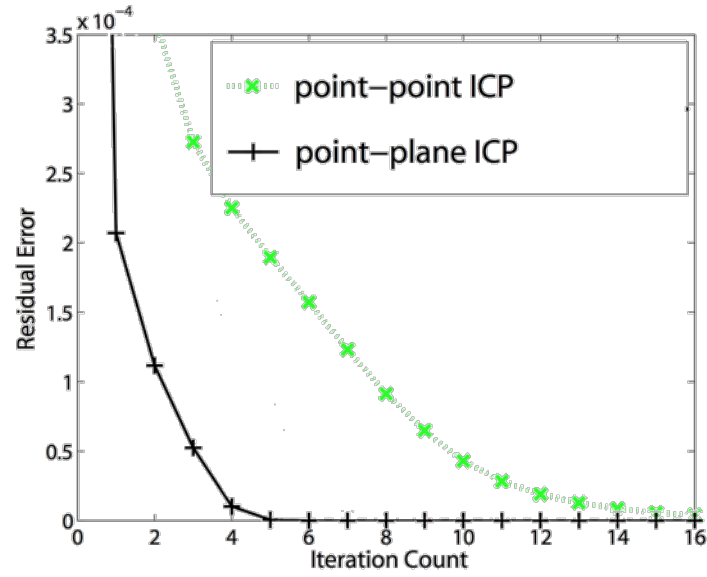
Minimize distance to  
the tangent plane

Chen, Medioni, '91



No longer a closed-form  
solution

# Iterative Closest Point

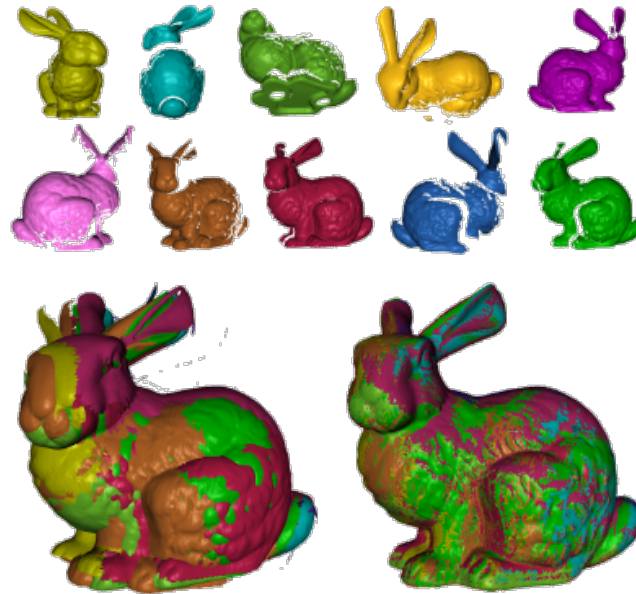


Aligning the bunny to itself:  
Point-to-plane always wins in the end-game.

# Global Matching Methods

# Global Matching

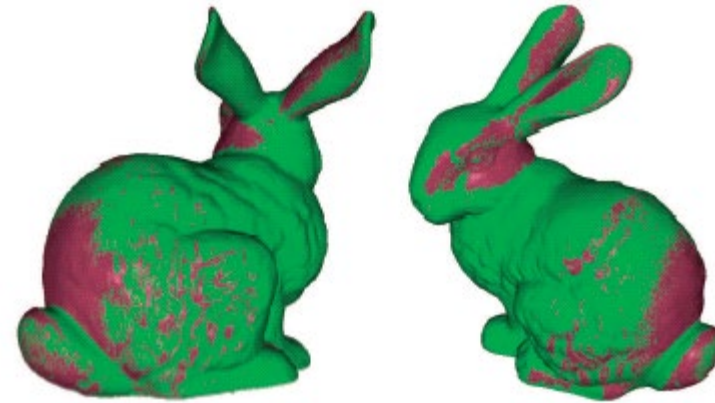
Given shapes in *arbitrary* positions, find their alignment:



*Robust Global Registration*  
Gelfand et al. SGP 2005

Can be approximate, since will refine later using e.g. ICP

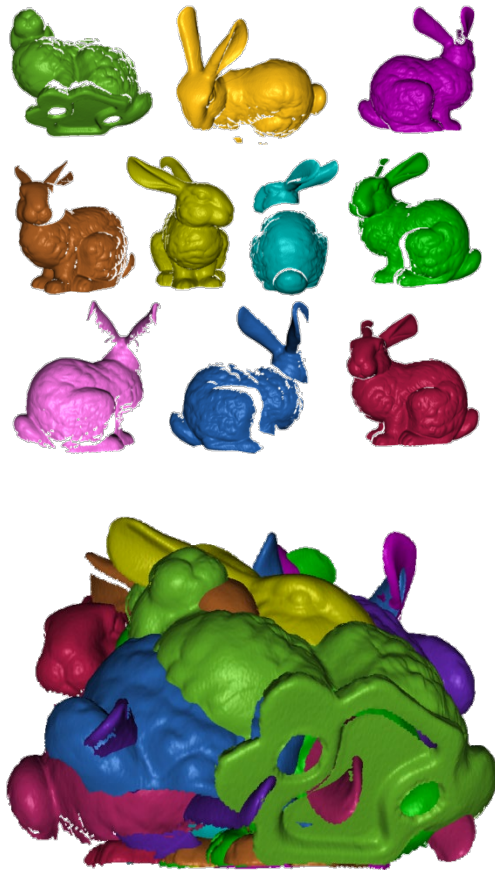
# Partial Alignment



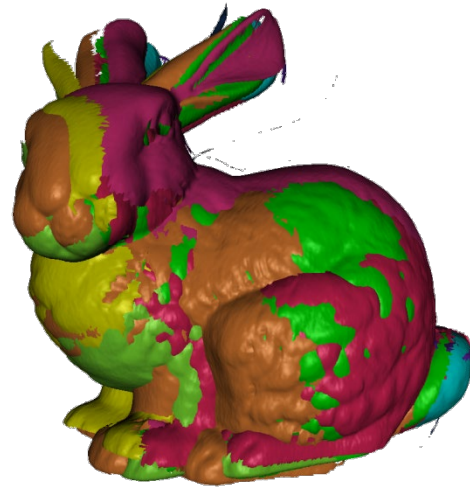
After 6 iterations

# Multiple Alignment Results

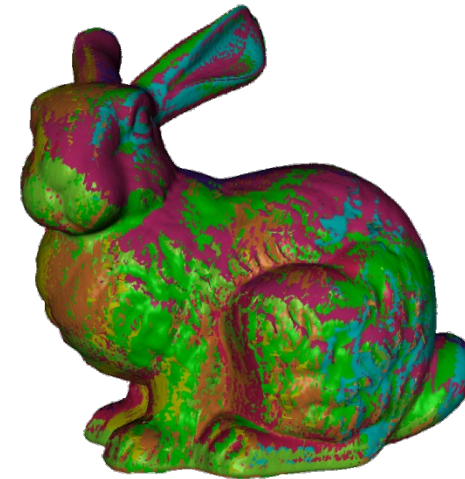
**Bundle adjustment:** build a scan graph  
keep re-aligning pairs so as to reduce global error



Input: 10 scans



Approximate alignment



Refined by ICP

# Global Matching – Approaches

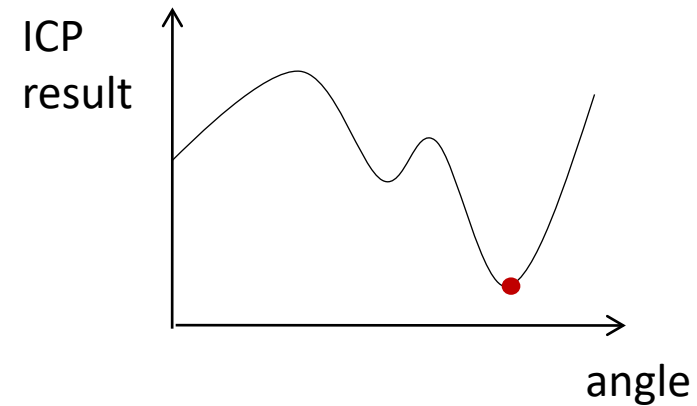
Several classes of approaches:

1. Exhaustive Search
2. Normalization
3. Random Sampling
4. Invariance

# Exhaustive Search:

Compare (ideally) all alignments

- Sample the space of possible initial alignments.
- Correspondence is determined by the alignment at which models are closest.



Very common in biology: e.g., protein docking

# Exhaustive Search:

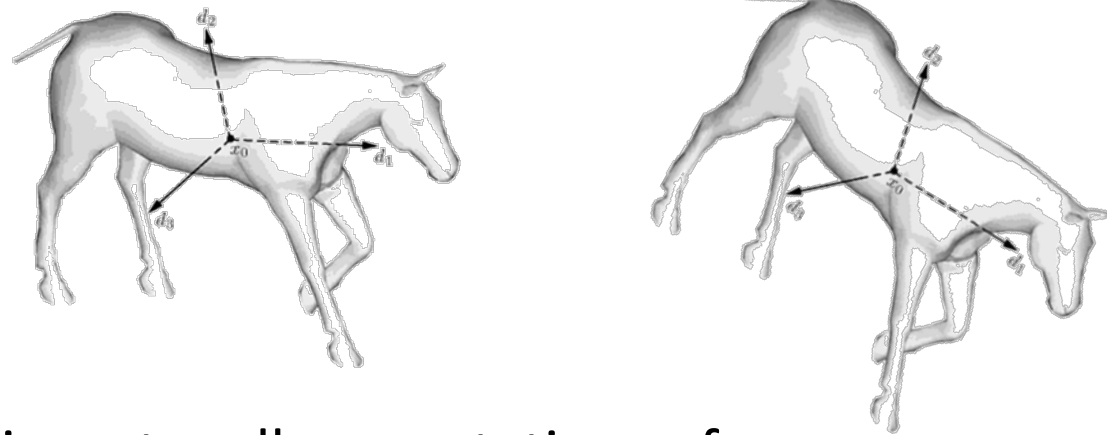
## Compare at all alignments

- Sample the space of possible initial alignments
- Correspondence is determined by the alignment at which models are closest
- Provides optimal result
- Can be unnecessarily slow
- Does not generalize well to non-rigid deformations

# Normalization – Canonical Poses

There are only a handful of initial configurations that are important.

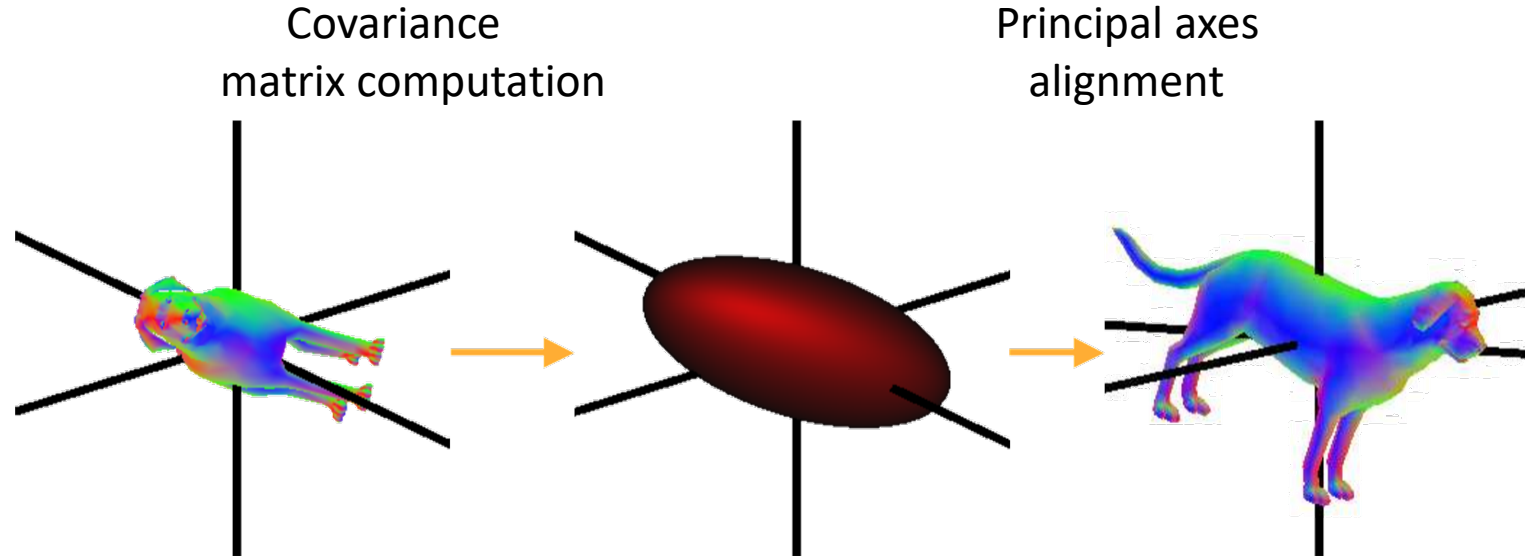
Can center all shapes at the origin and use PCA to find the principal directions of the shape.



In addition sometimes try all permutations of x-y-z.

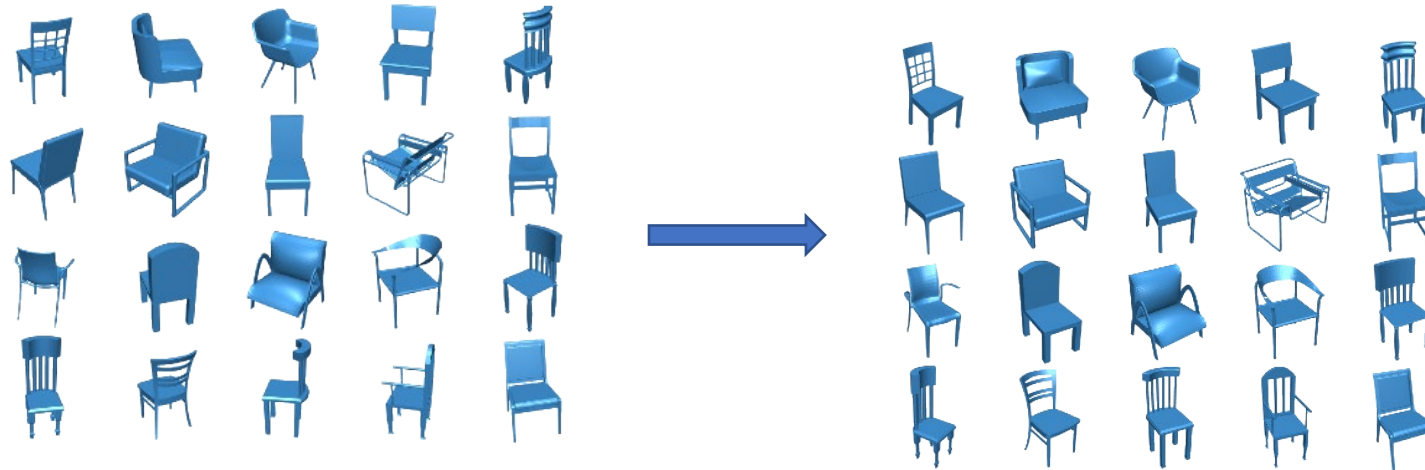
# PCA-Based Alignment

- ◆ Use PCA to place models into canonical coordinate frames
- ◆ Then align those frames



# Normalization – Canonical Poses

There are only a handful of initial configurations that are important.

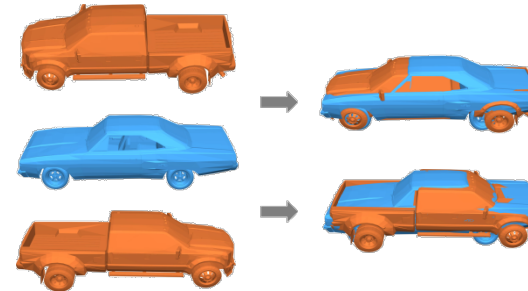


Works well if we have complete shapes and no noise.

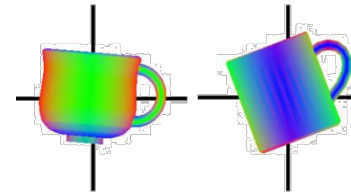
Fails for partial scans, outliers, high noise, etc.

# Problems with PCA

- ◆ Principal axes are not consistently oriented
  - ◆ Symmetries cause problems



- ◆ Axes are unstable when principal values are similar



- ◆ Partial similarity

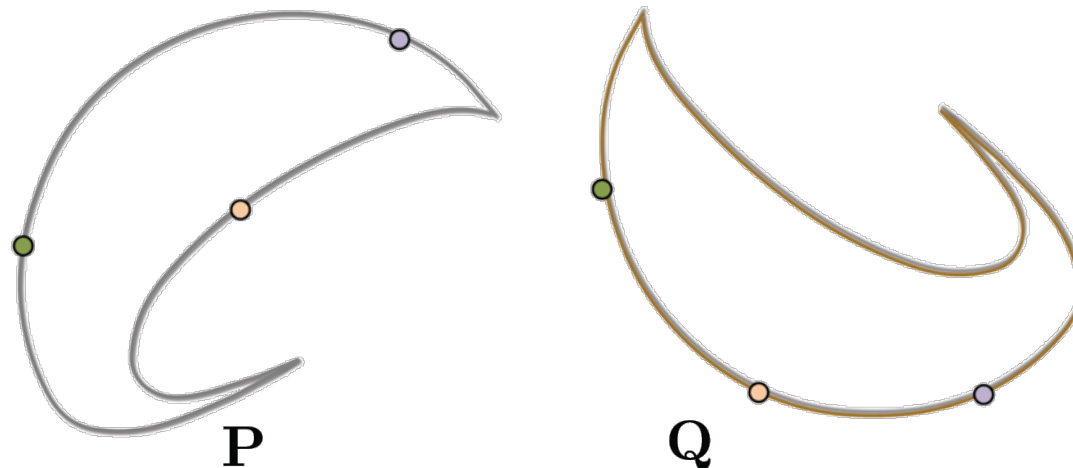


# Random Sampling (RANSAC)

ICP only needs 3 point pairs! – Rigid motion space is 6-dimensional.

Robust and Simple approach. Iterate between:

1. Pick a random pair of 3 points on model & scan
2. Estimate alignment, and check for error.



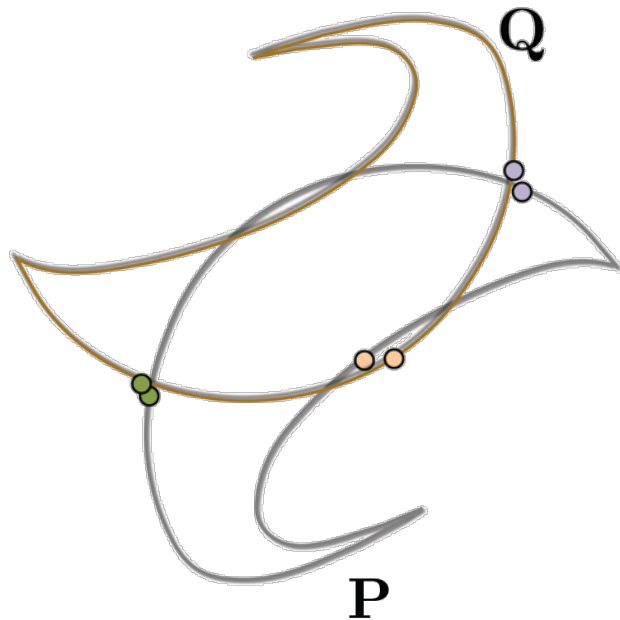
Guess and  
verify

# Random Sampling (RANSAC)

ICP only needs 3 point pairs! – Rigid motion space is 6-dimensional.

Robust and simple approach. Iterate between:

1. Pick a random pair of 3 points on model & scan
2. Estimate alignment, and check for error.



Guess and  
verify

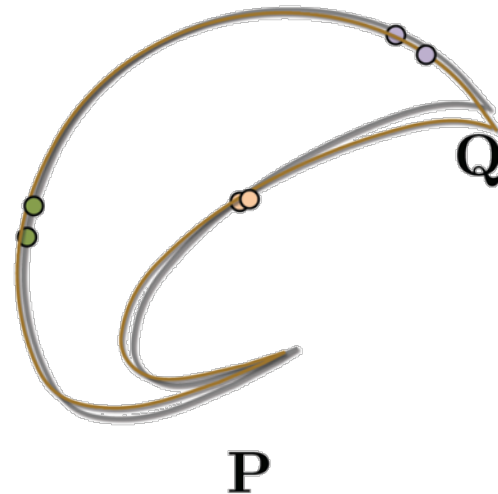
# Random Sampling (RANSAC)

ICP only needs 3 point pairs! – Rigid motion space is 6-dimensional.

Robust and simple approach. Iterate between:

1. Pick a random pair of 3 points on model & scan
2. Estimate alignment, and check for error.

Can be expensive!



Can also refine the final result. Picks don't have to be exact.

Guess and verify

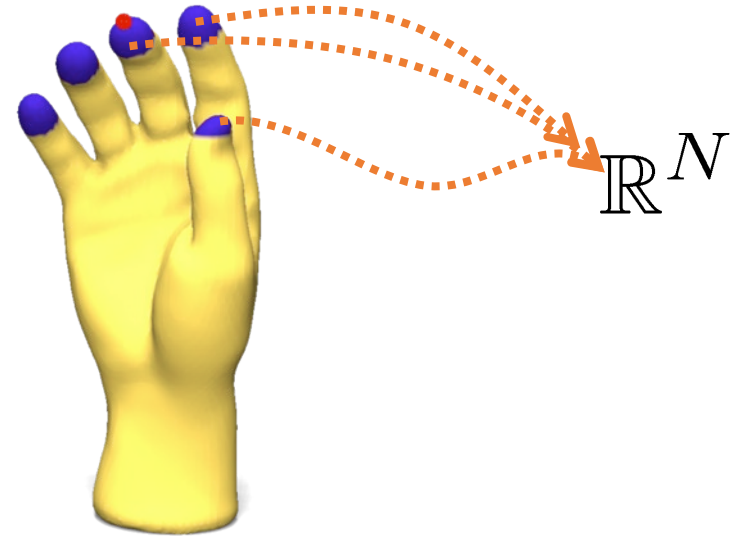
# Global Matching – Invariant Features

Try to characterize the shape using properties that are invariant under the desired set of transformations.

Conflicting interests – invariance vs. informativeness.

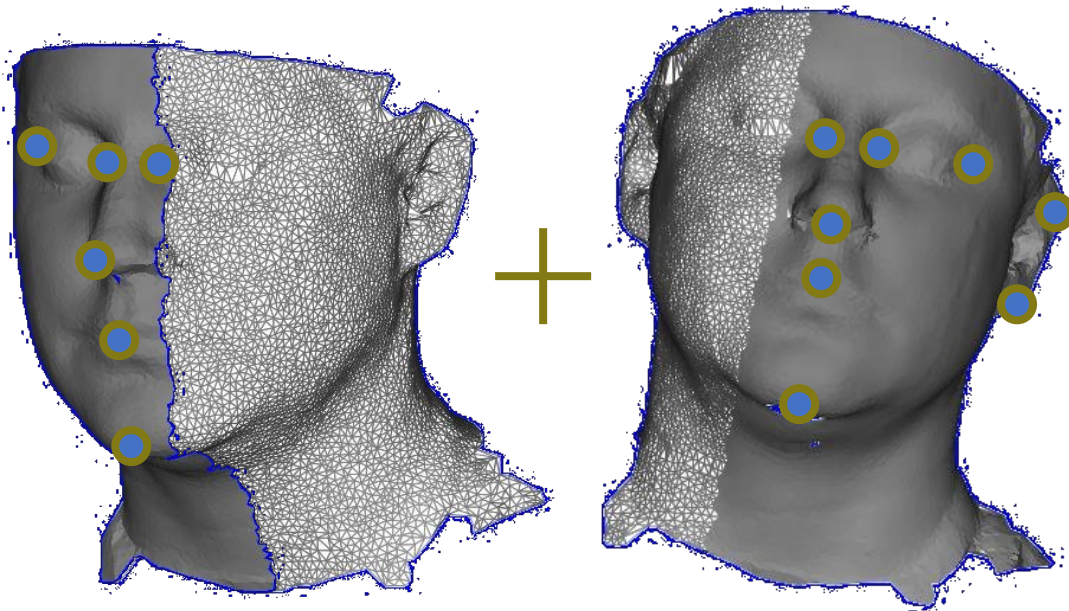
The most common pipeline:

1. identify salient feature points
2. compute informative and commensurable descriptors.



# Matching Using Feature Points

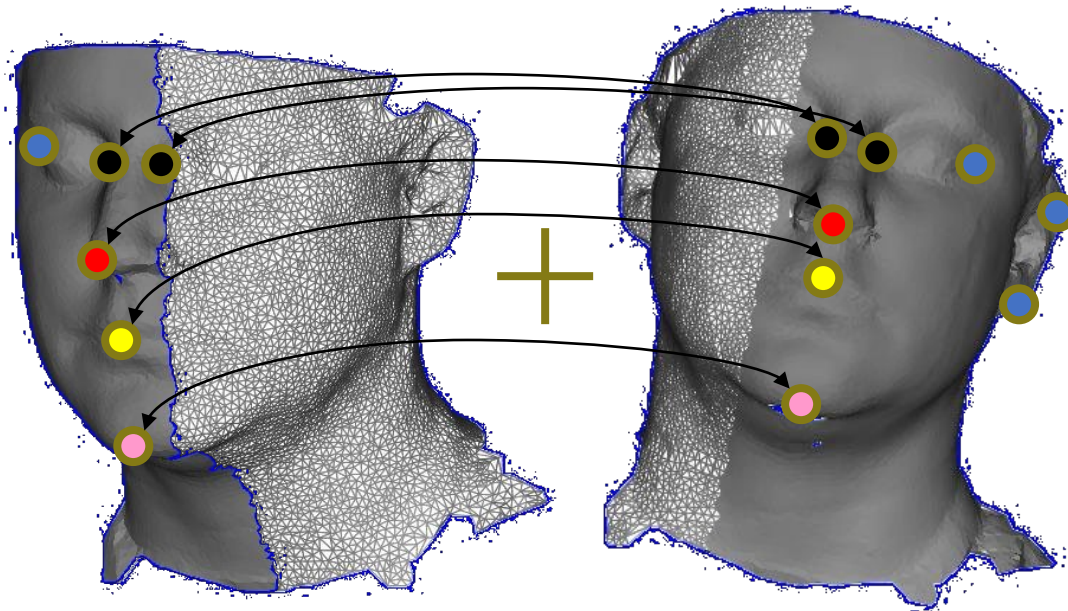
1. Find **feature points** on the two scans (we'll come back to that issue)



Partially Overlapping Scans

# Approach

1. (Find feature points on the two scans)
2. Establish **correspondences**

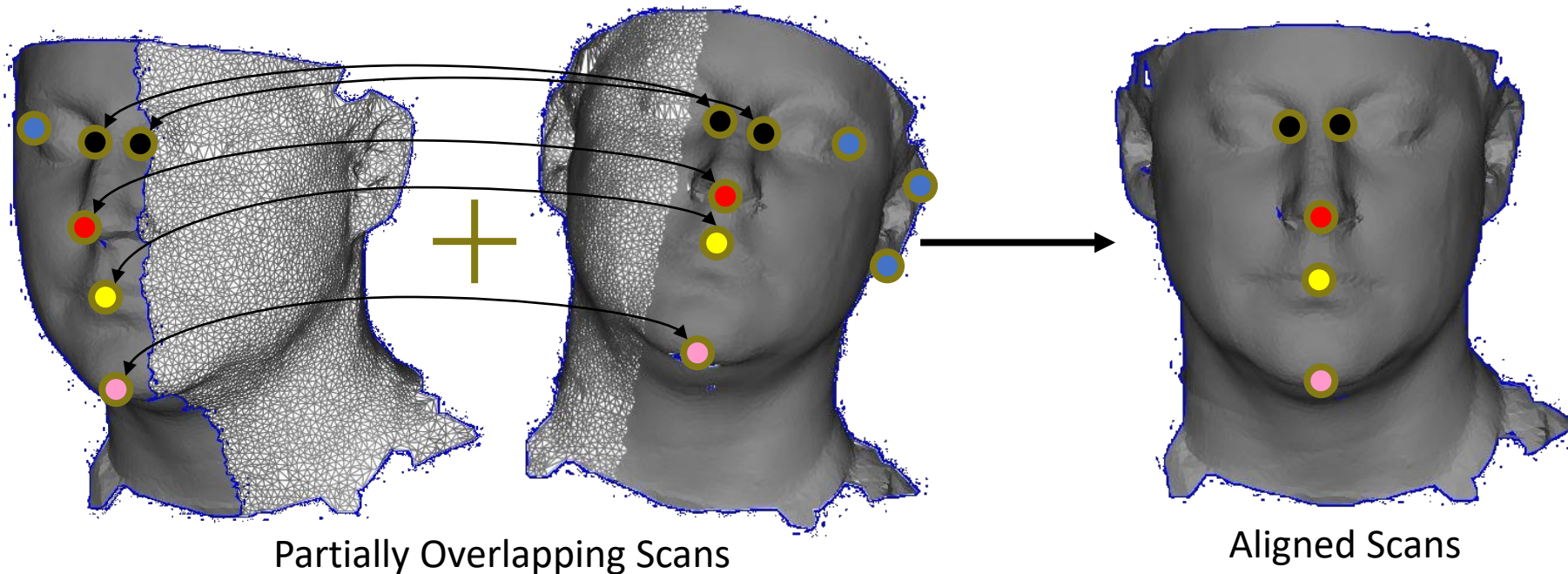


Partially Overlapping Scans

# Approach

1. (Find feature points on the two scans)
2. Establish correspondences
3. Compute the aligning transformation

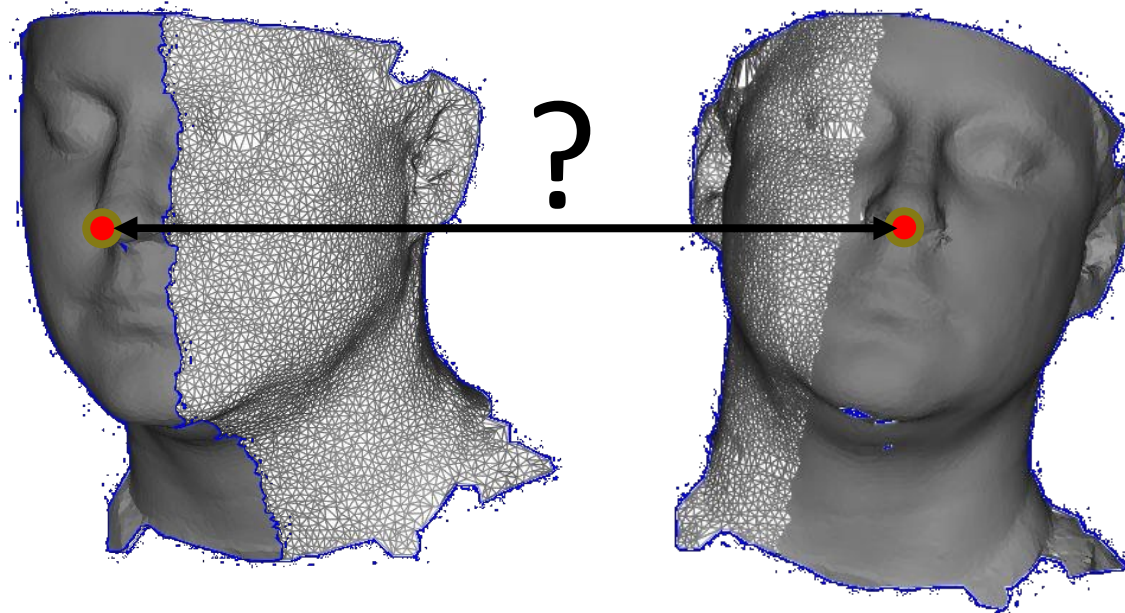
Preserve features  
Various regularizers



# Correspondence

## Goal:

Identify when two points on different scans represent the same feature

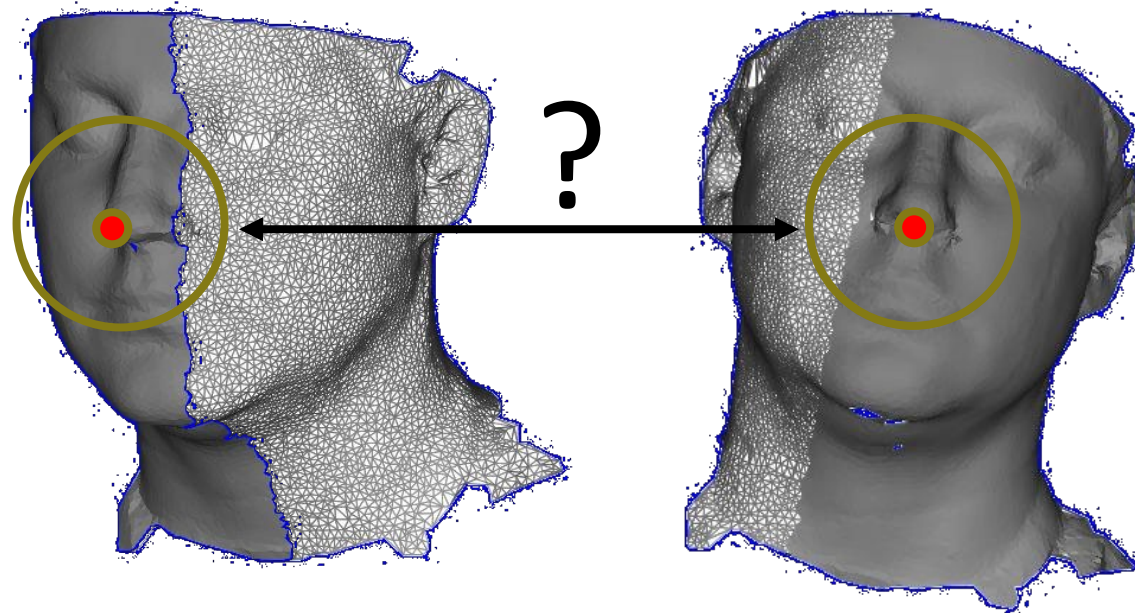


# Correspondence

## Goal:

Identify when two points on different scans represent the same feature:

Are the surrounding regions similar?

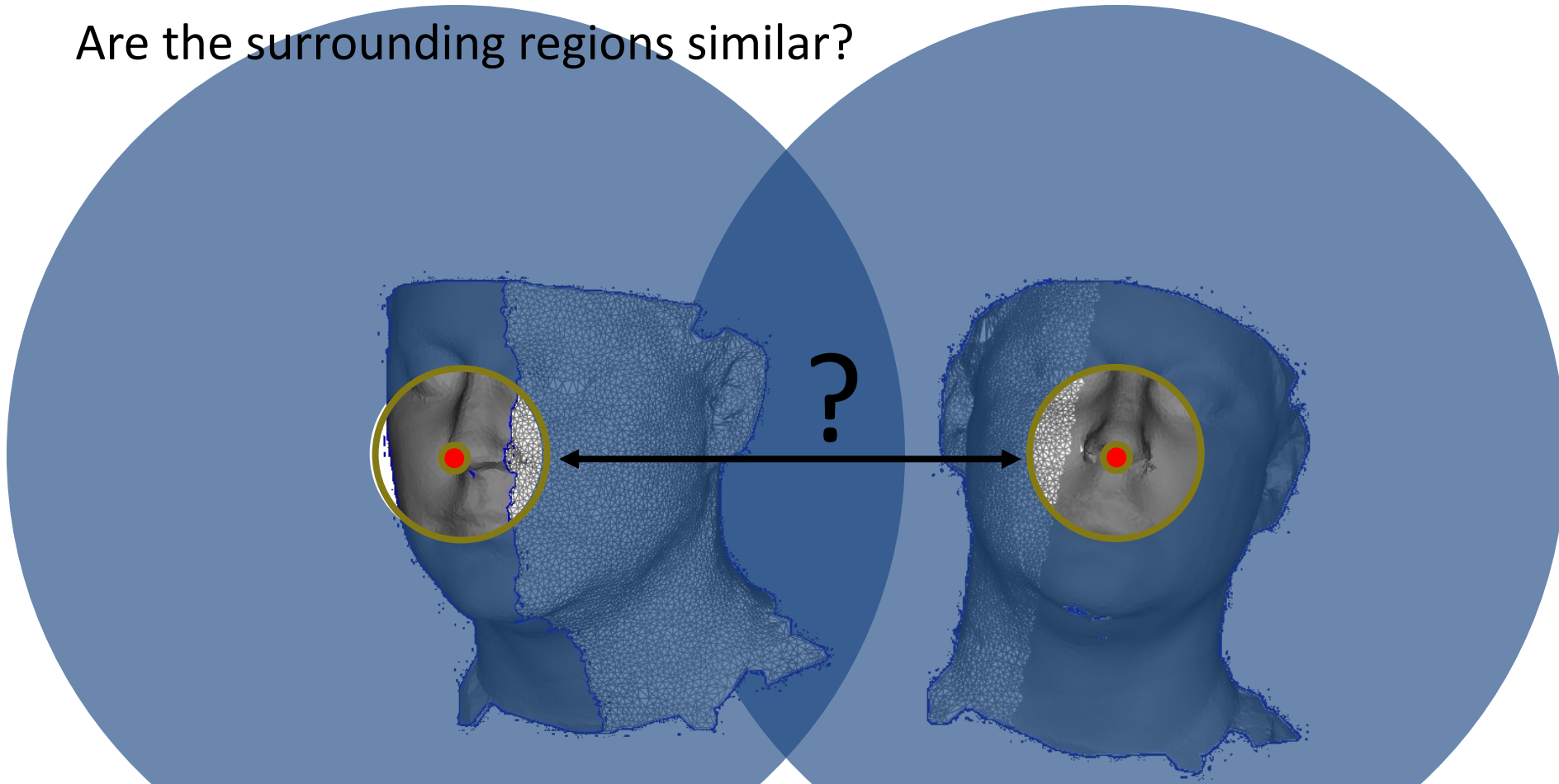


# Correspondence

## Goal:

Identify when two points on different scans represent the same feature:

Are the surrounding regions similar?



# Shape Descriptors

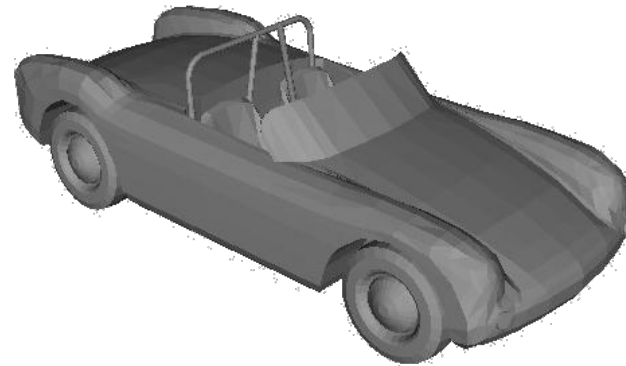
# Global Shape Similarity

# Global Similarity

Given two 3D models, determine if they represent the same/similar shapes



?



# Global Similarity

Given two models, determine if they represent the same/similar shapes.



Models can have different:  
representations, tessellations, topologies, etc.

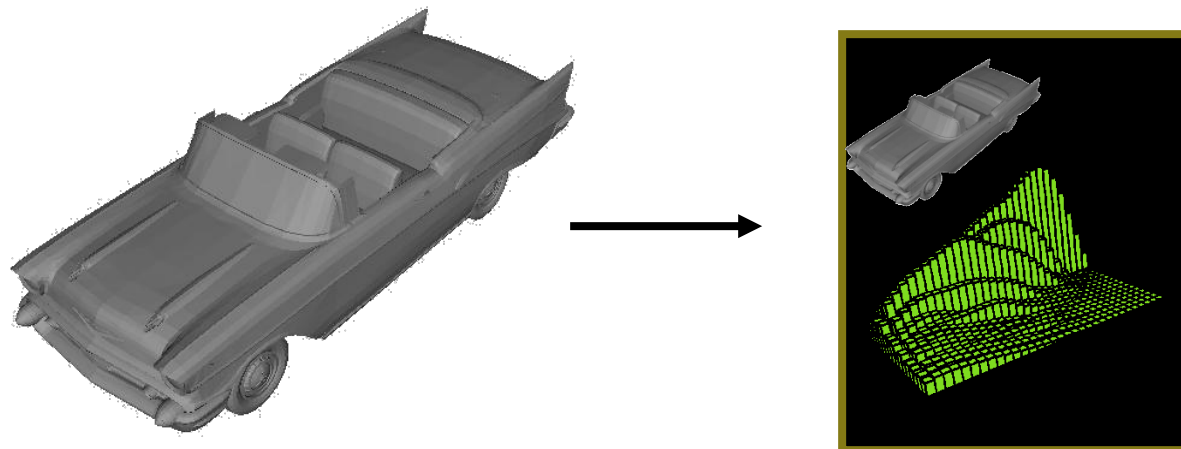
# Global Similarity

## Approach:

### 1. Represent each model by a **shape descriptor**:

- A structured abstraction of a 3D model
- That captures salient shape information

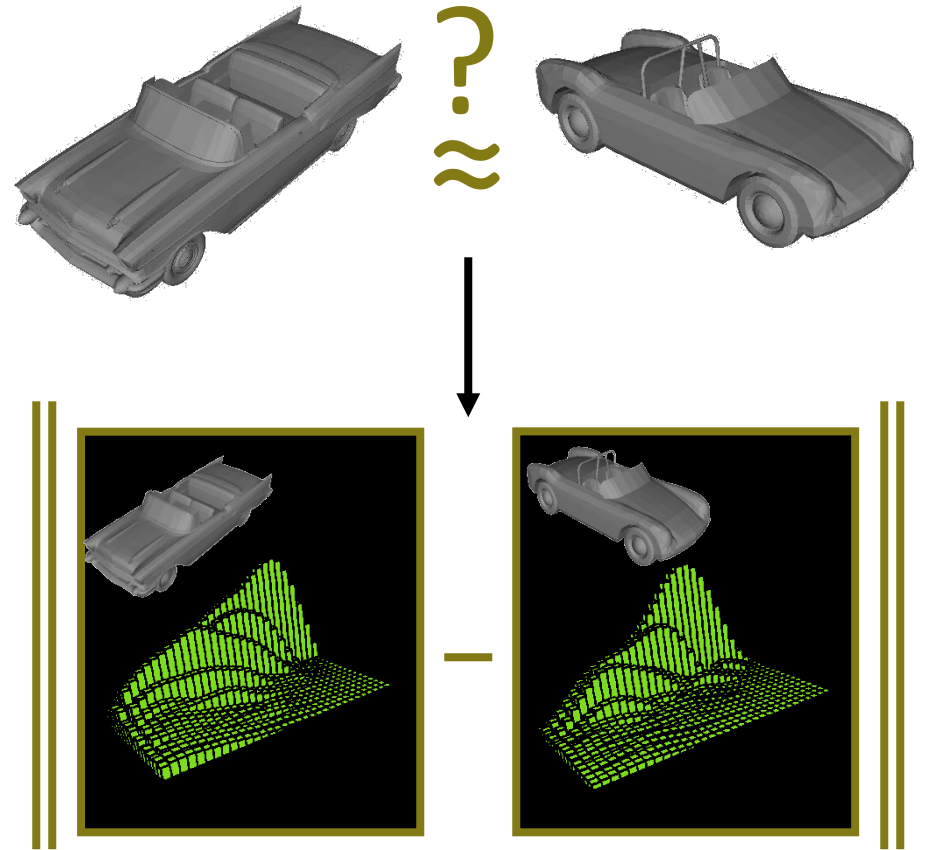
Typically a  
high-dimensional vector



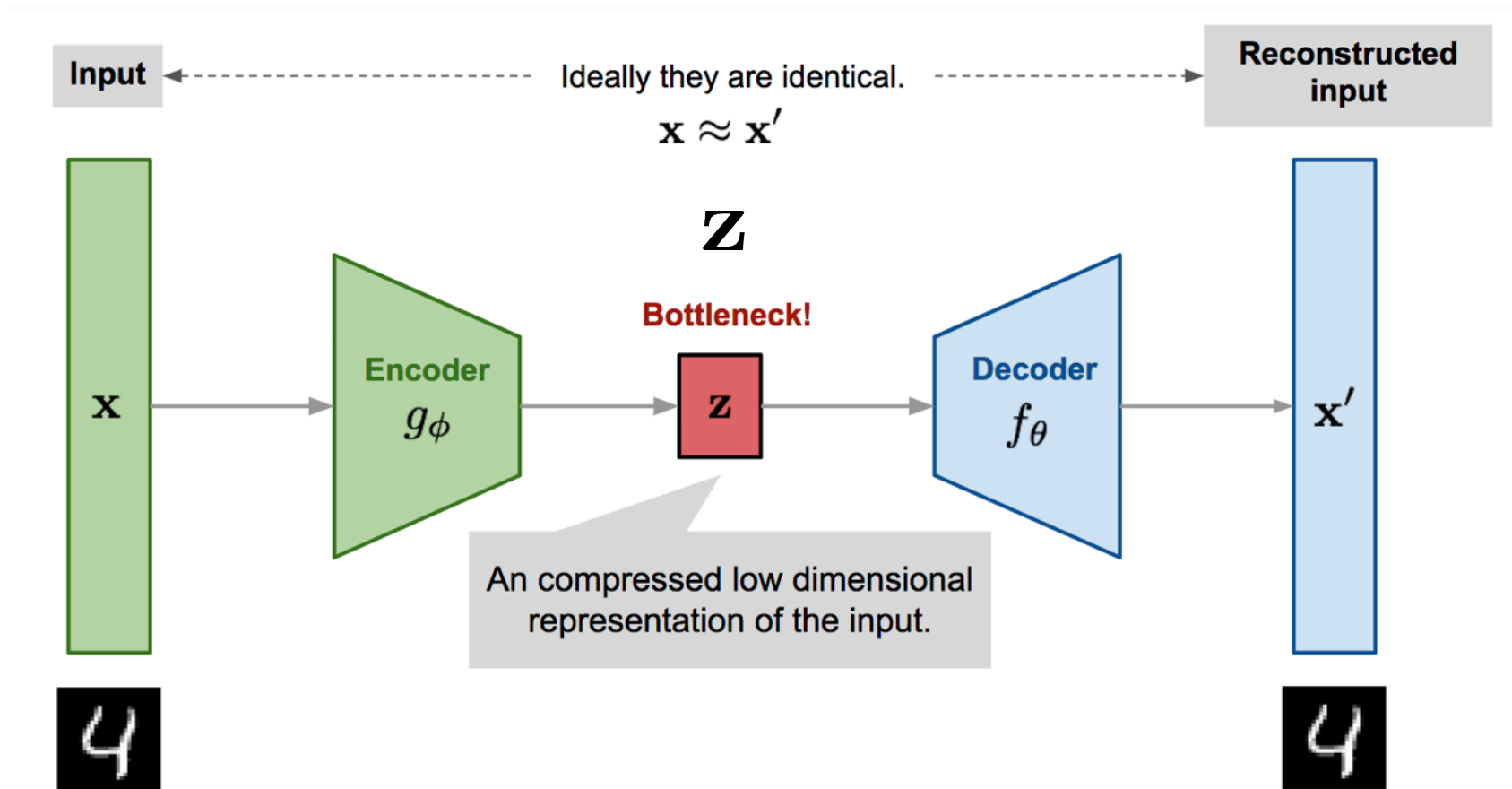
# Global Similarity

## Approach:

1. Represent each model by a **shape descriptor**
2. Compare shapes by comparing their shape descriptors
3. Is the descriptor designed, or learned?



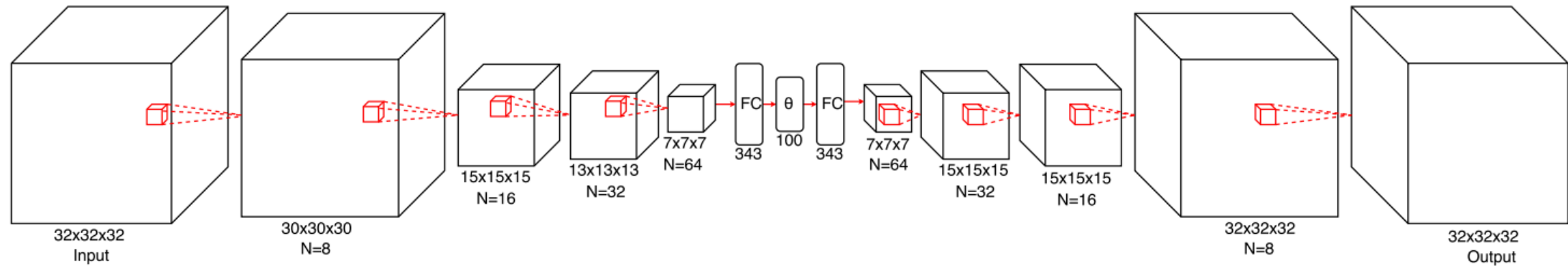
# Auto-Encoders (AE)



**Task:** Learn to encode the input and decode itself

**Reconstruction loss:** measuring the distance between the input/output

# Volumetric AE



**Binary Cross-Entropy Loss:**  $\mathcal{L} = -t \log(o) - (1 - t) \log(1 - o)$



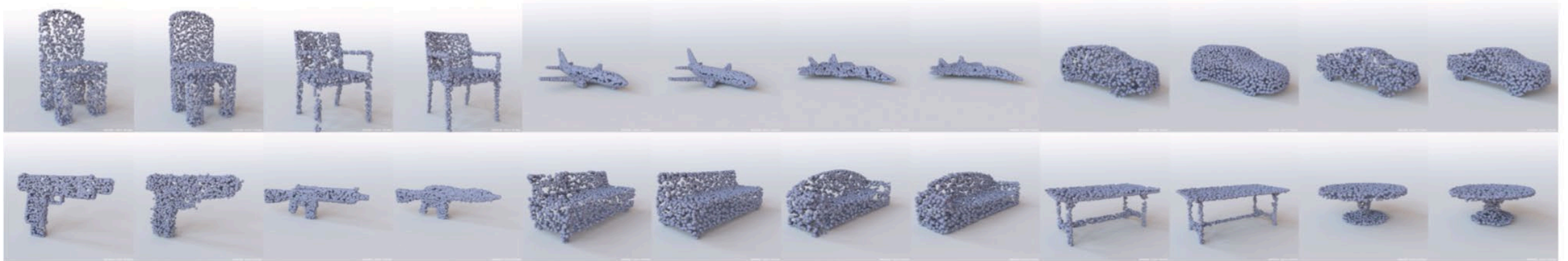
NeurIPS 2016

Generative and Discriminative Voxel Modeling with Convolutional Neural Networks

# Point Cloud AE

Encoder: PointNet

Decoder: MLP



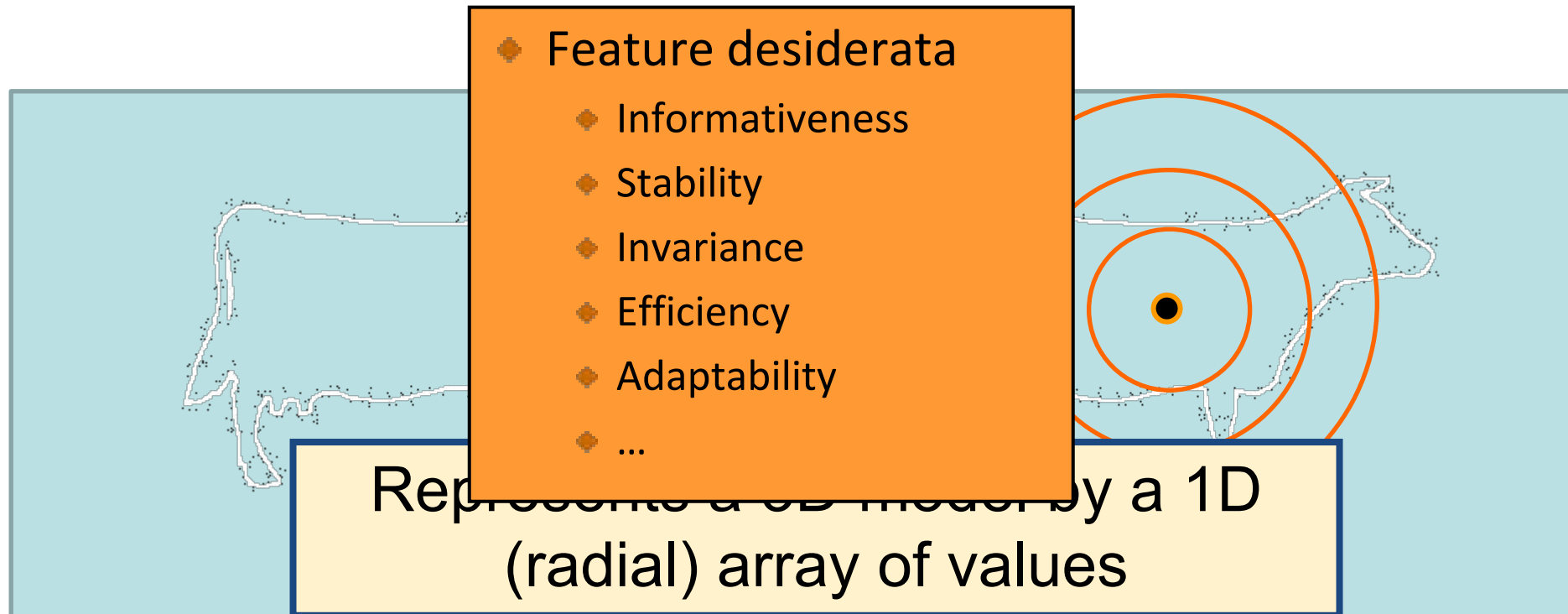
**ICML 2018, Learning Representations and Generative Models for 3D Point Clouds, Panos Achlioptas, et. al.**

# Shape Descriptors: Examples

## Shape Histograms

[Ankerst *et al.* 1999]

Shape descriptor stores a histogram of how much surface area resides within different concentric shells in space

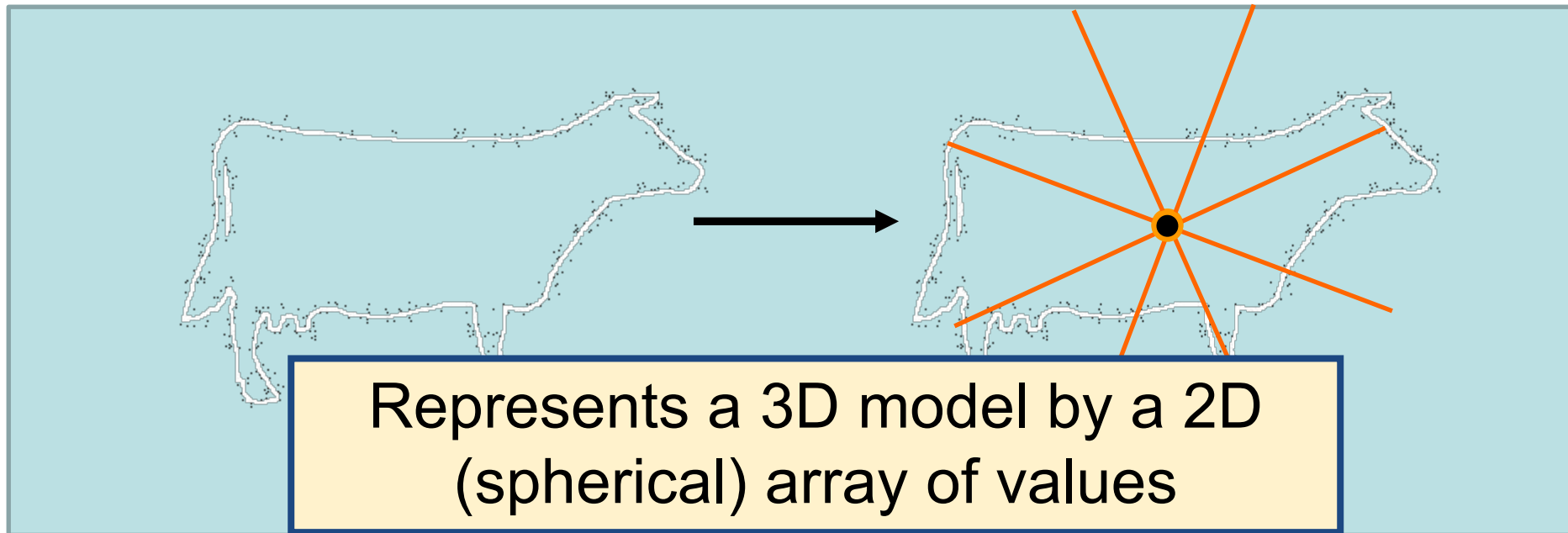


# Shape Descriptors: Examples

## Shape Histograms

[Ankerst *et al.* 1999]

Shape descriptor stores a histogram of how much surface area resides within different sectors in space

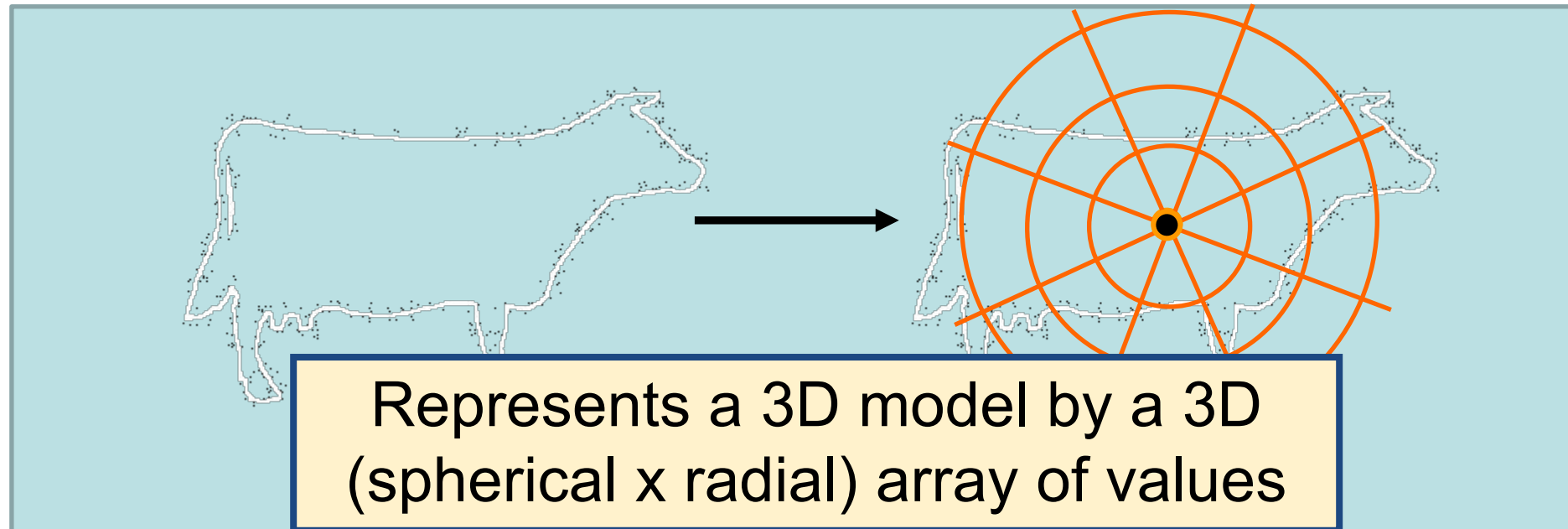


# Shape Descriptors: Examples

## Shape Histograms

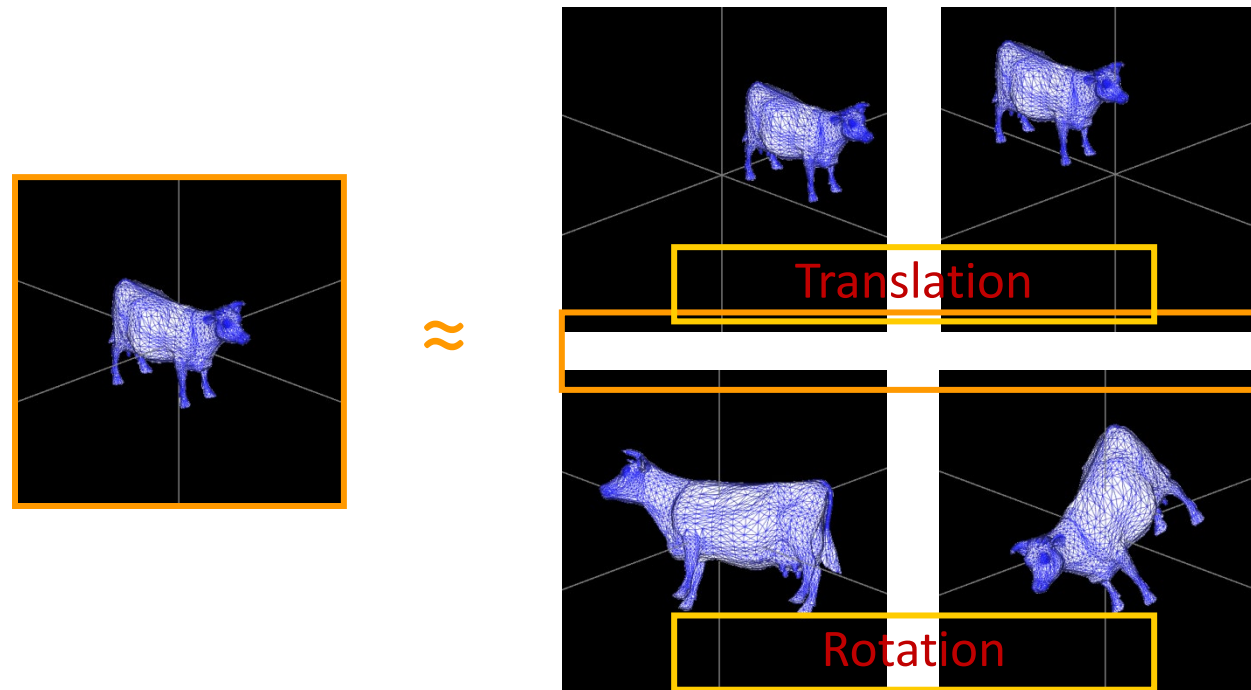
[Ankerst *et al.* 1999]

Shape descriptor stores a histogram of how much surface area resides within different shells and sectors in space



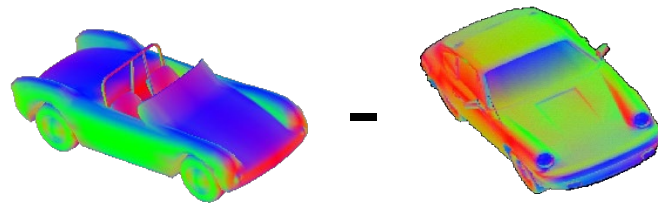
# Shape Descriptors: Challenge

The descriptor must not change when a rigid body transformation (e.g., translation, rotation) is applied to the model



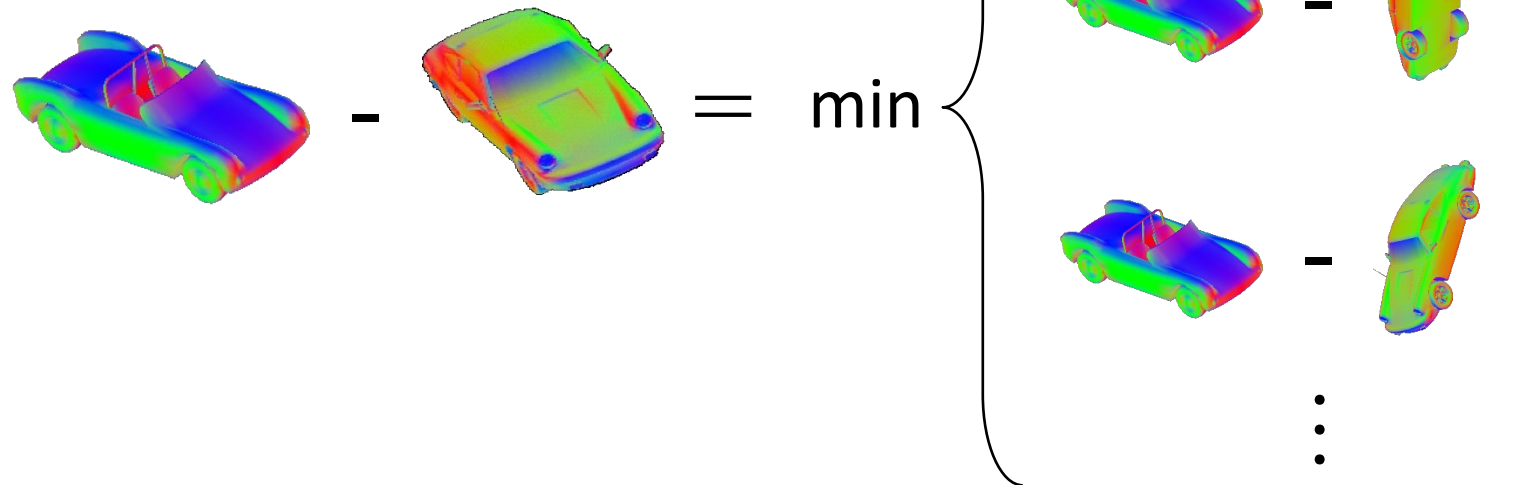
# Shape Descriptors: Challenge

In order to compare two 3D models, we must either make descriptors invariant to rigid motions, or we need to compare the shapes at their optimal alignment



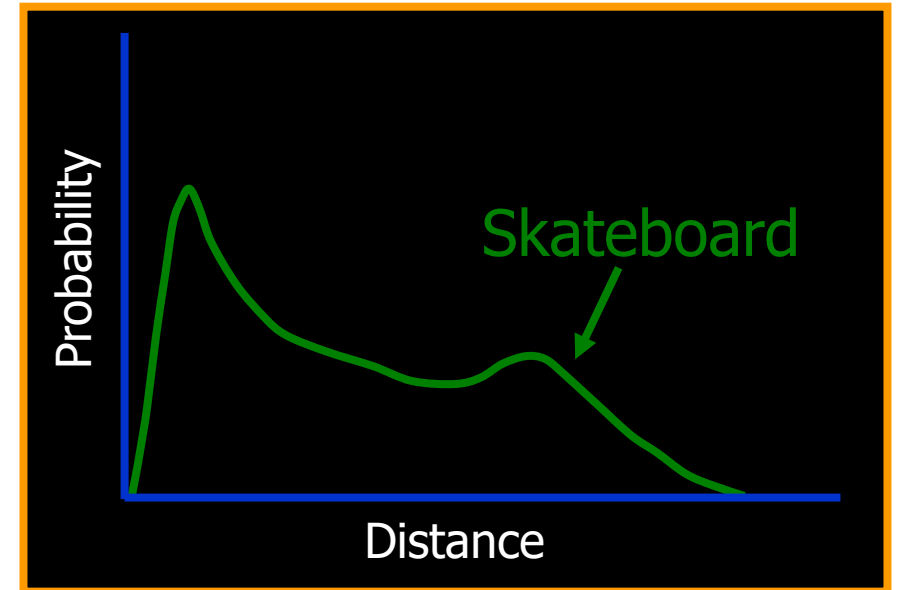
# Shape Descriptors: Challenge

In order to compare two models,  
we need to compare them  
at their optimal alignment



# D2 Shape Distributions

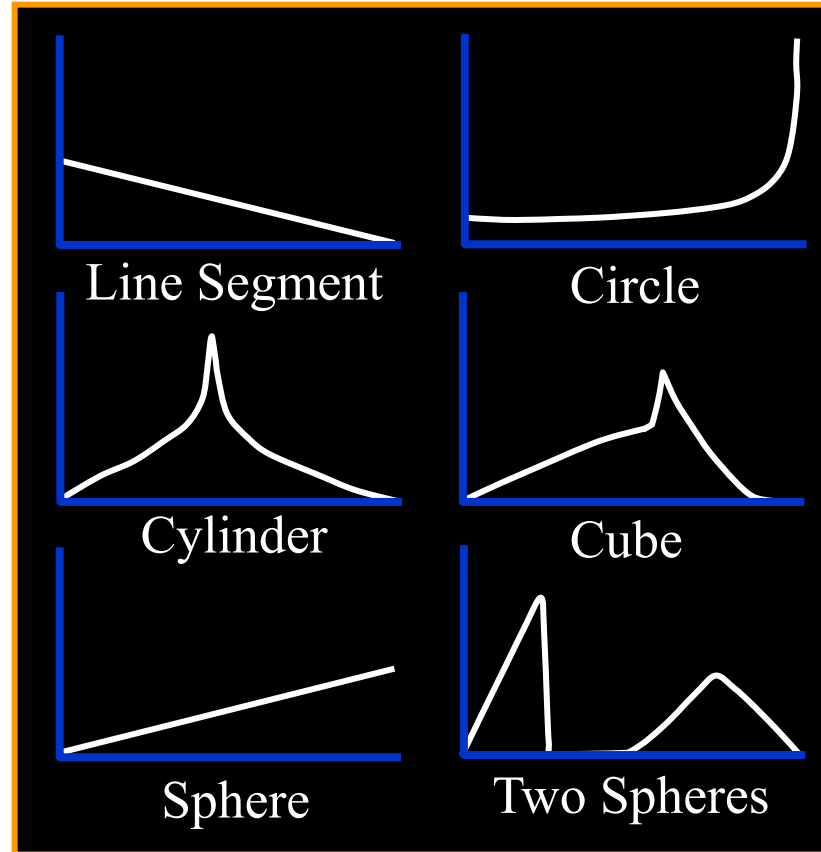
- Properties
  - Concise to store?
  - Quick to compute?
  - Invariant to transforms?
  - Efficient to match?
  - Insensitive to noise?
  - Insensitive to topology?
  - Robust to degeneracies?
  - Invariant to deformations?
  - Discriminating?



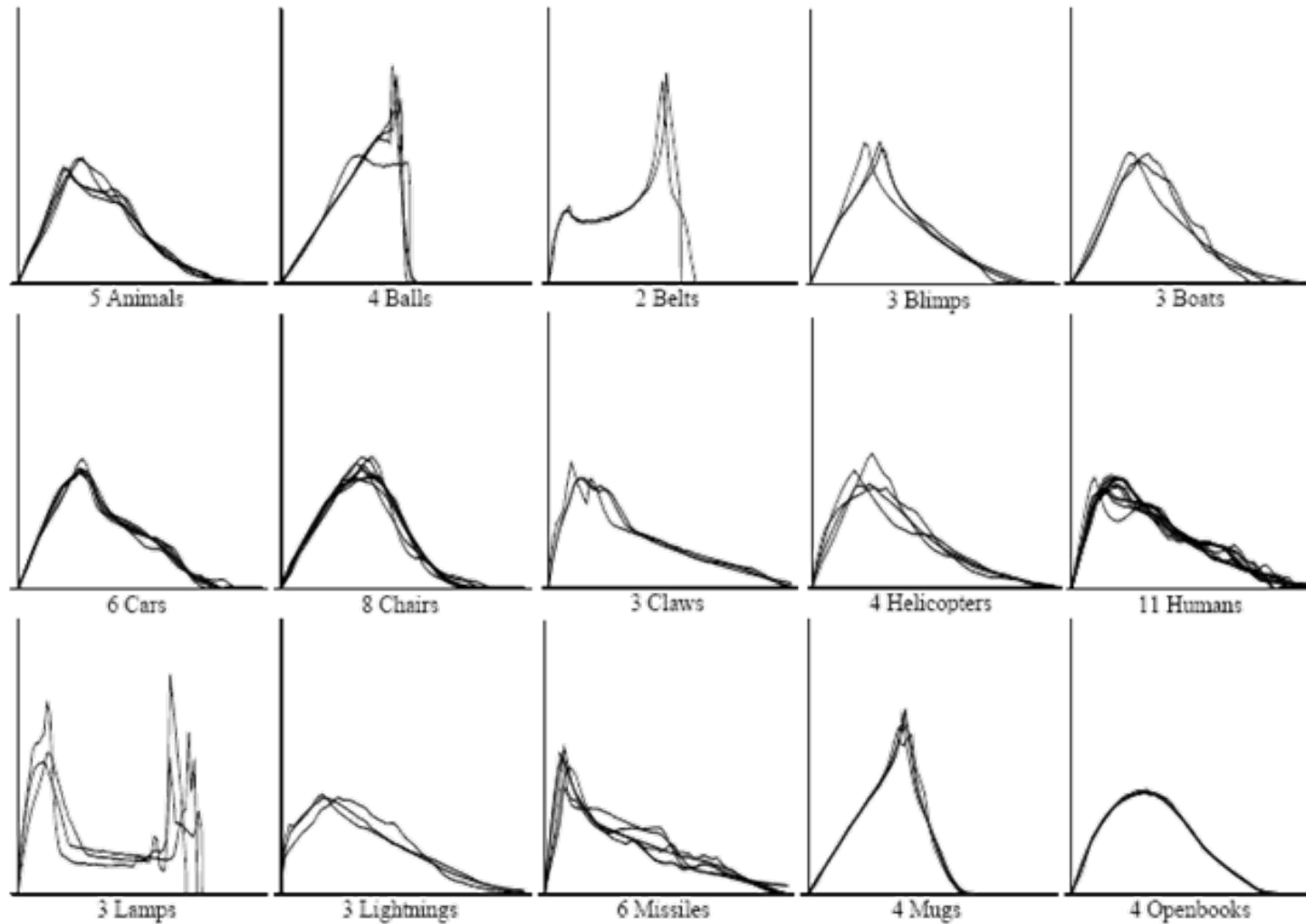
512 bytes (64 values)

0.5 seconds ( $10^6$  samples)

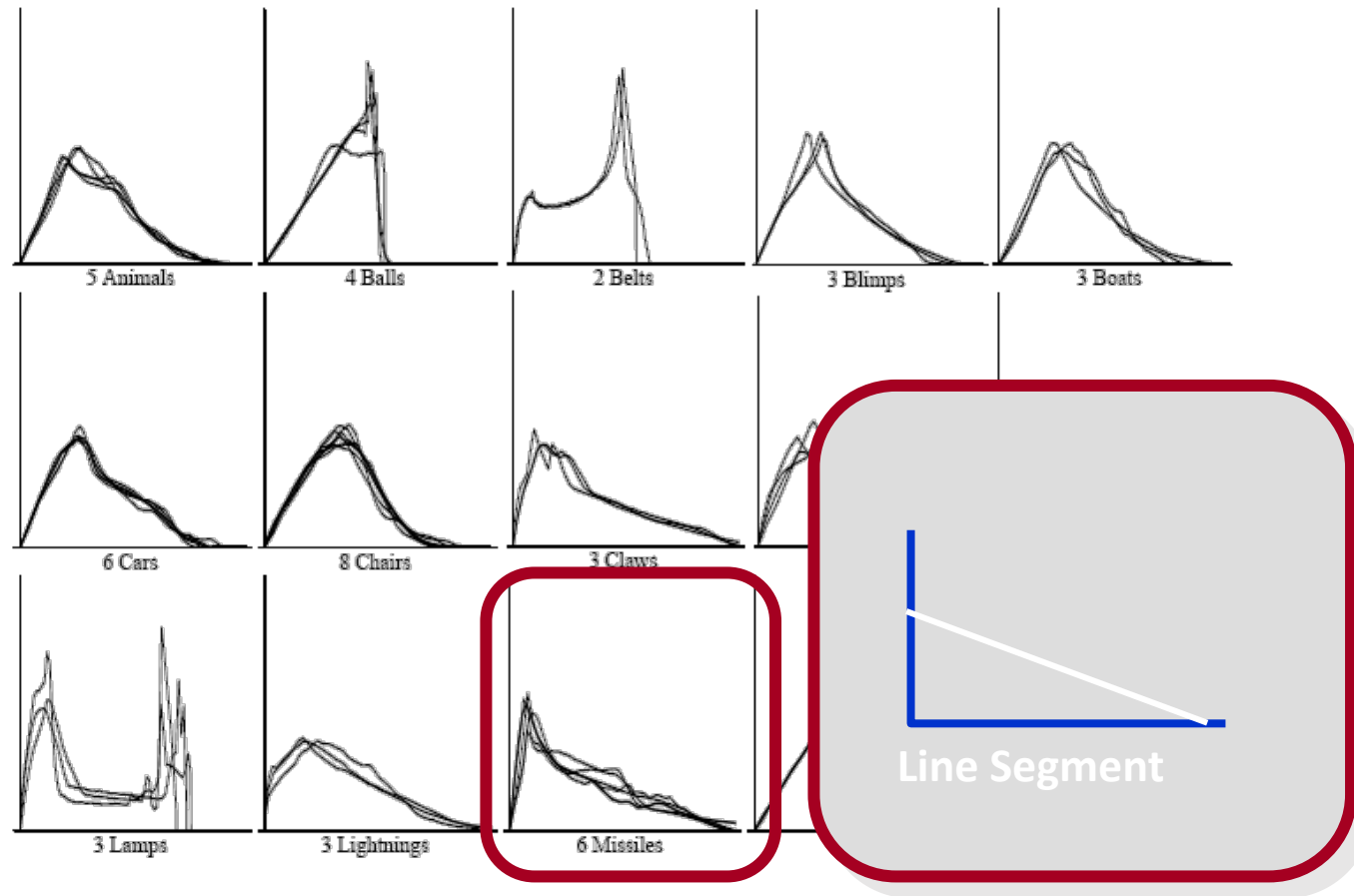
# Discriminating?



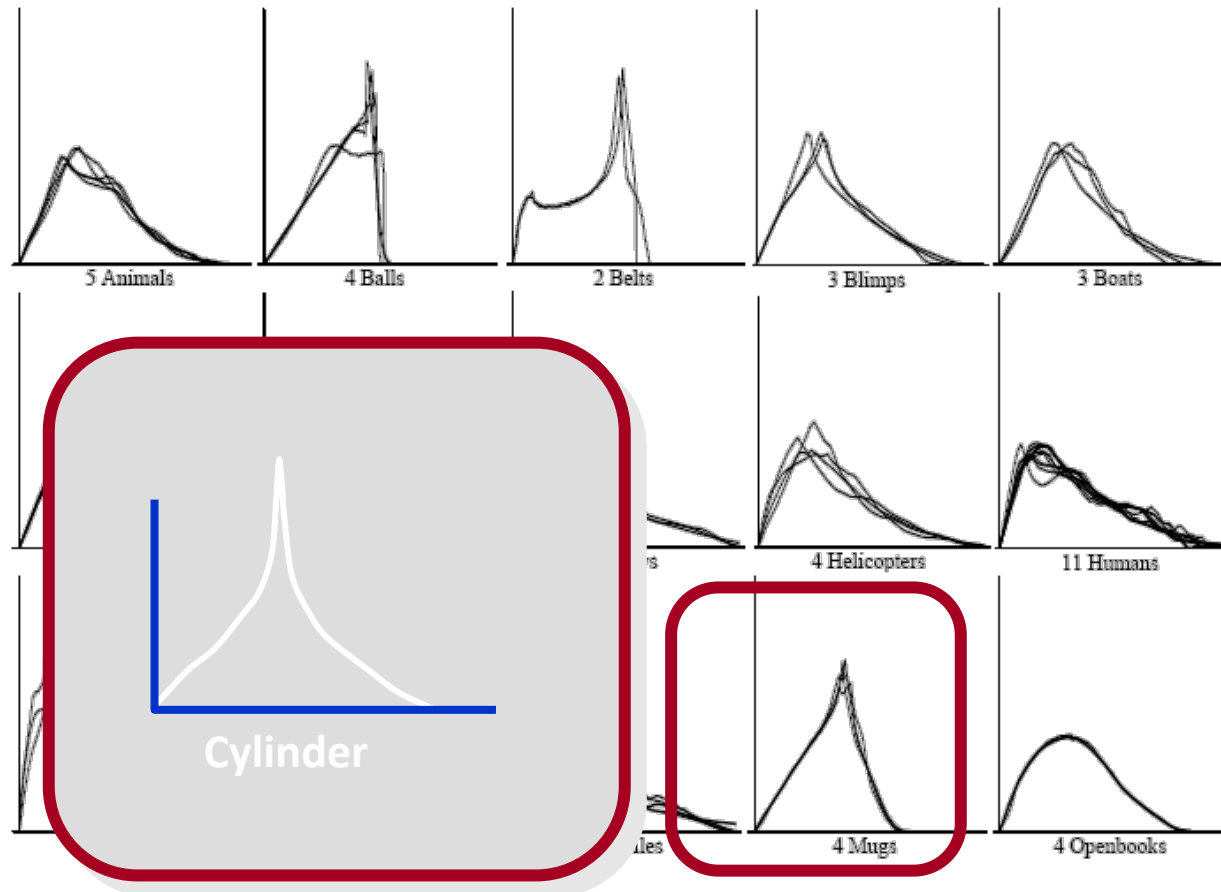
# Stable?



# Stable and Discriminating?



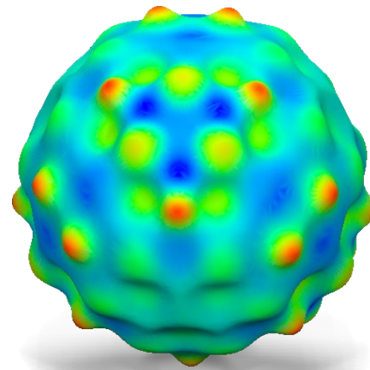
# Stable and Discriminating



# Local Features and Local Shape Similarity

# Classical Curvature

- Differential features can be noisy on meshes



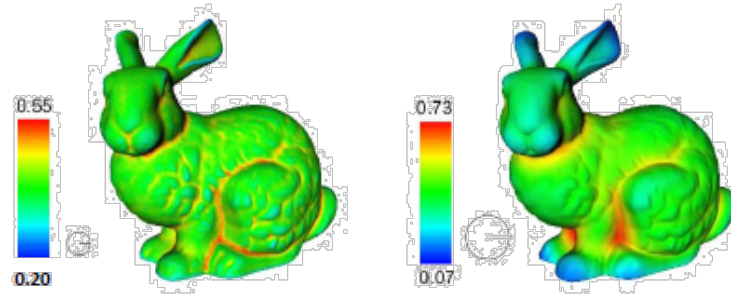
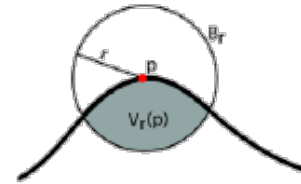
Curvature

# Integral Volume Descriptor

*Integral invariant signatures*, Manay et al. ECCV 2004

*Integral Invariants for Robust Geometry Processing*, Pottmann et al. 2007-2009

$$V_r(p) = \int_{B_r(p) \cap S} dx$$



## Relation to mean curvature

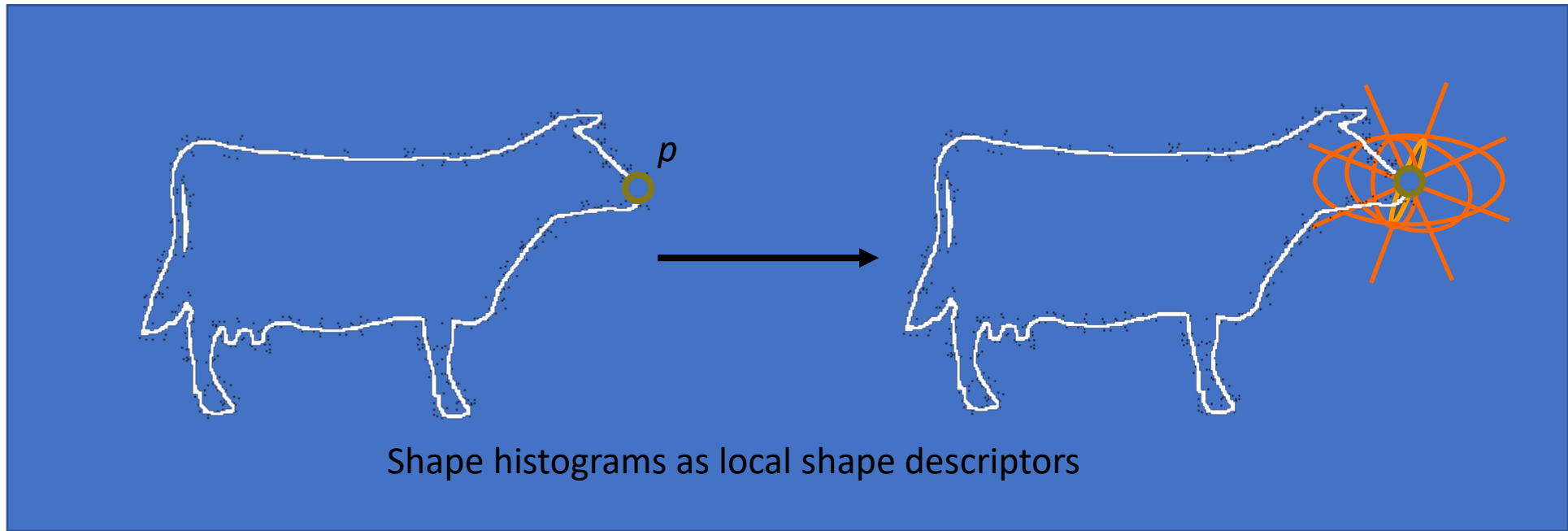
$$V_r(p) = \frac{2\pi}{3}r^3 - \frac{\pi H}{4}r^4 + O(r^5)$$

*Robust Global Registration*,  
Gelfand et al. 2005

# From Global to Local

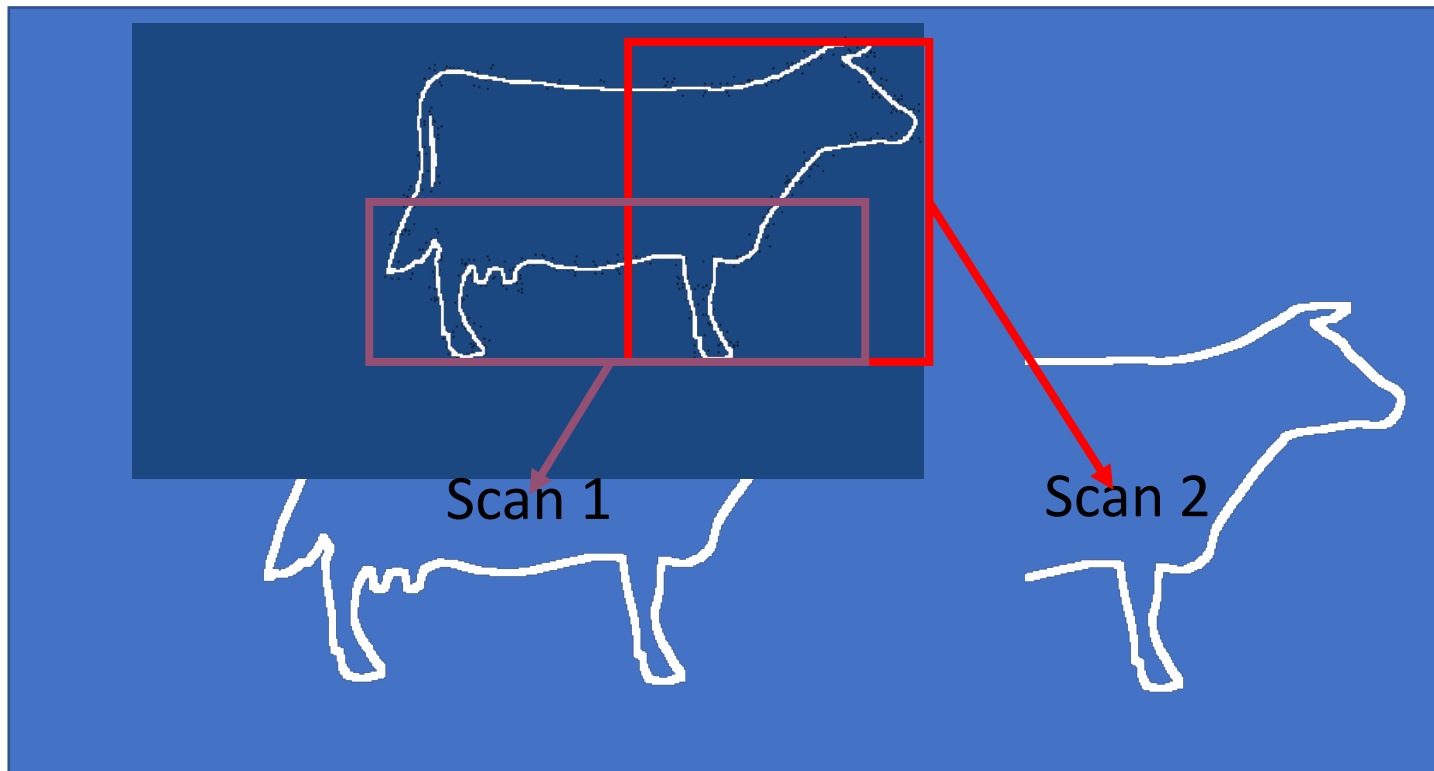
To characterize the surface about a point  $p$ , take a global descriptor and:

- center it about  $p$  (instead of the COM), and
- restrict the extent to a small region about  $p$ .



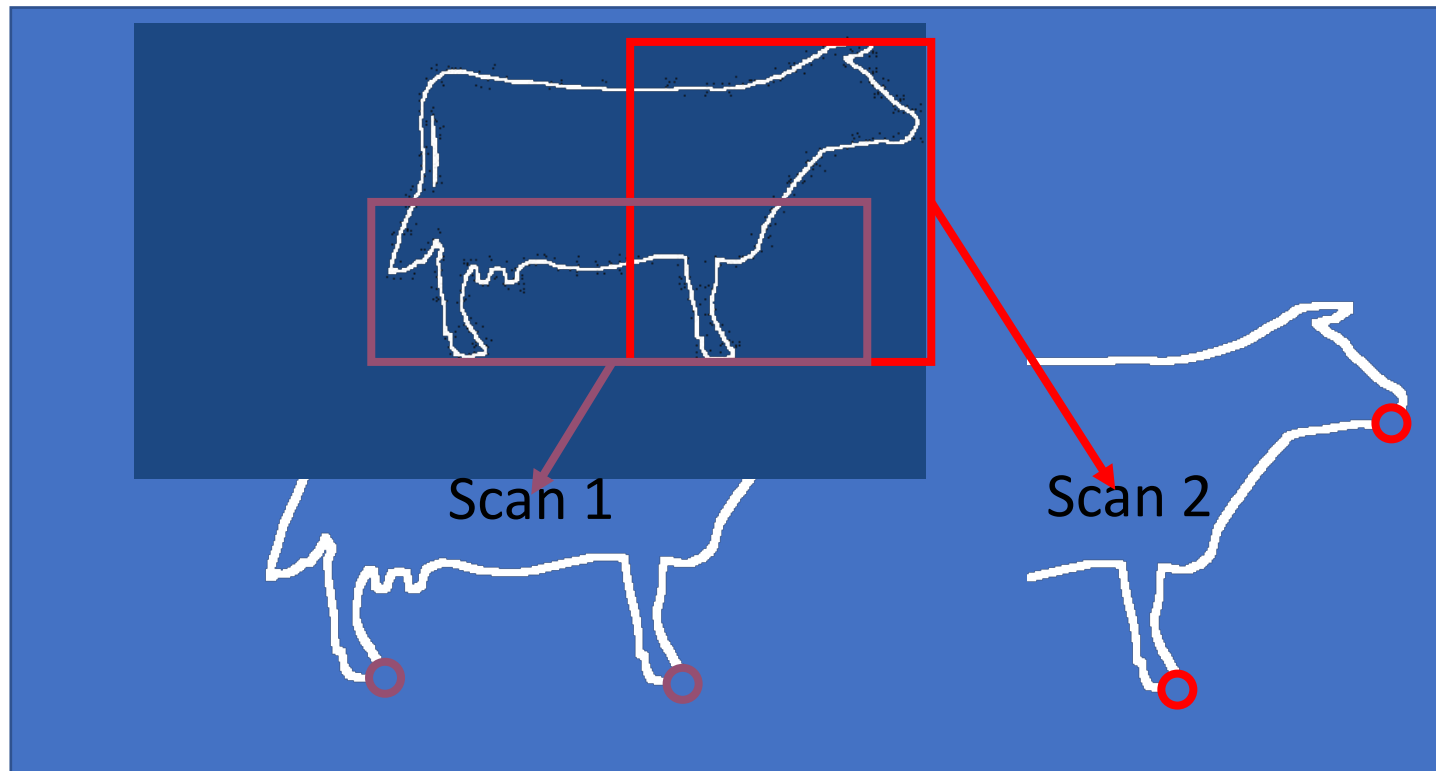
# From Global to Local

Given scans of a model:



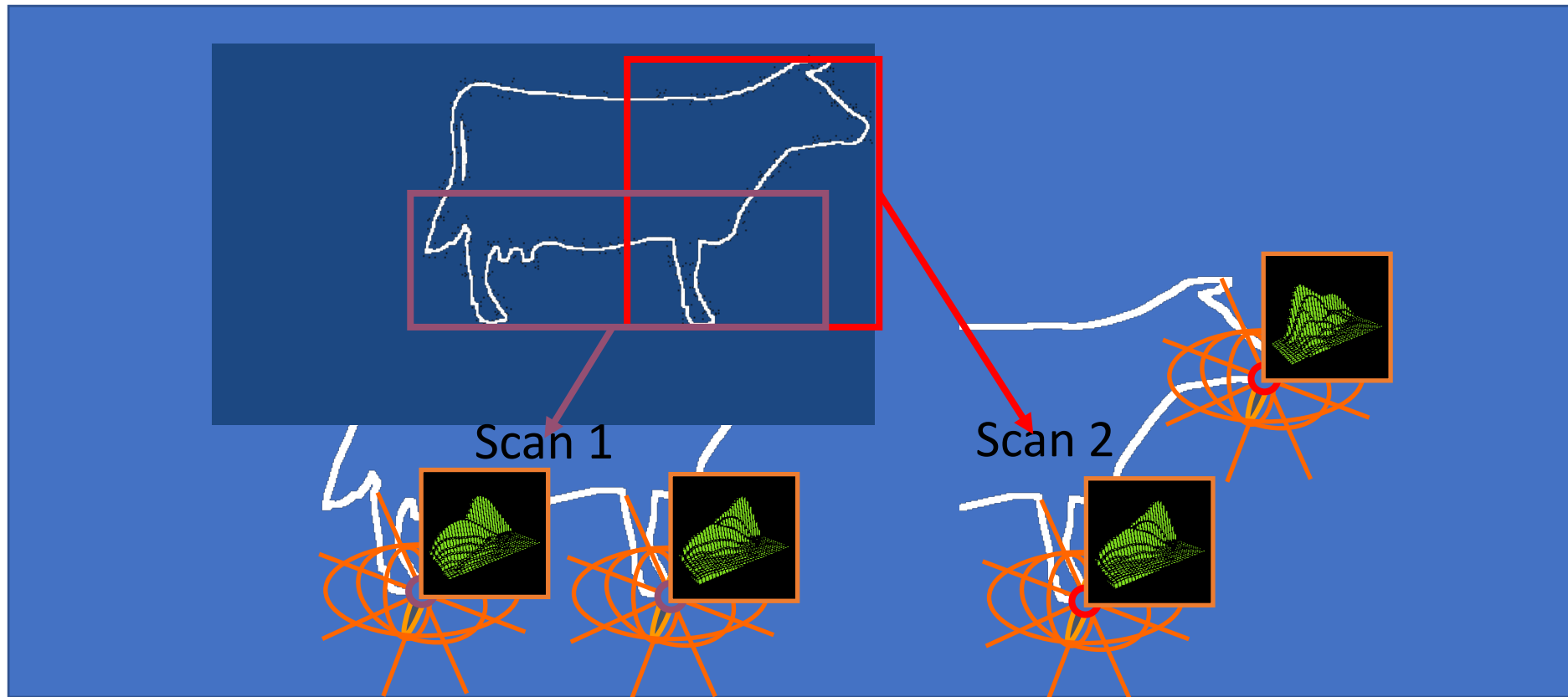
# From Global to Local

- Identify the feature points



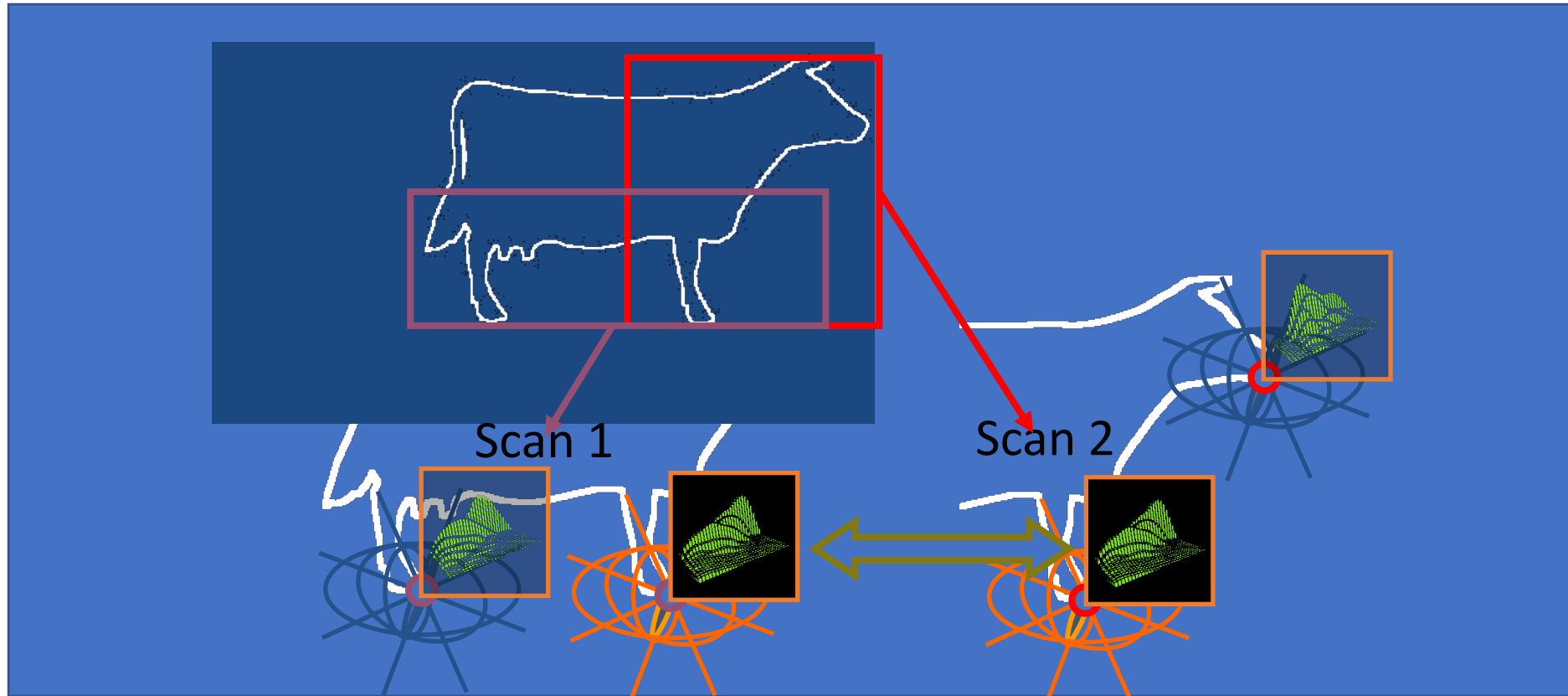
# From Global to Local

- Identify the features points
- Compute a local descriptor for each feature



# From Global to Local

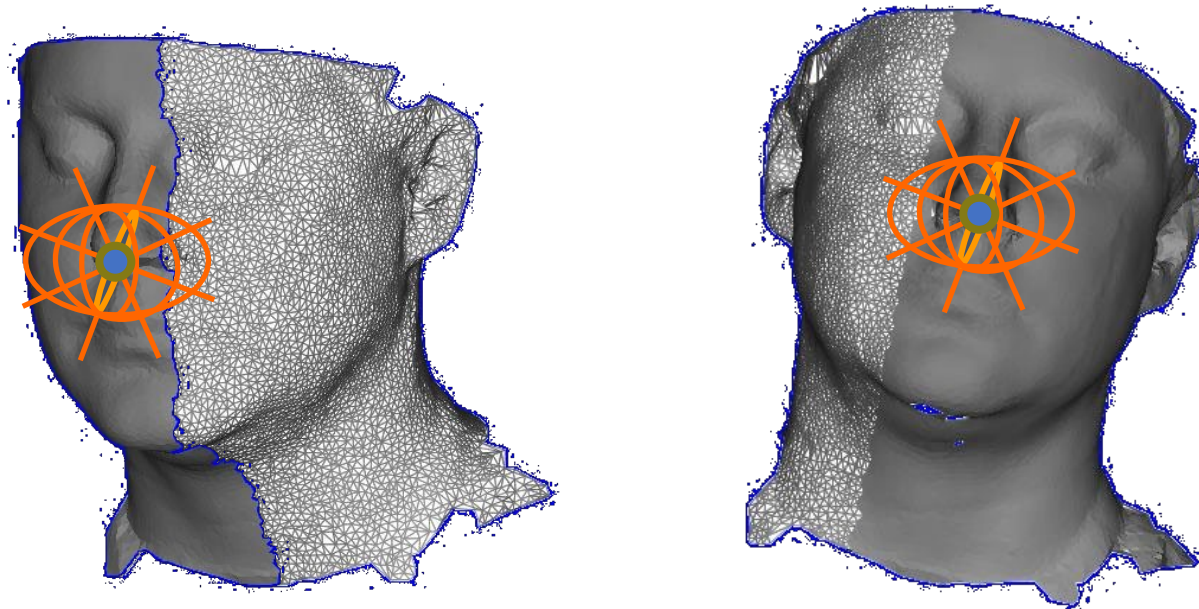
- Identify the features
- Compute a local descriptor for each feature
- For features correspond  $\rightarrow$  descriptors are similar



# Pose Normalization

## From Global to Local

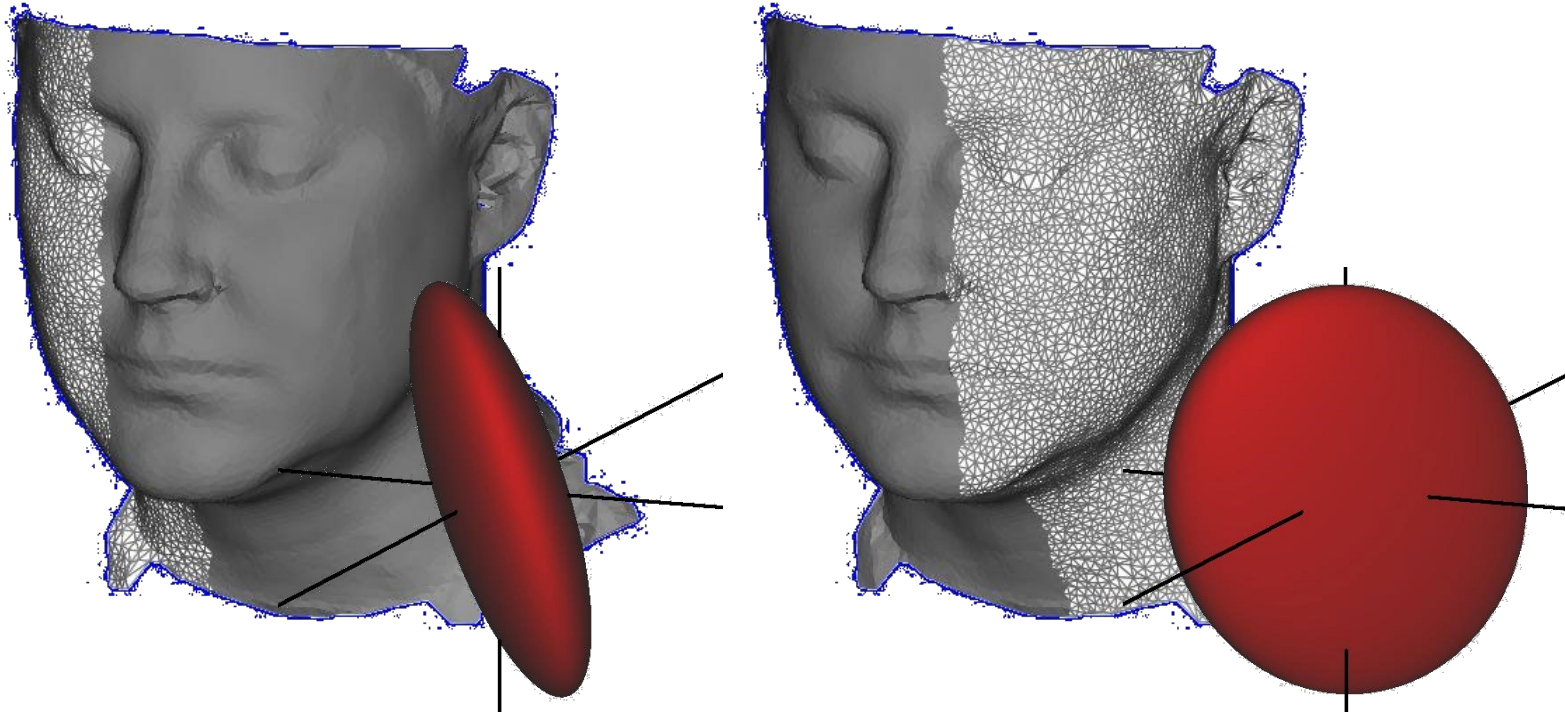
- ✓ Translation: Accounted for by centering the descriptor at the point of interest.
- ✗ Rotation: We still need to be able to match descriptors across different rotations.



# Pose Normalization

## Challenge

- Since only parts of the models are given, we cannot use global normalization to align the local descriptors



# Pose Normalization

## Challenge

- Since only parts of the models are given, we cannot use global normalization to align the local descriptors

## Solutions

- Normalize using local information

# Spin Images

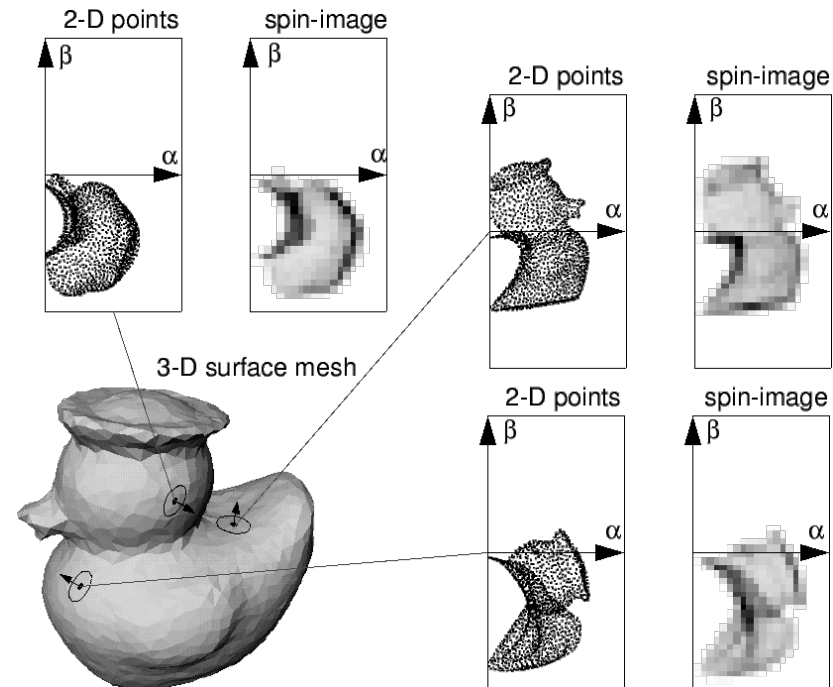
Creates an image associated with a neighborhood of a point.

Compare points by comparing their *spin images* (2D).

Given a point and a normal, every other point is indexed by two parameters:

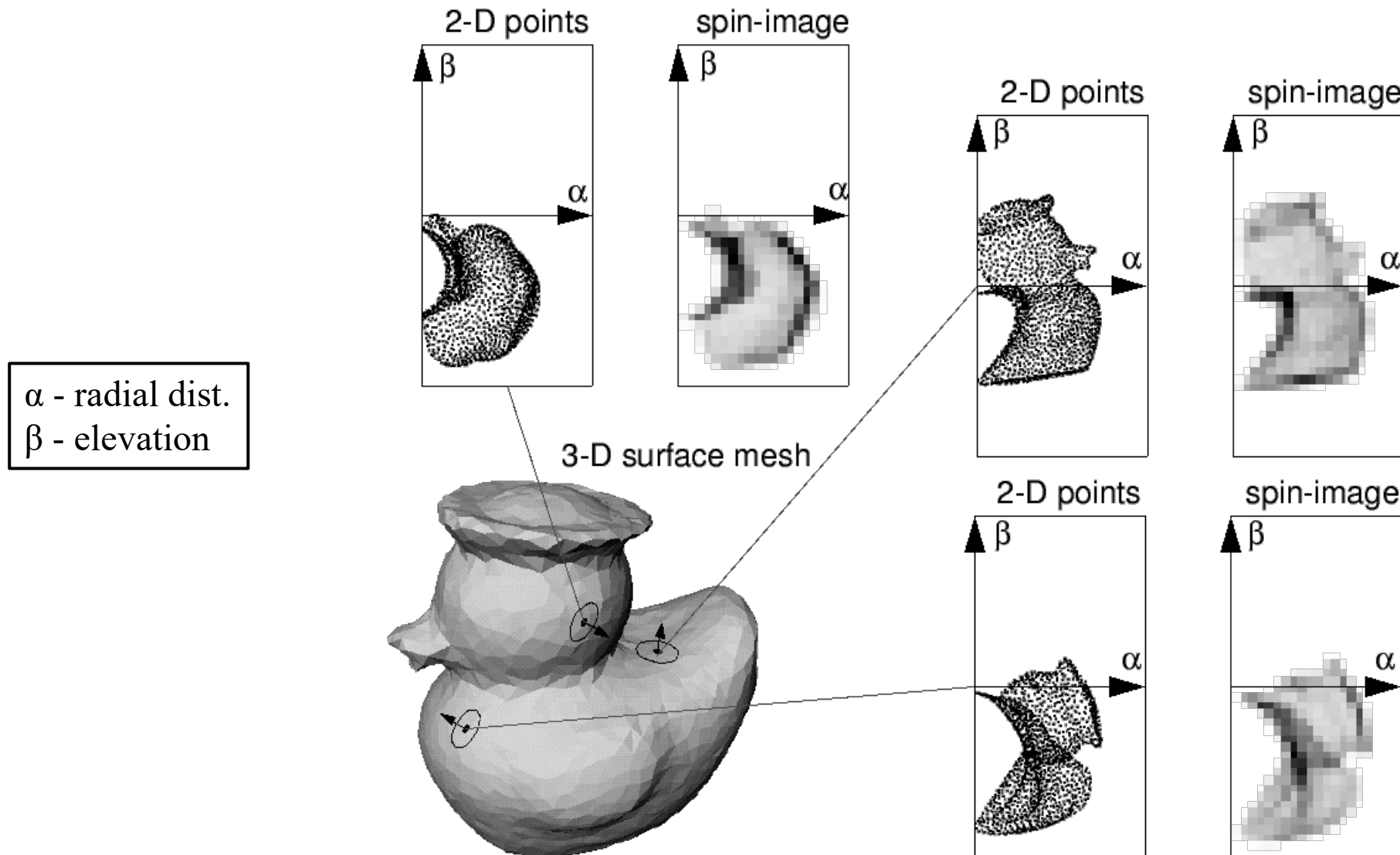
$\beta$  distance to tangent plane

$\alpha$  distance to normal line



*Using Spin Images for Efficient Object Recognition in Cluttered 3D Scenes*  
Johnson et al, PAMI 99

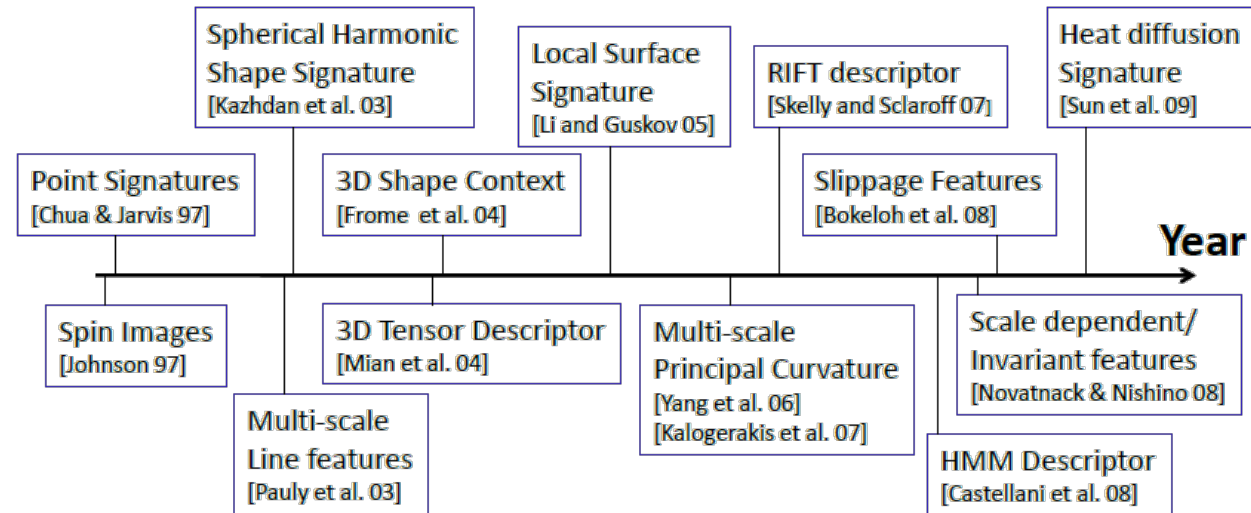
# Spin Images



# Main Question

How to compare regions on the shape in an invariant manner?

A large variety of *descriptors* have been suggested.

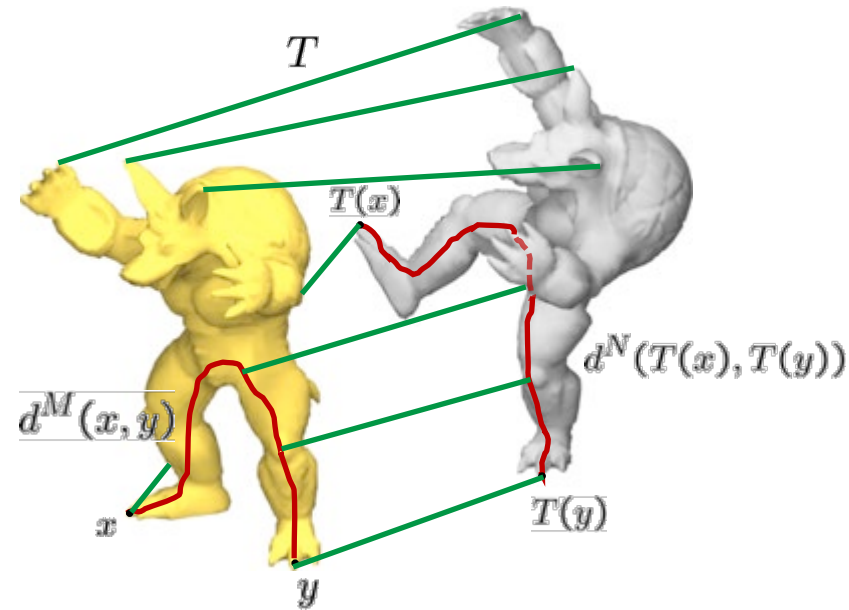


# Intrinsic Descriptors for Deformable Matching

# Laplace-Beltrami – Isometry Invariant

## Isometry invariance (LB is intrinsic)

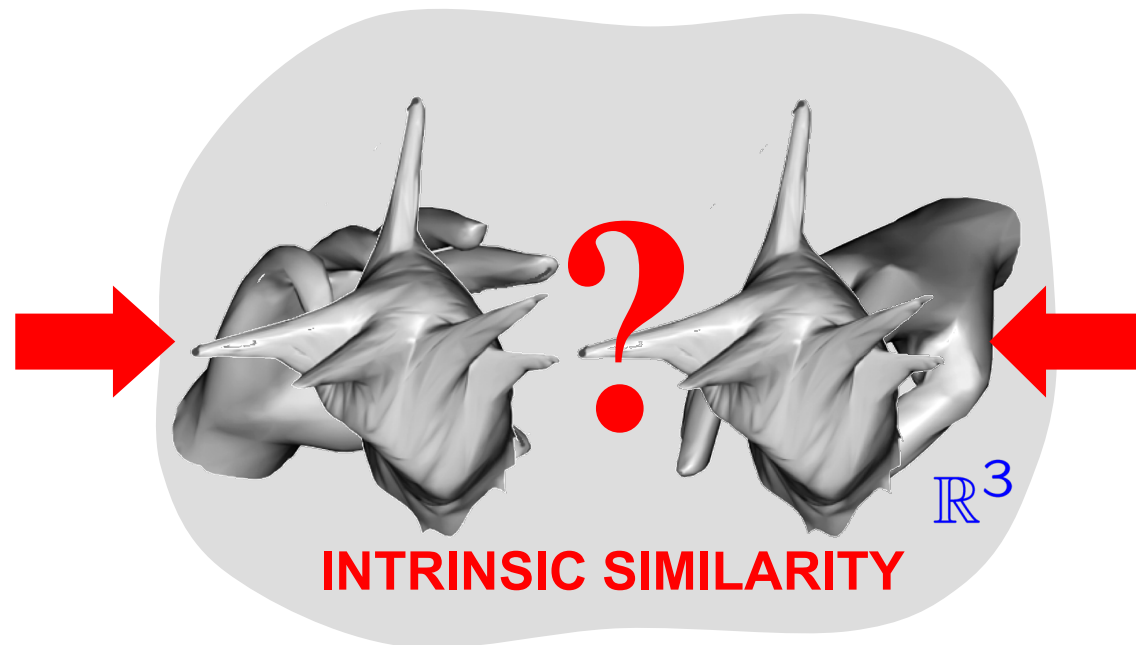
If two shapes are isometric then their LB operators agree.



Any quantity derived from the LB operator has to be invariant to isometries.

# Global Point Signature (GPS)

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

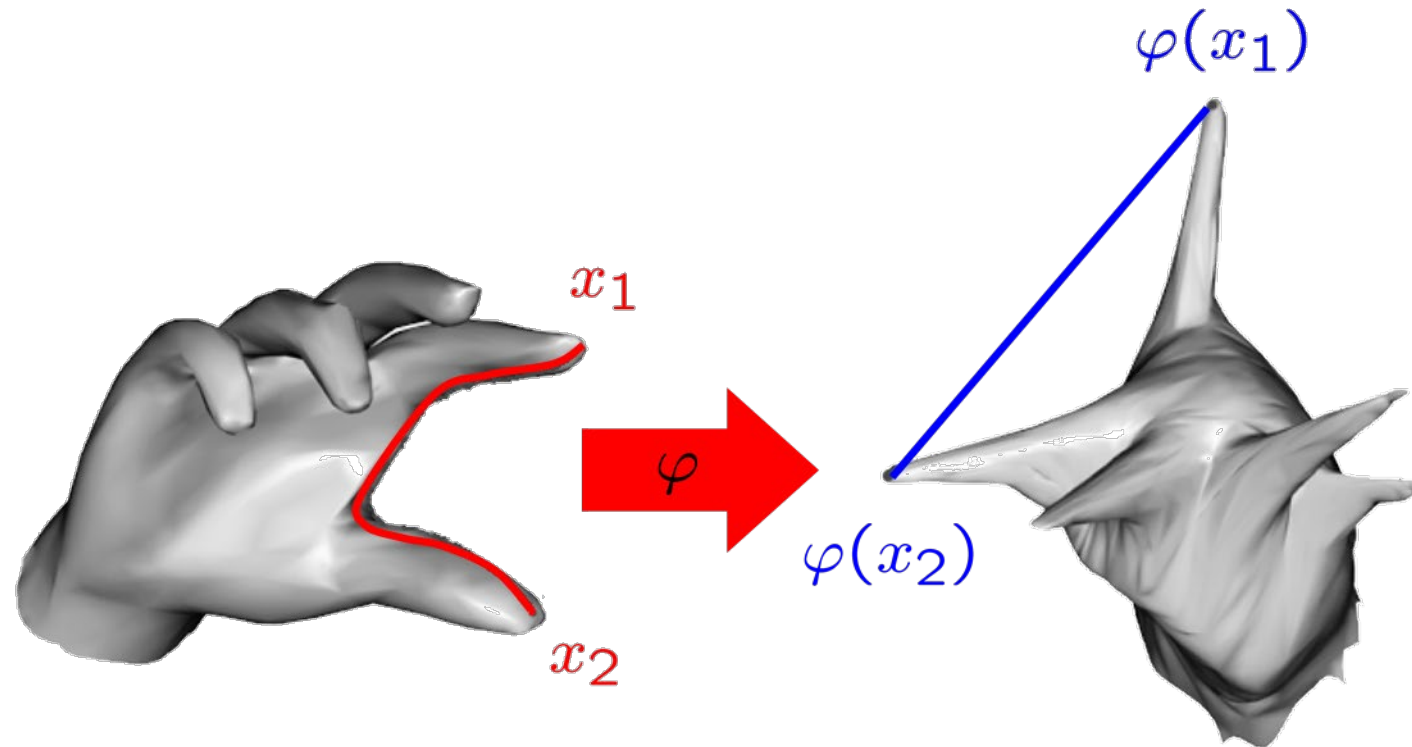


but there is a sign ambiguity

# Global Point Signature

almost invariant under isometries – but not completely canonical

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



Diffusion distances are also intrinsic  
and also canonical

# Global Point Signature

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

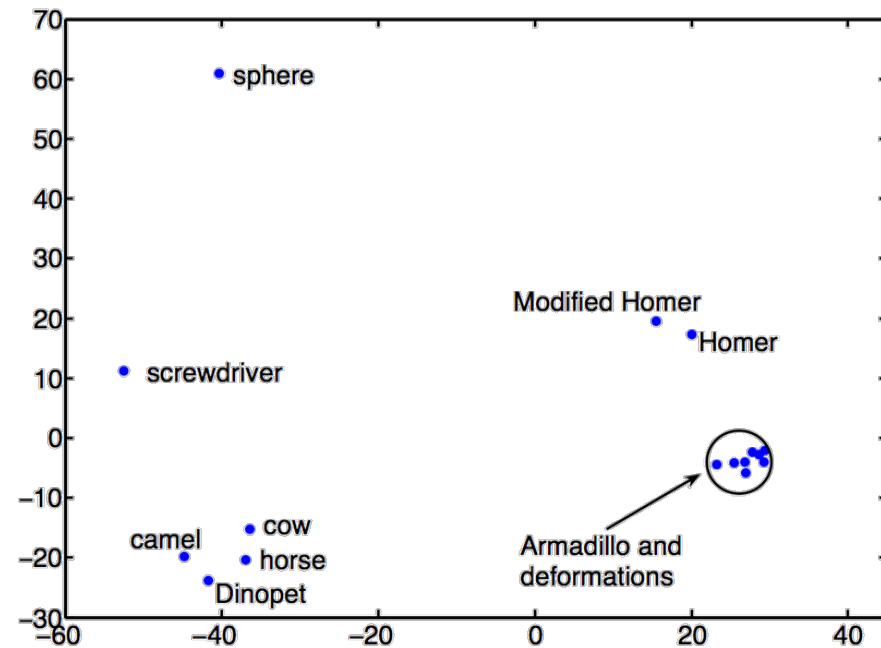
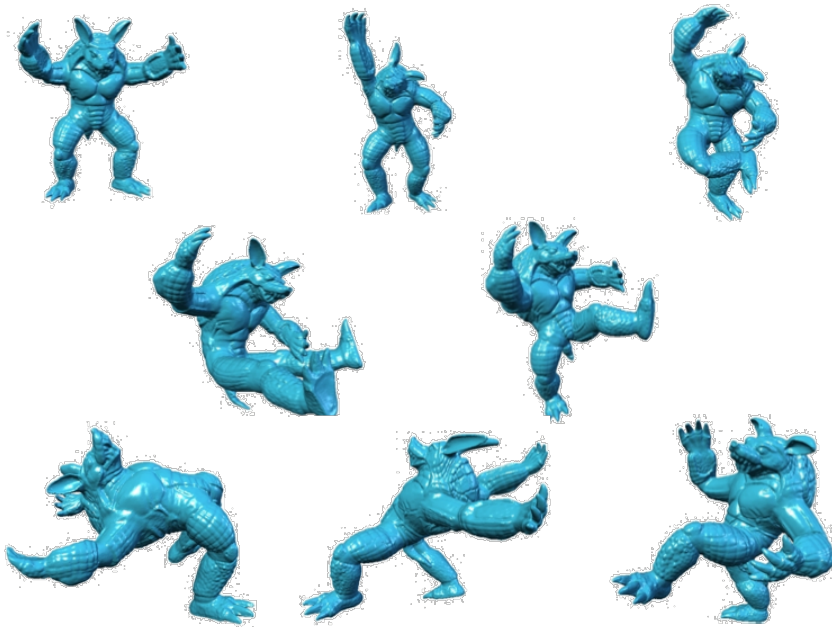


Figure 4: Armadillo and its deformations.

Similar to D2, but use histograms in embedded space  
(rather than Euclidean)

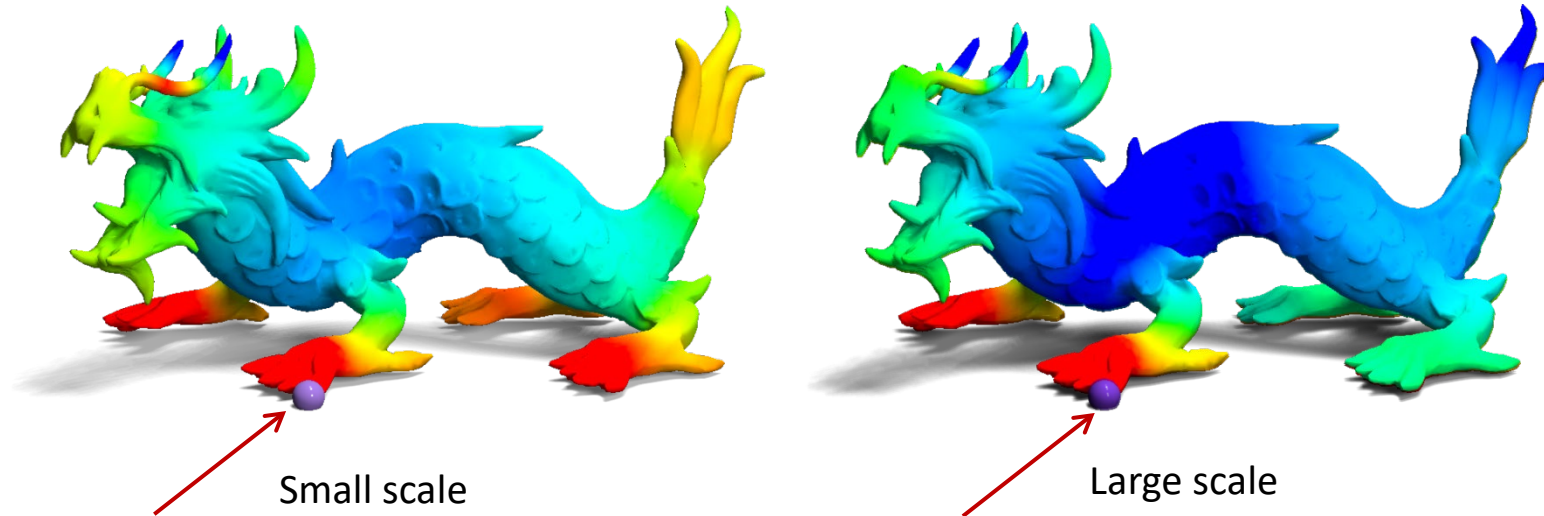
# Global Point Signature

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

- Pros
  - Isometry-invariant
  - Nearly canonical
- Cons
  - Eigenfunctions may flip sign
  - Eigenfunctions might change positions due to deformations
  - Only global info – a point descriptor depends on the entire shape

# The Issue of Scale

- Given a point (●) on a shape, find other points with “similar” neighborhoods



- Inherently multiscale question: on a manifold, locally all points are the same. Need a meaningful way to compare point neighborhoods at different scales
- At what scale do neighborhoods become unique?

# (Heat) Diffusion on Manifolds

- Heat diffusion on a Riemannian manifold:

If  $u(x, t)$  is the amount of heat at point  $x$  at time  $t$ ,  
then

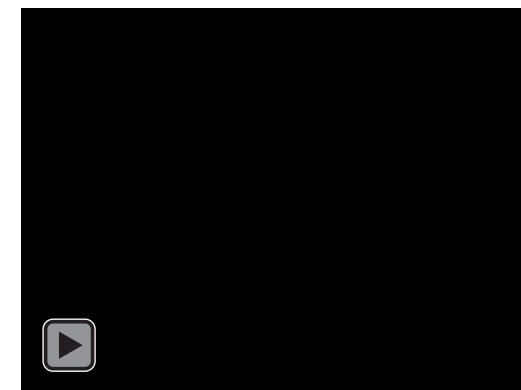
$$\frac{\partial u}{\partial t} = \Delta u$$

$\Delta$  : Laplace-Beltrami Operator (div grad)

- Given an initial distribution  $f(x)$ . After time  $t$ :

$$f(x, t) = e^{-t\Delta} f$$

$H_t$  heat operator

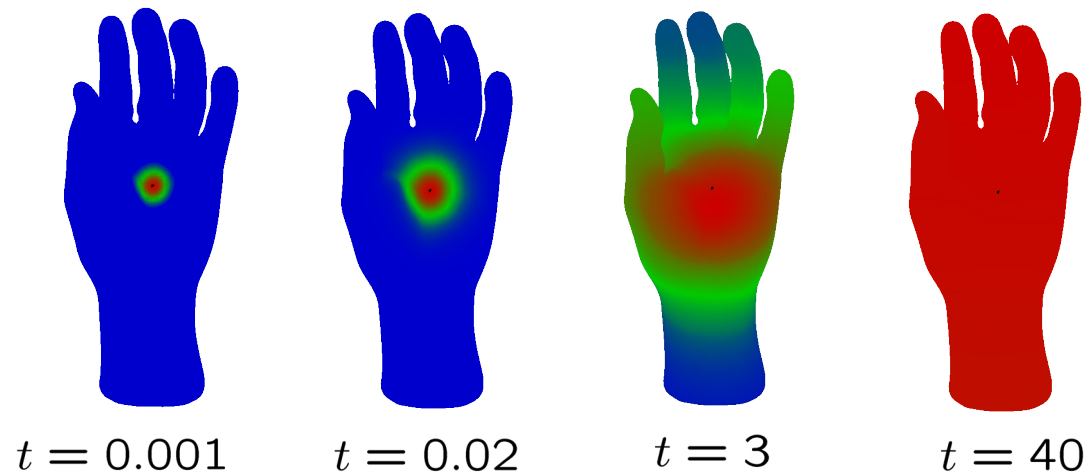


# The Heat Kernel

- Heat kernel  $k_t(x, y)$

$$f(x, t) = \int_{\mathcal{M}} k_t(x, y) f(y) dy$$

$k_t(x, y)$ : amount of heat transferred from  $x$  to  $y$  in time  $t$ .  
How well  $x$  and  $y$  are connected at scale  $t$



# Background

- Heat Kernel  $k_t(x, y)$ . Also the probability density function of Brownian motion on  $\mathcal{M}$ :

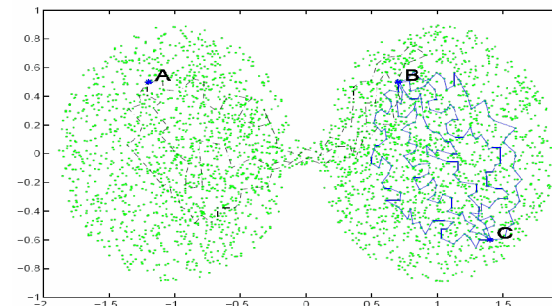
$$\mathbb{P} \left( W_x^t \in C \right) = \int_C k_t(x, y) dy$$

- Intuitively: weighted average over all paths possible between  $x$  and  $y$  in time  $t$

- Related to **Diffusion Distance**:

$$D_t(x, y) = k_t(x, x) - 2k_t(x, y) + k_t(y, y)$$

a robust multi-scale measure  
of proximity



# Heat Kernel Properties

## Basic Properties

- $k_t(x, y) = k_t(y, x)$
- $k_{t+s}(x, y) = \int_M k_t(x, z) k_s(z, y) dz$
- $k_t(x, y) = \sum_{i=0}^{\infty} e^{-\lambda_i t} \phi_i(x) \phi_i(y)$

Eigenfunctions of LB

# Heat Kernel Properties

- Invariant under isometric deformations

If  $T : X \rightarrow Y$  is an isometry, then:

$$k_t(X, Y) = k_t(T(x), T(y))$$

- Conversely: it characterizes the shape up to isometry.

If  $k_t(X, Y) = k_t(T(x), T(y)) \quad \forall x, y, t$  then:

$T$  is an isometry.

This is because:

$$\lim_{t \downarrow 0} (t \log k_t(x, y)) = -\frac{1}{4} d_{\mathcal{M}}^2(x, y) \quad \forall x, y$$

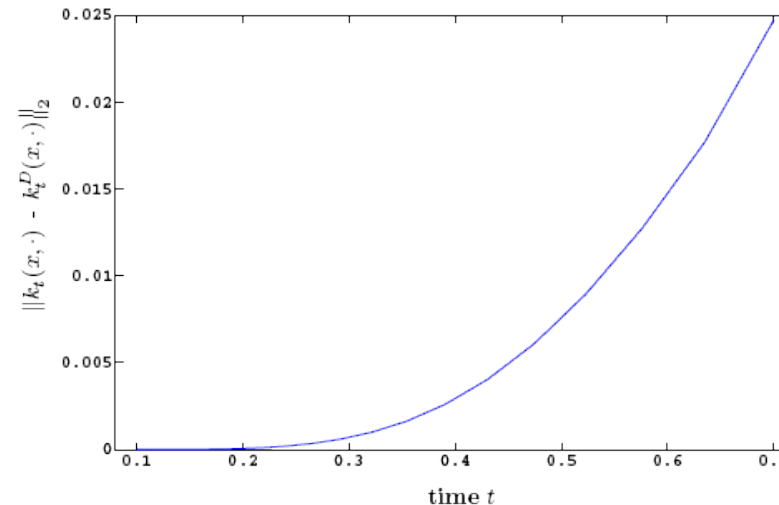
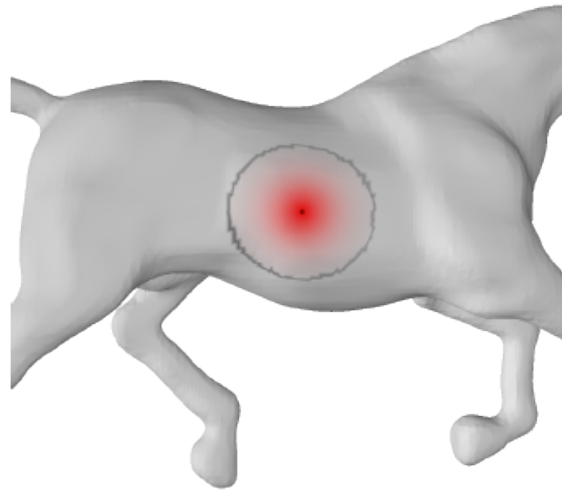
where  $d_{\mathcal{M}}(\cdot, \cdot)$  is the geodesic distance

# Heat Kernel Properties

## • Multiscale:

For a fixed  $x$ , as  $t$  increases, heat diffuses to larger and larger neighborhoods

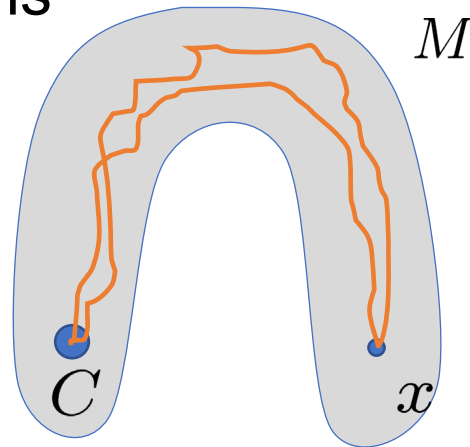
Therefore,  $k_t(x, \cdot)$  is determined by (reflects the properties of) a neighborhood that grows with  $t$



# Heat Kernel Properties

- **Robustness:**

$k_t(x, \cdot)$  is the probability density function of a Brownian motion, a weighted average over all paths, which is generally not very sensitive to local perturbations

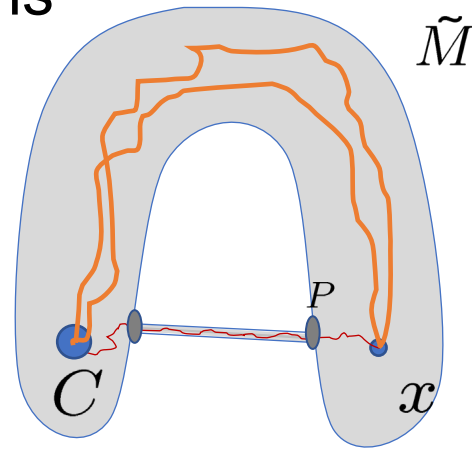


$$k_t^M(x, C) = \mathbb{P}(W_x^t \in C)$$

# Heat Kernel Properties

- **Robustness:**

$k_t(x, \cdot)$  is the probability density function of a Brownian motion, a weighted average over all paths, which is generally not very sensitive to local perturbations

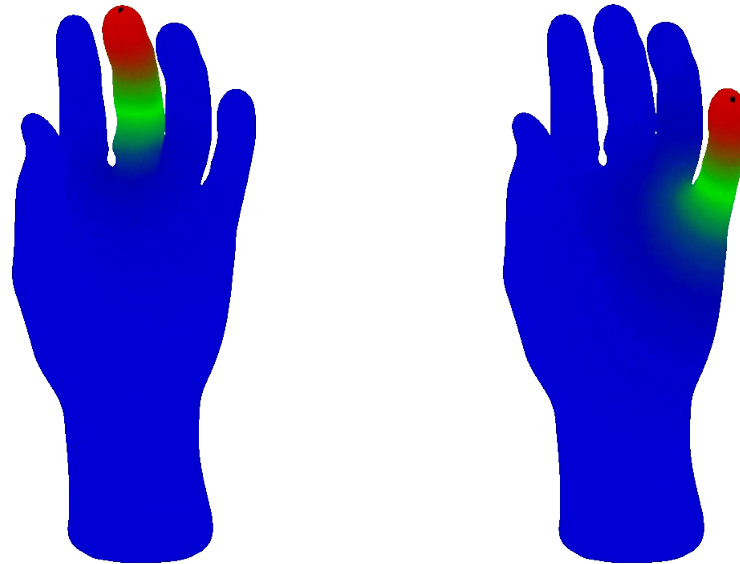


$$k_t^{\tilde{M}}(x, C) = \mathbb{P}(\tilde{W}_x^t \in C)$$

Only paths through the modified area  $P$  will change

# Defining a Signature

- Let  $k_t(x, \cdot)$  be the signature of  $x$  at scale  $t$ 
  - The heat kernel has all the properties we want
  - Except easy comparison ...



- $k_t(x, \cdot)$  is a function on the entire manifold
- Nontrivial to align the domains of such functions across different shapes, or even for different points of the same shape

# The Heat Kernel Signature

- Let  $k_t(x, \cdot)$  be the signature of  $x$  at scale  $t$   
The heat kernel has all the properties we want.  
Except easy comparison ...

- We define the **Heat Kernel Signature** (HKS), by restricting to the diagonal:

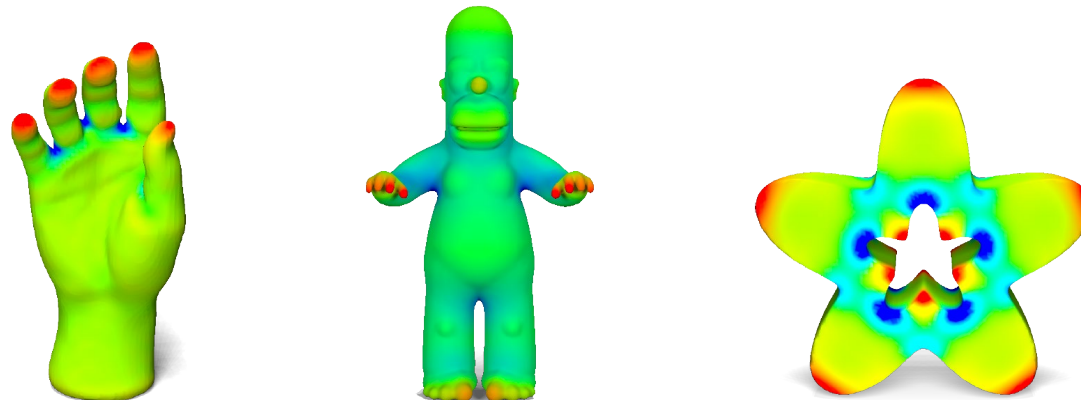
$$\text{HKS}(x) = \{k_t(x, x), t \in \mathbb{R}^+\}$$

- Now HKSs of two points can be easily compared since they are defined on a common domain (time)

# Defining a Signature

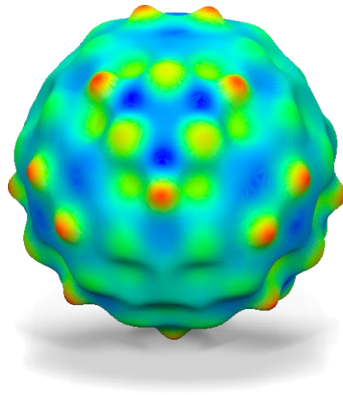
- Since HKS is a restriction of the heat kernel, it is:
  - Robust
  - Multiscale
- Question: How informative is it?
  - Related to Gaussian curvature for small  $t$  :

$$k_t(x, x) = \frac{1}{4\pi t} \sum_{i=0}^{\infty} a_i t^i \quad a_0 = 1, a_1 = \frac{1}{6}K$$

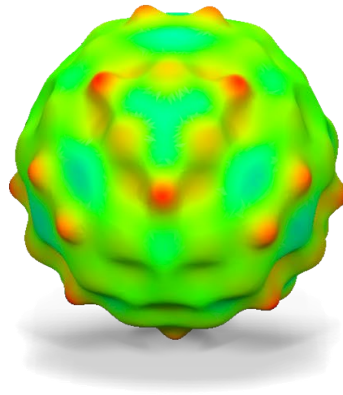


# Defining a Signature

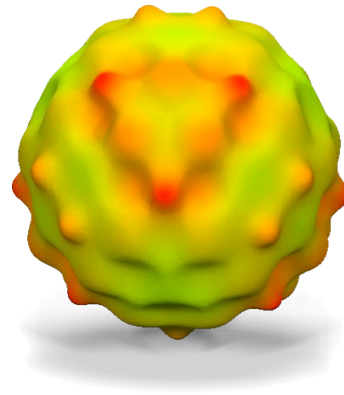
- HKS can be interpreted as a multiscale, robust, intrinsic curvature:



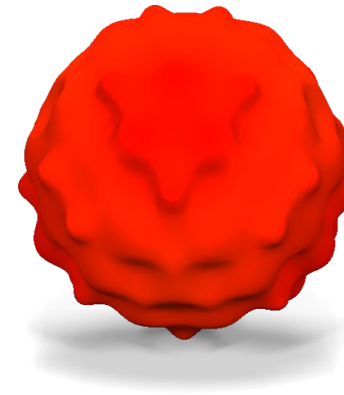
$t = 0.004$



$t = 0.008$



$t = 0.02$



$t = 2$

# Theory Perspective: Informative Theorem

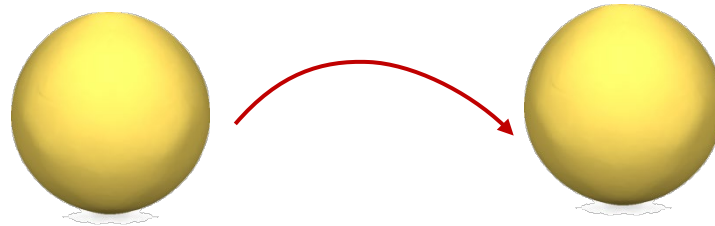
- The set of all HKSs on a shape almost always defines it up to isometry!
- **Theorem:** If  $X$  and  $Y$  are two compact manifolds, such that  $\Delta_X$  and  $\Delta_Y$  have only non-repeating eigenvalues, then a homeomorphism  $T : X \rightarrow Y$  is an isometry **if and only if**, for all  $x$

$$\text{HKS}(x) = \text{HKS}(T(x))$$

- The set of all HKSs characterizes the intrinsic structure of the manifold

# Theory Perspective: Informative Theorem

- How general is the theorem?
  - If there are repeated eigenvalues, it does not hold:



On the sphere,  $\text{HKS}(x) = \text{HKS}(y) \forall x, y$  but there are non-isometric maps between spheres.

- Uhlenbeck's Theorem (1976): for "almost any" metric on a 2-manifold  $X$ , the eigenvalues of  $\Delta_X$  are non-repeating

# Informative Theorem

- Heat kernel is related to the eigenvalues and eigenfunctions of the LB-operator:

$$\text{HKS}(x, t) = \sum_{i=0}^{\infty} e^{-\lambda_i t} \phi_i^2(x)$$

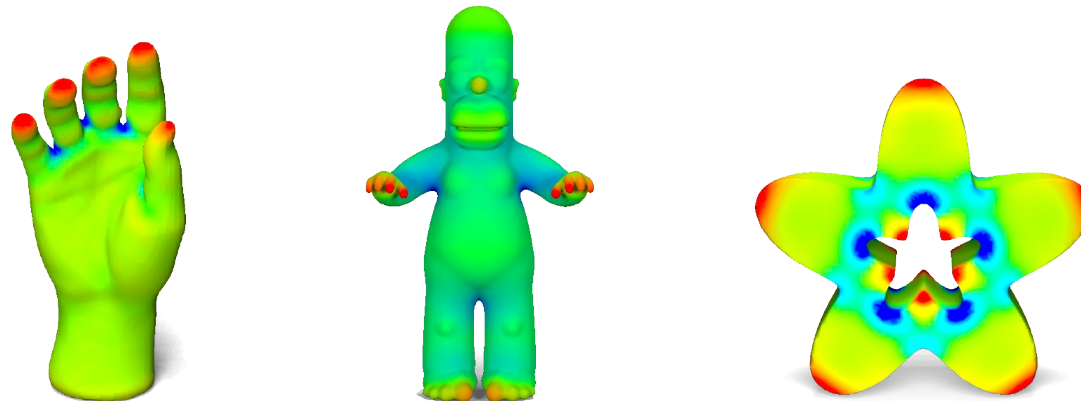
- Invariant to rotations within the eigenspace

# Informative Property

- Conclusion:
  - HKS is informative for individual points
  - And, as a set, for the entire shape

Can be used both for multiscale point matching  
and for shape comparison

$$\text{HKS}(x) = \{k_t(x, x), t \in \mathbb{R}^+\}$$



# Multiscale Matching

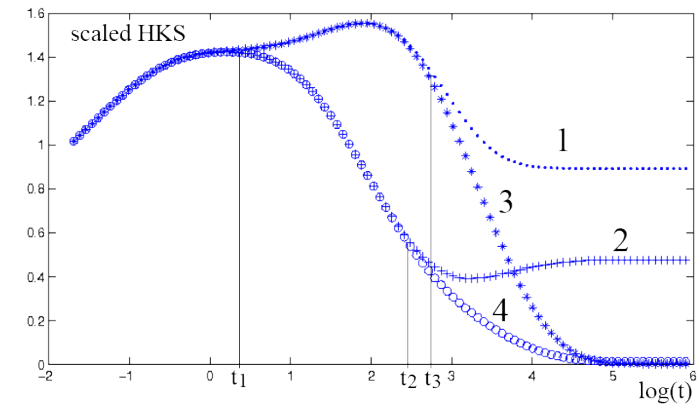
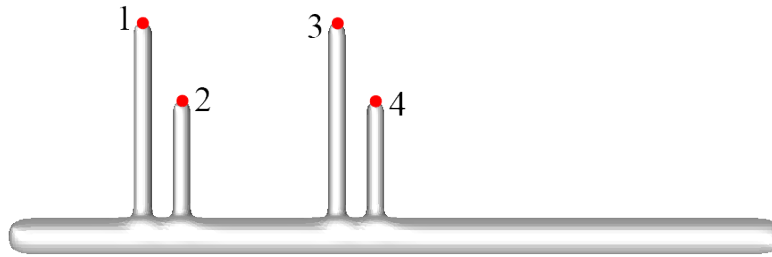
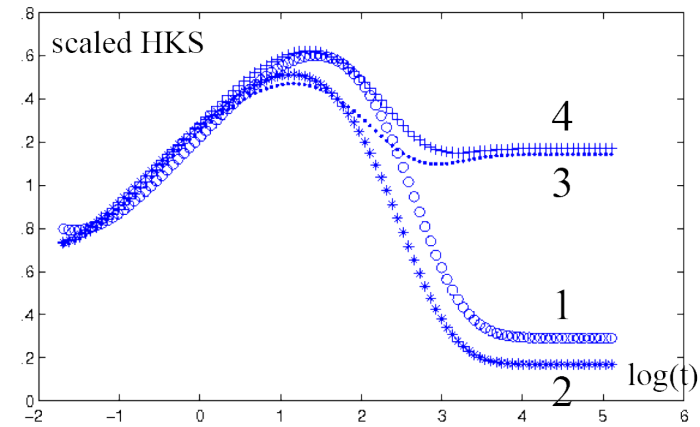
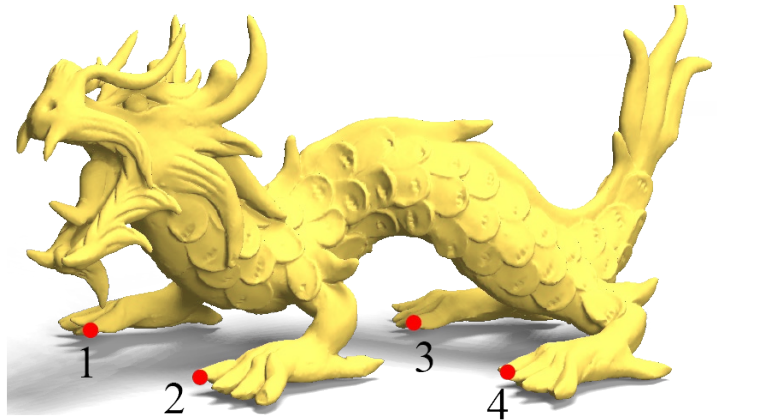
- Two heuristics for making HKSs commensurable:
  - For a fixed point  $x$ , sample HKS on a logarithmic scale at times  $t_i$
  - For a fixed time  $t$  scale each HKS, by the sum over all points of  $M$

$$\text{HKS}(x) = \left\{ \frac{k_{t_i}(x, x)}{\sum_j e^{-t_i \lambda_j}}, i \in 1, 2, \dots, 100 \right\}$$
$$t_i = \alpha^i t_0$$

- Compare using L2 norm of the HKS vectors.

# Multiscale Matching

- Comparing points through their HKS signatures:

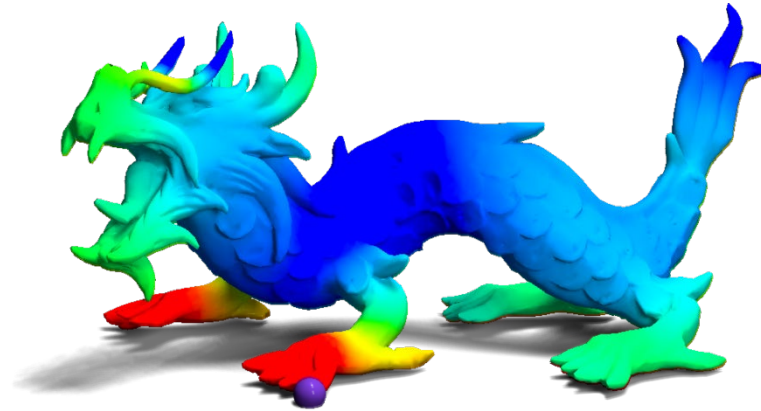


# Multiscale Matching

- Comparing points through their HKS signatures:



Medium scale



Full scale

# Multiscale Matching

- Finding similar points – robustly:



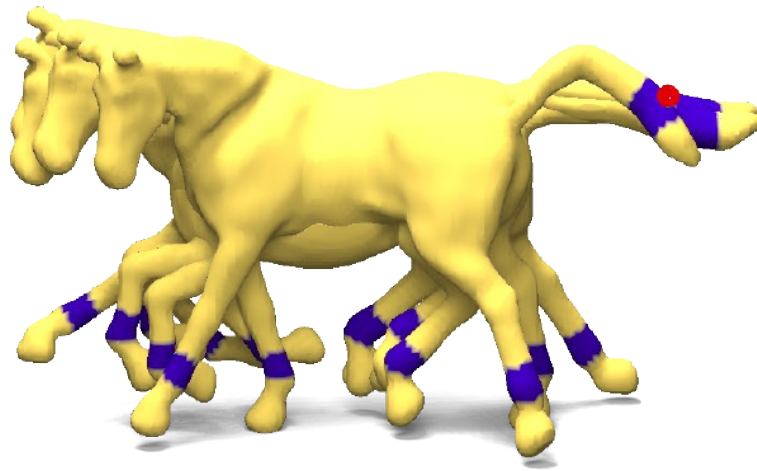
Medium scale



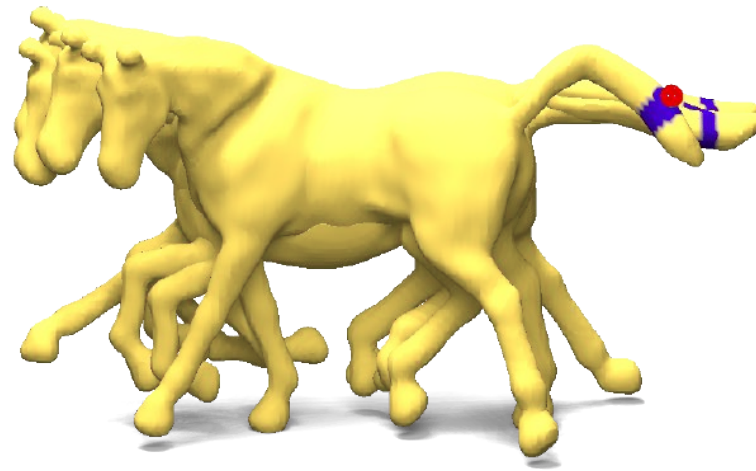
Full scale

# Multiscale Matching

- Finding similar points across multiple shapes:



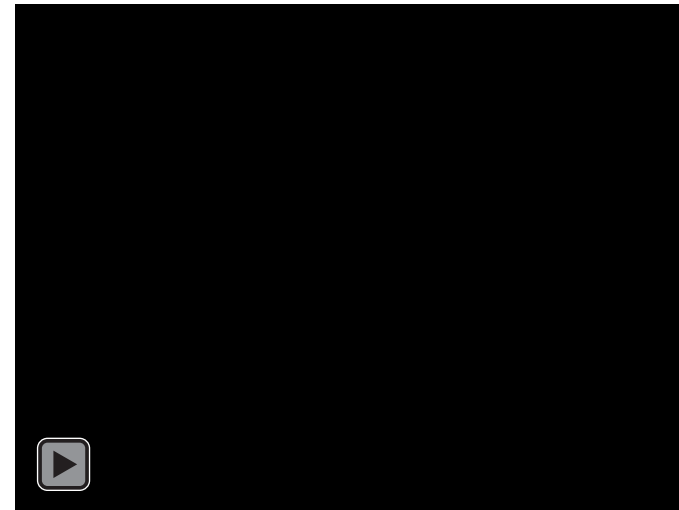
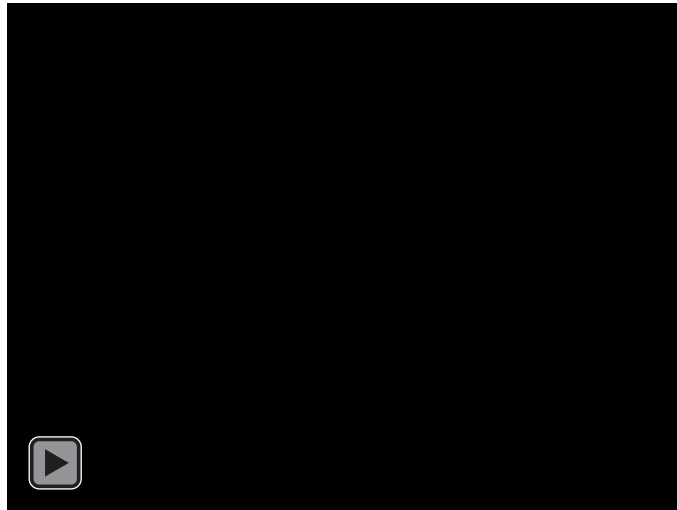
Medium scale



Full scale

# Feature Detection

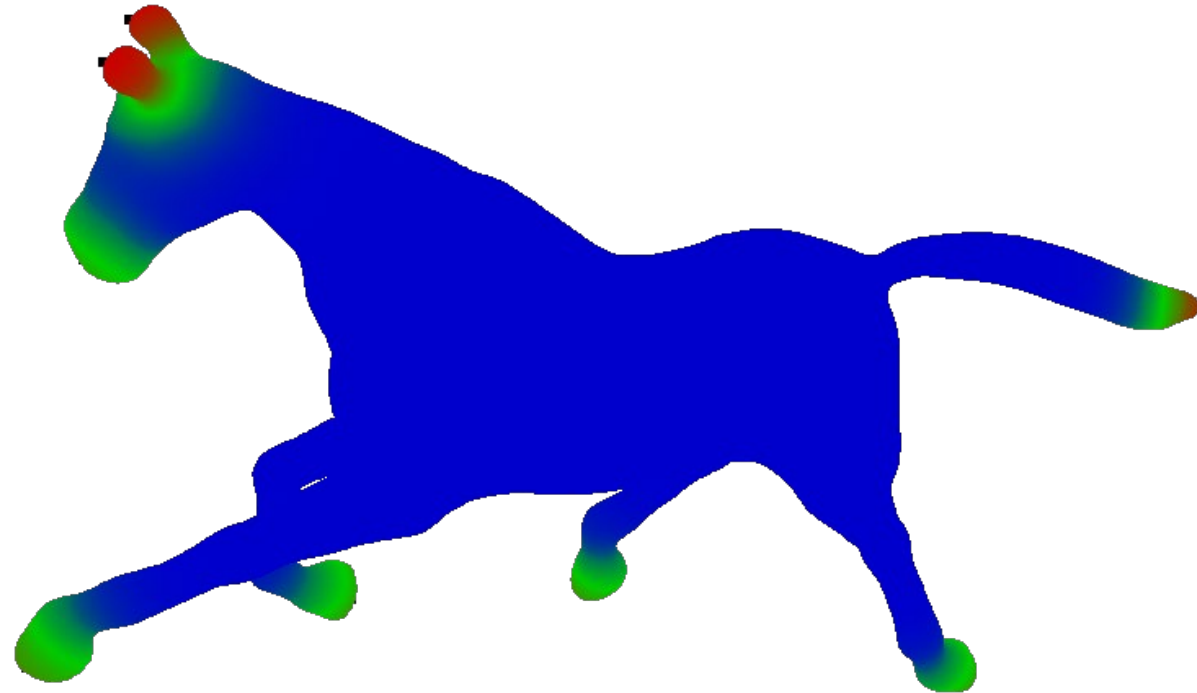
- Persistent feature detection:
  - Intuition: heat diffuses slower at points with high curvature. Heat will tend to concentrate in “hot spots” – extremities of the surface
  - Approach: track the local maximum of the heat kernel for increasing  $t$



# Feature Detection

- Persistent feature detection:
  - Find points that are long term maxima of their heat kernels:

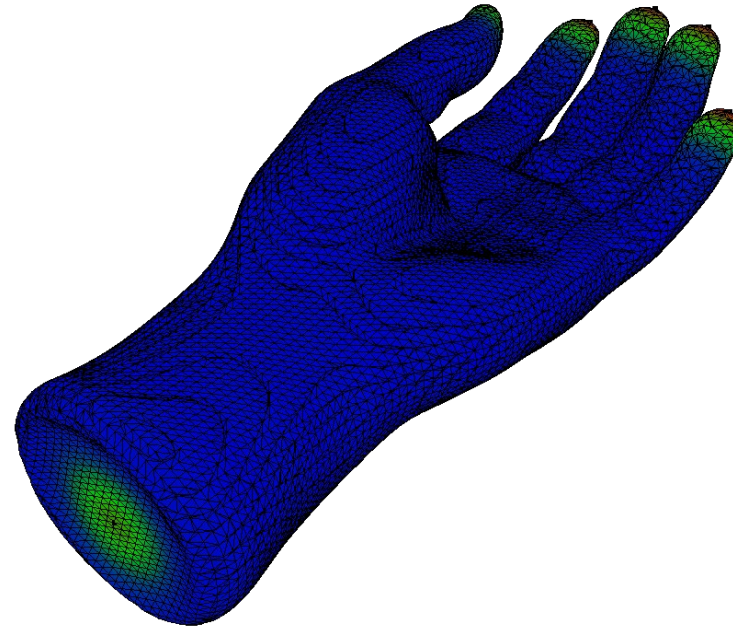
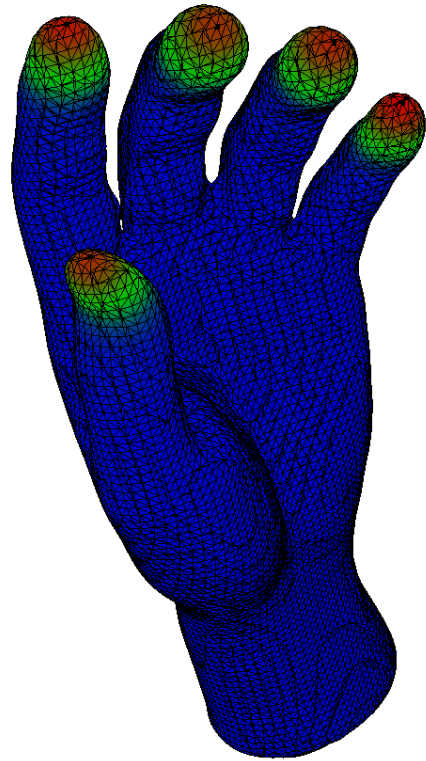
$$k_t(x, \cdot)$$



# Feature Detection

- Persistent feature detection:
  - Find points that are long term maxima of their heat kernels:

$$k_t(x, \cdot)$$



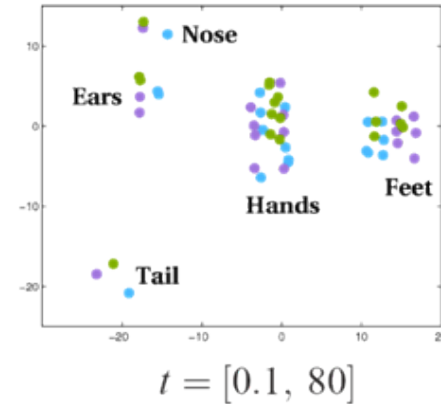
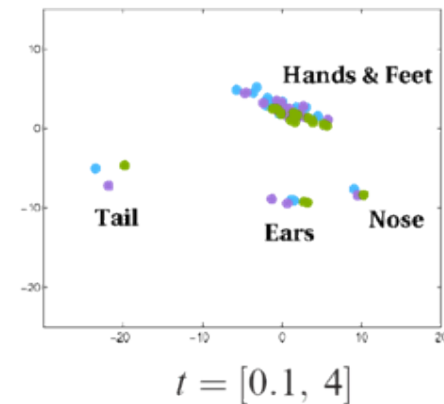
# Feature Detection

- Persistent feature detection:
  - Find points that are long term maxima of their heat kernels:
$$k_t(x, \cdot)$$
  - This may be expensive since the heat kernel at every point is a function over the whole shape. However, long term behavior at nearby points is similar due to mixing
  - Approximation: find points that are local maxima of
$$k_t(x, x)$$
for large enough  $t$



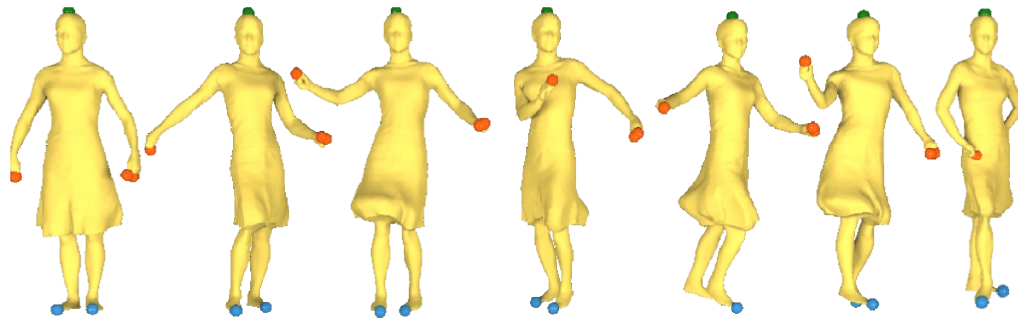
# Shared Structure

- 2D MDS embedding of feature points on three shapes according to distances of their HKS

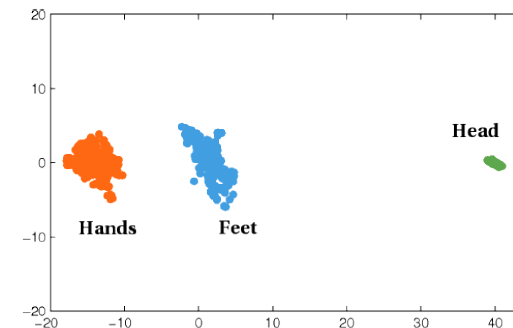


# Shared Structure

- 2D MDS embedding of feature points on **175 shapes** according to distances of their HKS.

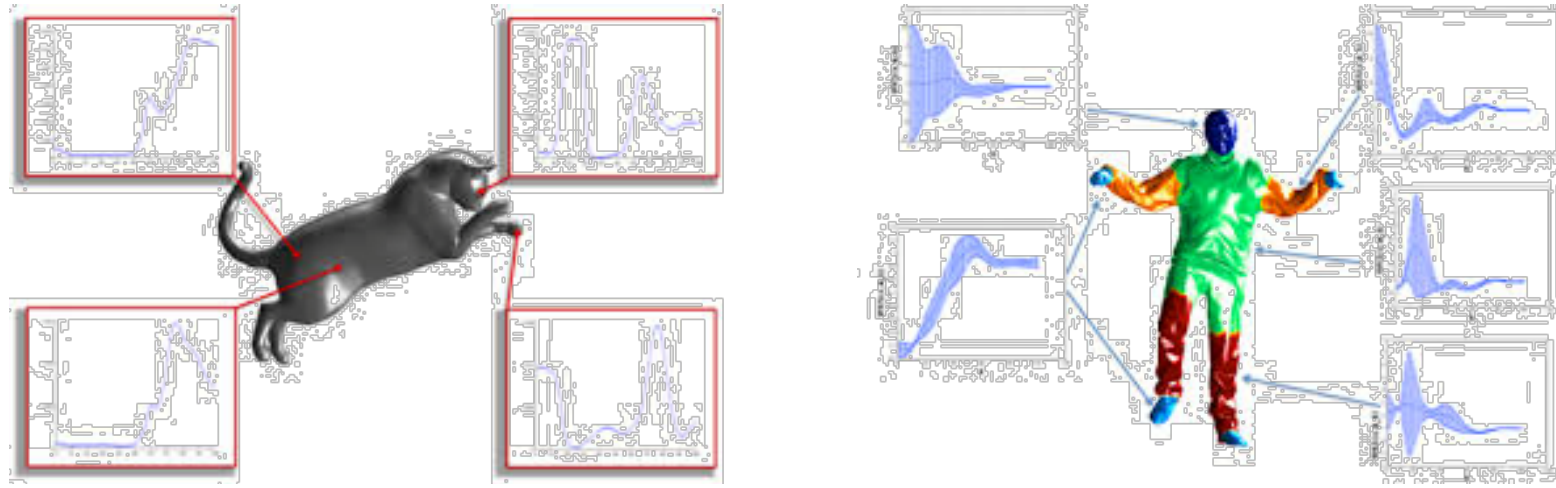


Feature points found on a few poses of the dancer model by Vlasic *et al.*



MDS of features from all 175 poses using a full range of scales

# The Wave Kernel Signature (WKS)

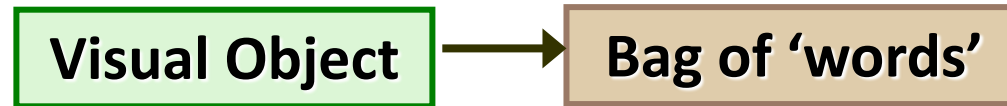


Based on solutions of the quantum Schrödinger equation

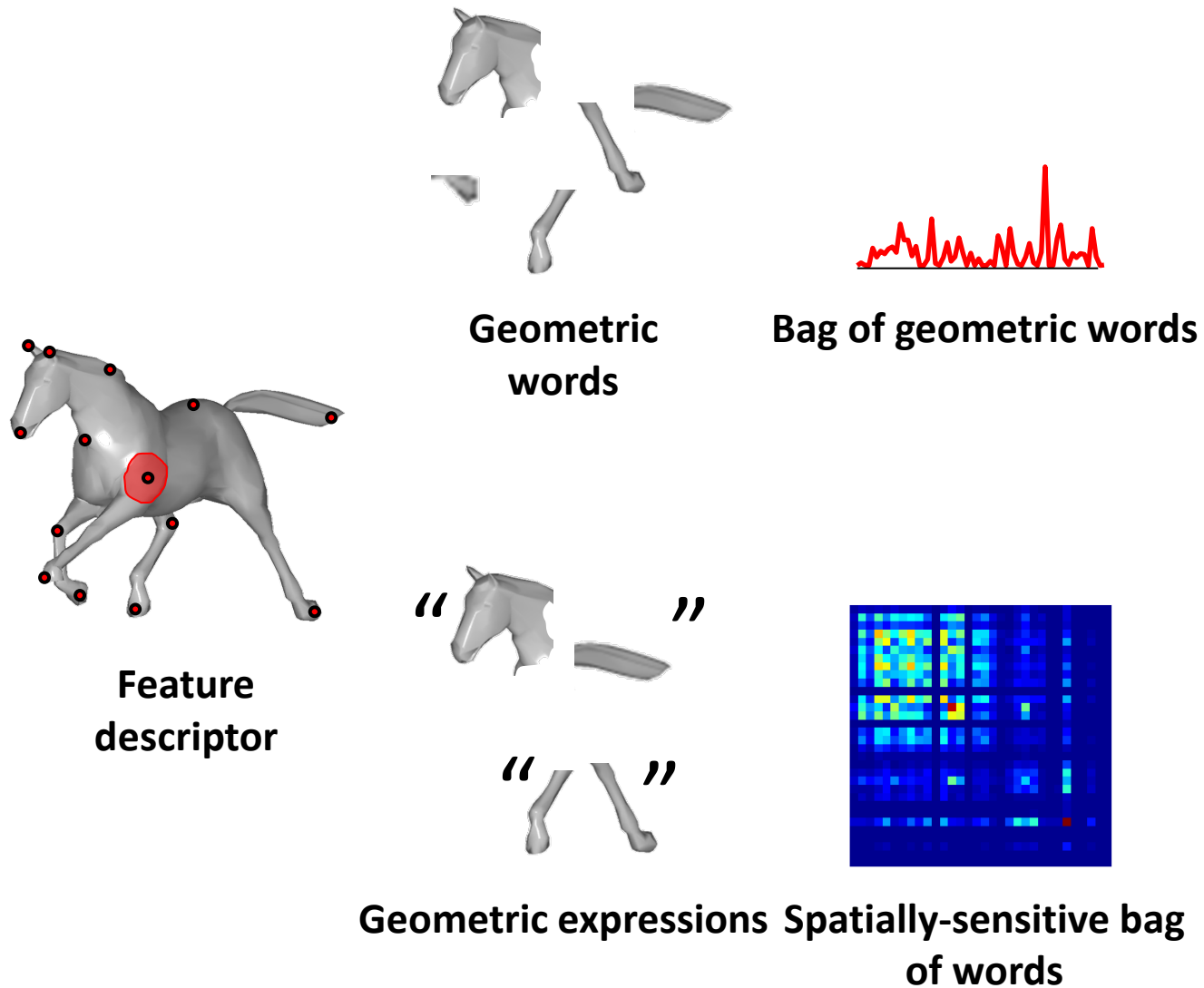
$$\frac{\partial \psi}{\partial t}(x, t) = i\Delta \psi(x, t)$$

# Shape Search

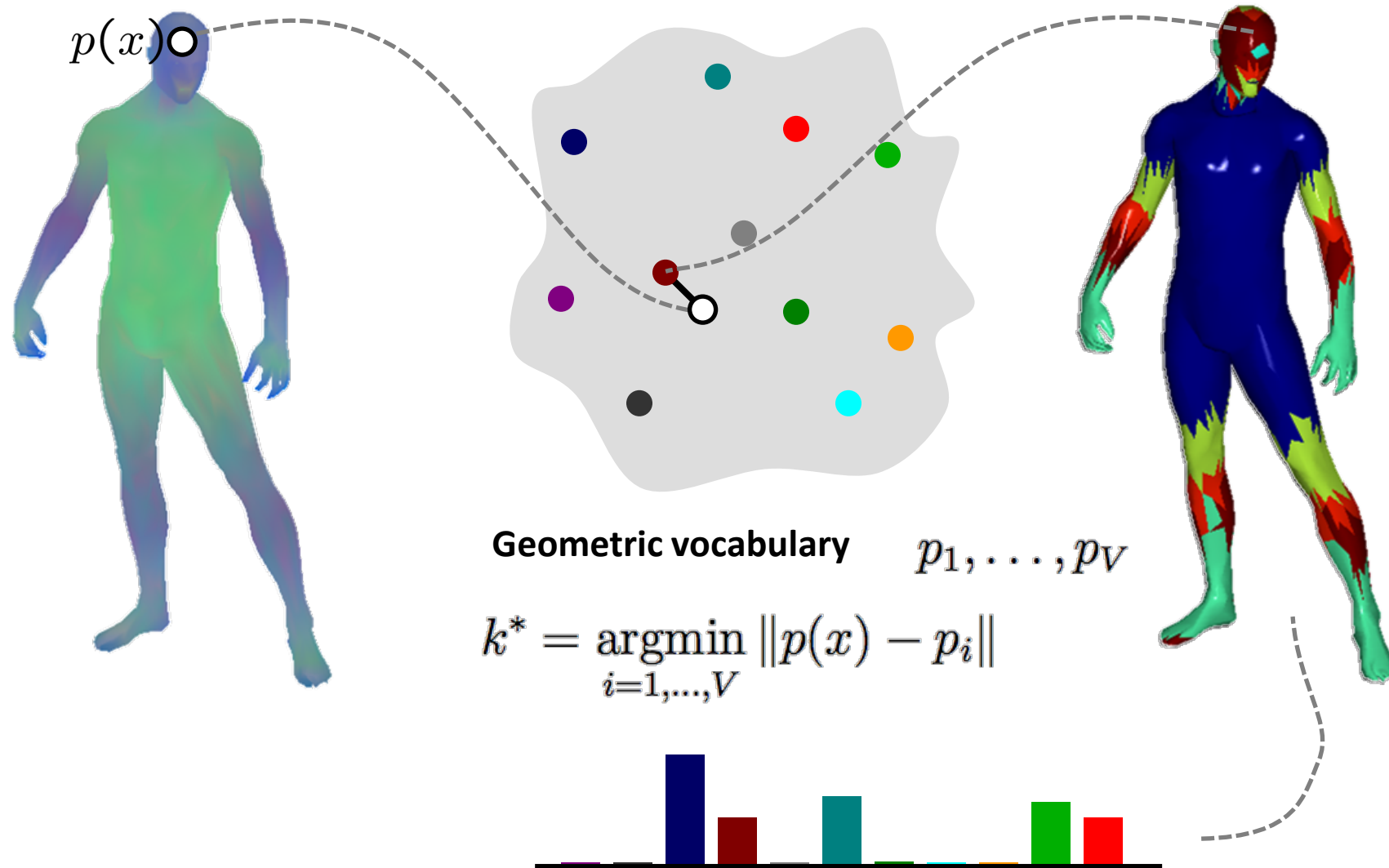
# Bag-of-Words Models (BoW)



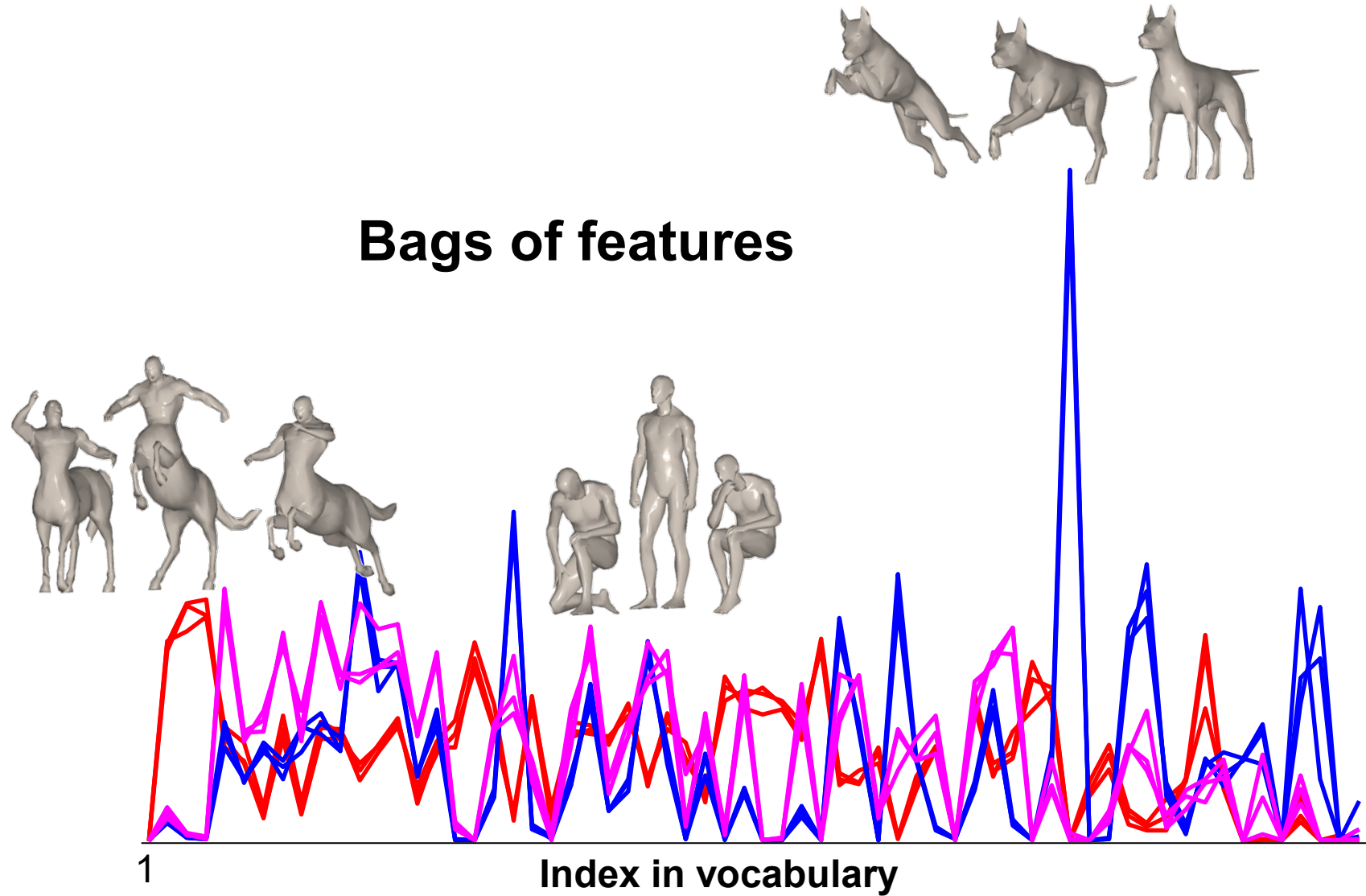
# Spatial Words



# ShapeGoogle: HKS-Based BoW Shape Search



# Shape Signatures



# That's All

