Tutorial 2
Biological shape descriptors

Patrice Koehl and Joel Hass

University of California, Davis, USA
Deciphering Biological Shapes

-How do we understand shapes?
  The Mumford experiments

-Shape Descriptors
Deciphering Biological Shapes

-How do we understand shapes?
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-Shape Descriptors
Start with an easy case:

Before moving to the problem of comparing surfaces in $R^3$, we ask a simpler question:

**Problem**: How similar are two *regions in the plane*?

This is already an important problem.

Question: How close is a square to a circle?
Distance between shapes

Which of these nine shapes is closest to?

Which is second closest?
Application - Facial Recognition

Start with a 2D photograph.
Create some planar regions from a face.
Compare their shapes.
Application - Computer Vision

“Purring Test”  Cat or Dog?

Flip a coin - correct 50% of the time
Software fifteen years ago - not much better
Today - 99%
Application - Computer Vision

Dog or Muffin? Still a challenge
Application - Computer Vision

Puppy or Bagel?
Application - Character Recognition

What letter is this?

This is a handwritten example for GOCR.
Write as good as you can.
Test Case

How close are these two shapes?

Can either compare curves or enclosed regions:

Our Goal: Find a mathematical framework to measure the similarity of two shapes.
Goal for 2D shapes:
A metric on curves in the plane

1. $d(C_1, C_2) = 0 \iff C_1 \text{ is isometric to } C_2$ (isometry)
2. $d(C_1, C_2) = d(C_2, C_2)$ (symmetry)
3. $d(C_1, C_3) \leq d(C_1, C_2) + d(C_2, C_3)$ (triangle inequality)
Why these three metric properties?

1. \(d(C_1, C_2) = 0 \iff C_1 \text{ is isometric to } C_2\) (isometry)

2. \(d(C_1, C_2) = d(C_2, C_2)\) (symmetry)

3. \(d(C_1, C_3) \leq d(C_1, C_3) + d(C_1, C_3)\) (triangle inequality)

Each property plays an important role in applications.
Isometry: \[ d(C_1, C_2) = 0 \iff C_1 \text{ is isometric to } C_2 \]

Allows for identifying different views of the same object.

We want to consider these to be the same object. Our distance measure should not change if one shape is moved by a Euclidean Isometry.
Symmetry: \[ d(C_1, C_2) = d(C_2, C_2) \]

The distance between two objects does not depend on the order in which we find them.

If I own the square, and you own the circle, we can agree on the distance between them.
Triangle inequality: \( d(C_1, C_3) \leq d(C_1, C_2) + d(C_2, C_3) \)

Measurements should be stable under small errors.

\[ d(C_1, C_3) - d(C_2, C_3) \leq d(C_1, C_2) \]

If \( C_1 \) and \( C_2 \) are close, so \( d(C_1, C_2) \) is small, then the distance of \( C_1 \) and \( C_2 \) to a third shape \( C_3 \) is about the same.

\[ d(\text{square}, \text{circle}) - d(\text{rectangle}, \text{circle}) = d(\text{square}, \text{rectangle}) \]

This means that noise, or a small error, does not affect distance measurements very much.
What is a good metric on the shapes in $\mathbb{R}^2$?

David Mumford examined this question.

D. Mumford, 1991
*Mathematical Theories of Shape: do they model perception?*

There are many natural candidates for metrics giving distances between shapes.

We look at some of these metrics.
Hausdorff metric

\( d_H = \) Maximal distance of a point in one set from the other set, after a rigid motion.

\[
d_H(A, B) = \min_{\text{rigid motions}} \left\{ \sup_{x \in A} d(x, B) + \sup_{y \in B} d(y, A) \right\}
\]

What is the Hausdorff distance?

Add the distances of each red dot from the other set.

Gives a metric on \{compact subsets of the plane\}. 
Drawbacks: Hausdorff metric

\[ d_H(A, B) = 0 \]

\[ d_H(A, B) = 1 \]

\[ d_H(A, B) = 1 \]
Drawbacks: Hausdorff metric

The alignment that minimizes Hausdorff distance may not give the correspondence we want.

Can we fix this with a different metric?
Template metric

distance = Area of non-overlap after rigid motion.

\[ d_T(A, B) = \min \{\text{Area}(A-B) + \text{Area}(B-A)\} \]

rigid motions

Blue area at left + green area at right

\[ d_T(A, B) \approx 0 \]
Drawbacks: Template metric

The area overlap is small. \( d_T(A,B) \approx 1 \)

The area overlap is large. \( d_T(A,B) \approx 0 \)
Challenge- Intrinsic geometry.

These shapes are *intrinsically* close. Not picked up by Hausdorff or template metrics.

How can we see this?
Gromov-Hausdorff metric

One way to see that these are close:
Bend them in $\mathbb{R}^3$, and then use $\mathbb{R}^3$-Hausdorff metric.
This gives the *Gromov-Hausdorff* metric.
Optimal transport metric

Also called the *Wasserstein* or *Monge-Kantorovich* metric. Distance between two shapes is the cost of moving one shape to the other:

Distance = \[ \int \text{(area of subregion)} \times \text{(distance moved)} \]
Drawback - Optimal Transport

Can be discontinuous

Can be hard to compute
Optimal diffeomorphism metric

Define an energy that measures the stretching between two shapes. This energy defines a distance between two spaces that are diffeomorphic.

\[ E(f) = \int \int \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial x} \right)^2 \, dx \, dy \]

\[ d_D(A, B) = \min_{\text{diffeomorphisms}} \{ E(f) \} \]
Drawback: Optimal diffeomorphism

Requires diffeomorphic shapes
Maps with tears

Optimal diffeomorphism but allowing some tears.

Hard to compute.
Mumford Experiments

Two groups of subjects, and 15 polygons

a. Pigeons

b. Harvard undergraduates

*Experiment Conclusion*: Human and pigeon perception of shape similarity do not indicate an underlying mathematical metric.
Deciphering Biological Shapes

- How do we understand shapes?
  The Mumford experiments

- Shape Descriptors
Now look at surfaces and shapes in $\mathbb{R}^3$

How similar are these two shapes?
How do we compare two proteins?

“Feature space”

$P_1 \rightarrow \mathbf{V}_1 = (a_1, b_1, \ldots.)$

$d = \| \mathbf{V}_1 - \mathbf{V}_2 \|$

$P_2 \rightarrow \mathbf{V}_2 = (a_2, b_2, \ldots.)$
Fourier Analysis of Time Signal

\[ f_r = \frac{1}{N} \sum_{s=0}^{N-1} F_s e^{2\pi rs/N} \]

\[ F_s = \frac{1}{N} \sum_{r=0}^{N-1} f_r e^{-2\pi rs/N} \]
Harmonic Representation of Shapes

1. Surface-based shape analysis
   *Spherical harmonics*

2. Volume-based shape analysis
   *3D-Zernike moments*
The challenge of the elephant…

Enrico Fermi once said to Freeman Dyson:

“I remember my friend Johnny von Neumann used to say, with four parameters I can fit an elephant, and with five I can make him wiggle his trunk.”

The challenge of the elephant…


\[ x(t) = \sum_{k=0}^{K} \left( A_k^x \cos(kt) + B_k^x \sin(kt) \right) \]

\[ y(t) = \sum_{k=0}^{K} \left( A_k^y \cos(kt) + B_k^y \sin(kt) \right) \]

<table>
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<th>( A_k^x )</th>
<th>( B_k^x )</th>
<th>( A_k^y )</th>
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</tbody>
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The challenge of the elephant...
3D: Spherical harmonics

Any function $f$ on the unit-sphere can be expanded into spherical harmonics:

$$f(\theta, \varphi) = \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} c_{l,m} Y_{l}^{m}(\theta, \varphi)$$

where the basis functions are defined as:

$$Y_{l}^{m}(\theta, \varphi) = \sqrt{\frac{2l + 1}{4\pi}} \frac{(l - m)!}{(l + m)!} P_{l}^{m}(\cos \theta)e^{im\varphi}$$

The coefficients $c_{l,m}$ are computed as:

$$c_{l,m} = \int_{0}^{2\pi} \int_{0}^{\pi} f(\theta, \varphi)(Y_{l}^{m}(\theta, \varphi))^{*} \sin(\theta) d\theta d\varphi$$
Harmonic Decomposition

3D: Spherical harmonics

\[ \text{Harmonic Decomposition} = \text{Constant} + 1^{\text{st}} \text{Order} + 2^{\text{nd}} \text{Order} + 3^{\text{rd}} \text{Order} + \ldots \]
What are the spherical harmonics $Y_{l}^{m}$?

\[ Y_{0}^{0}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{1}{\pi}} \]

\[ Y_{1}^{-1}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-i\varphi} \]

\[ Y_{1}^{0}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta \]

\[ Y_{1}^{1}(\theta, \varphi) = \frac{-1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{i\varphi} \]

\[ Y_{2}^{-2}(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^{2} \theta e^{-2i\varphi} \]

\[ Y_{2}^{-1}(\theta, \varphi) = \frac{1}{2} \sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{-i\varphi} \]

\[ Y_{2}^{0}(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{5}{\pi}} (3 \cos^{2} \theta - 1) \]

\[ Y_{2}^{1}(\theta, \varphi) = \frac{-1}{2} \sqrt{\frac{15}{2\pi}} \sin \theta \cos \theta e^{i\varphi} \]

\[ Y_{2}^{2}(\theta, \varphi) = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^{2} \theta e^{2i\varphi} \]
Importance of Rotational Invariance

Shapes are unchanged by rotation

Shape descriptors may be sensitive to rotation: for example, the $c_{l,m}$ are not rotation invariant
Restoring Rotational Invariance

Note that:

\[ f(x) = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \neq \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = f(Rx) \]

However:

\[ \|f(x)\| = \sqrt{a_1^2 + a_2^2} = \sqrt{b_1^2 + b_2^2} = \|f(Rx)\| \]

Invariant spherical harmonics descriptors:

\[ c_{l,m} \text{ for all } l, m \quad \rightarrow \quad g_l = \sqrt{\sum_{m=-l}^{l} c_{l,m}^2} \]
Invariant spherical harmonics descriptors
Some issues with Spherical Harmonics

*Spherical harmonics are surface-based:*
- They require a parametrization of the surface (usually triangulation)
- They are appropriate for star-shaped objects
- They lose content information
From Surface to Volume

- Consider a set of concentric spheres over the object.
- Compute harmonic representation of each sphere independently.
Problem: insensitive to internal rotations
A natural extension to Spherical Harmonics: The 3D Zernike moments

Surface-based

\[ f(\theta, \varphi) = \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} c_{l,m} Y^m_l(\theta, \varphi) \]

Volume-based

\[ f(\theta, \varphi, r) = \sum_{n=0}^{+\infty} \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} c_{l,m} R_{n,l} Y^m_l(\theta, \varphi) \]

with:

\[ Y^m_l(\theta, \varphi) = \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}} P^m_l(\cos \theta) e^{im\varphi} \]

and

\[ R_{n,l}(r) = \begin{cases} \sum_{k=0}^{(n-l)/2} N_{n,l,k} r^{n-2k} & \text{n - l even} \\ 0 & \text{n - l odd} \end{cases} \]
How does it work?
Applications
Comparing Old World Monkey Skulls
Old World Monkey Skulls: DNA Tree

- Macaca sylvanus
- Macaca nemestrina (Borneo)
- Macaca spp. Sulawesi
- Macaca pogensis
- Macaca fascicularis
- Macaca fuscata
- Macaca mulatta
- Macaca assamensis
- Theropithecus
- Papio h. ursinus (Southern)
- Papio h. Kindae
- Papio h. ursinus (Grisseides)
- Papio h. cynocepalus (Southern)
- Papio h. papio
- Papio h. anubis (Western)
- Lophocebus
Old World Monkey Skulls: Distance Tree

- Papio h. ursinus (Southern)
- Papio h. ursinus (Griseides)
- Papio h. anubis (Western)
- Theropithecus
- Papio h. cynocephalus (Southern)
- Papio h. papio
- Lophocebus
- Papio h. Kindae
- Macaca sylvanus
- Macaca mulatta
- Macaca spp. Sulawesi
- Macaca pagensis
- Macaca fuscata
- Macaca fascicularis
- Macaca nemestrina (Borneo)
- Macaca assamensis
Analysis of the McGill Shape databases
458 objects, in 10 categories

A) Fraction of TP vs. Fraction of FP

B) ROC area vs. Max. order of Zernike invariants

Legend:
- ○ N=1
- × N=5
- + N=40
- □ N=50