MSRI
Mathematical Sciences Research Institute

17 Gauss Way Berkeley, CA 94720-5070 p: 510.642.0143 f: 510.642.8609 www.msri.org

NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: Malgorzata Marciniak **Email/Phone:** mmarciniak@lagcc.cuny.edu 5734620411

Speaker's Name: Joel Hass

Talk Title: Geometric and topological methods for aligning and comparing shapes (Comparing genus-zero surfaces)

Date: 10 /02 /2018 **Time:** 9 :30 am / pm (circle one)

Please summarize the lecture in 5 or fewer sentences:
Applied geometry and topology is used in problems in science. Evolutionary tree was reconstructed using only metatarsal bone shapes and a distance between shapes, without any human input. Machine learning approach seems to be more efficient than traditional approaches and works well for problems of recognition such as decision whether the given picture represents a cat or a dog. A new way of measuring distances between surfaces that involves conformal diffeomorphisms is implemented.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

- ☑ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- ☑ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
  - **Computer Presentations**: Obtain a copy of their presentation
  - **Overhead**: Obtain a copy or use the originals and scan them
  - **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
  - **Handouts**: Obtain copies of and scan all handouts
- ☑ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- ☑ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)
- ☑ Email the re-named files to notes@msri.org with the workshop name and your name in the subject line.

Comparing genus-zero surfaces

MSRI
October 2, 2018

joint work with Patrice Koehl

Applied Geometry and Topology

Many problems in science are concerned with the geometry of two and three-dimensional objects.

Mathematicians have developed powerful tools to study such problems and these are now starting to be used.

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Anthropologists dig up a fossilized primate bone.
What species does it belong to?

Lemur?

Chimpanzee?

Baboon?

What bone from a known species does it most closely resemble?

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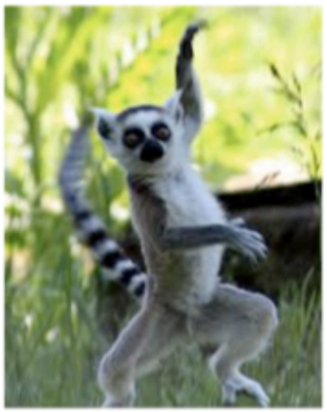
This is a problem in geometry.

Example: Metatarsal Bones

Proximal first metatarsals from 38 prosimian primates, and 23 New and Old World simian monkeys



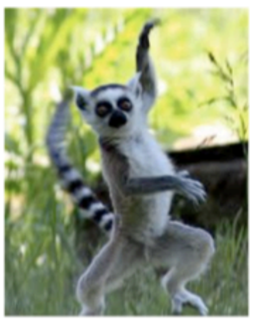
Prosimian:
lemur

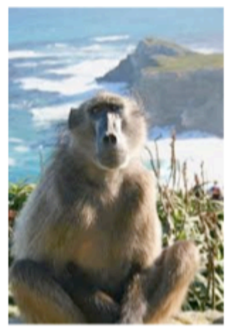
Simian:
Cape baboon
(old world)

Simian:
White eared titi
(new world)

Which Bone is “Closest”?

Proximal first metatarsals from 38 prosimian primates, and 23 New and Old World simian monkeys





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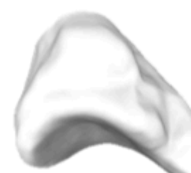
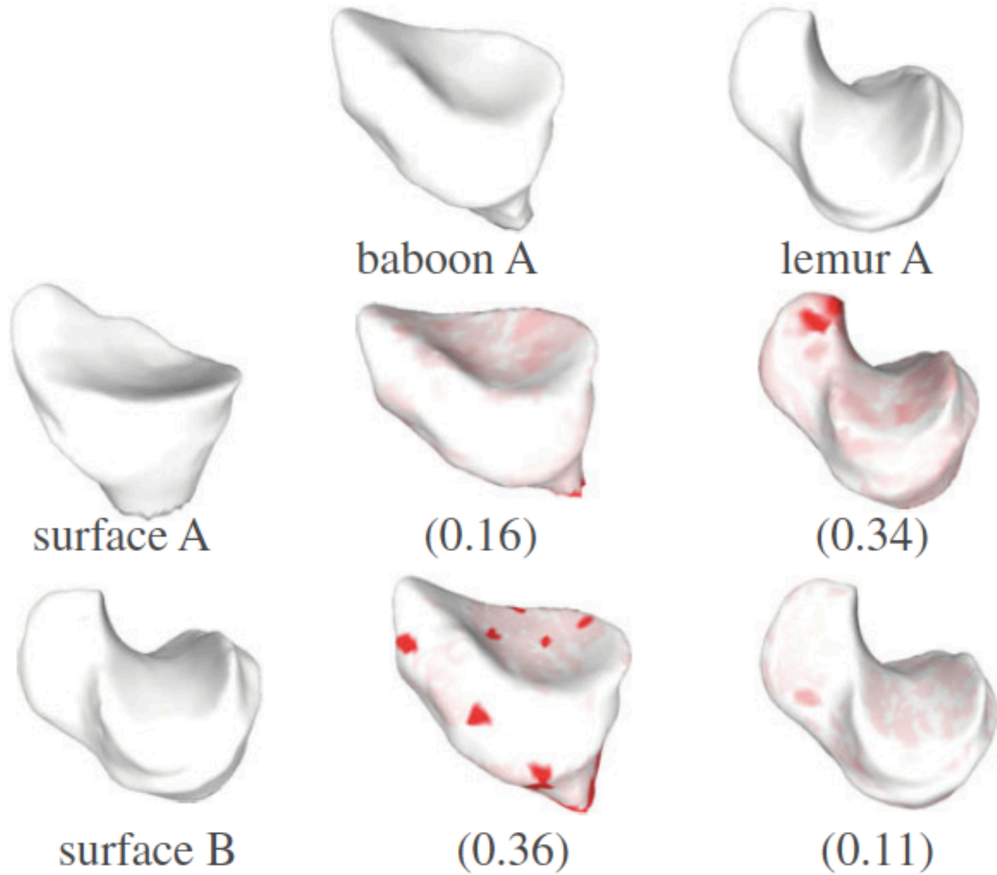


Simian:
White eared titi
(new world)

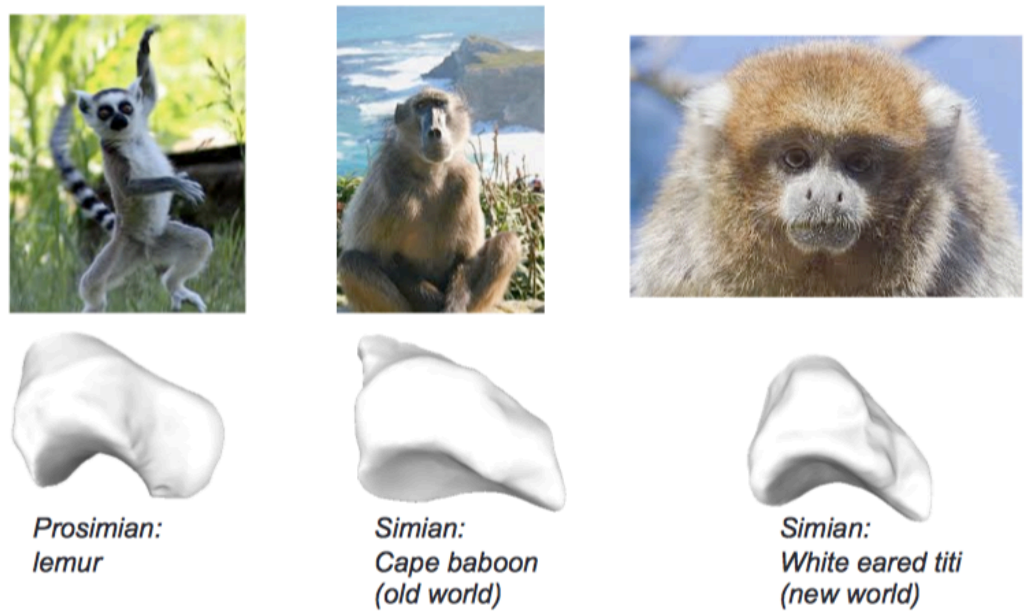
Find a *distance* between shapes



A number that tells us if two shapes are close (look similar) or far (look different).

Experiment - Bone Surfaces

Proximal first metatarsals from 38 prosimian primates, and 23 New and Old World simian monkeys



Compare metatarsal (toe) bones from 23 old and new world monkeys and 38 prosimians
(Data from Boyer, Lipman, St. Clair, Puente, Patel, Funkhouser, Jernvall, Daubechies, PNAS, 2012)

Experiment - Bone Surfaces

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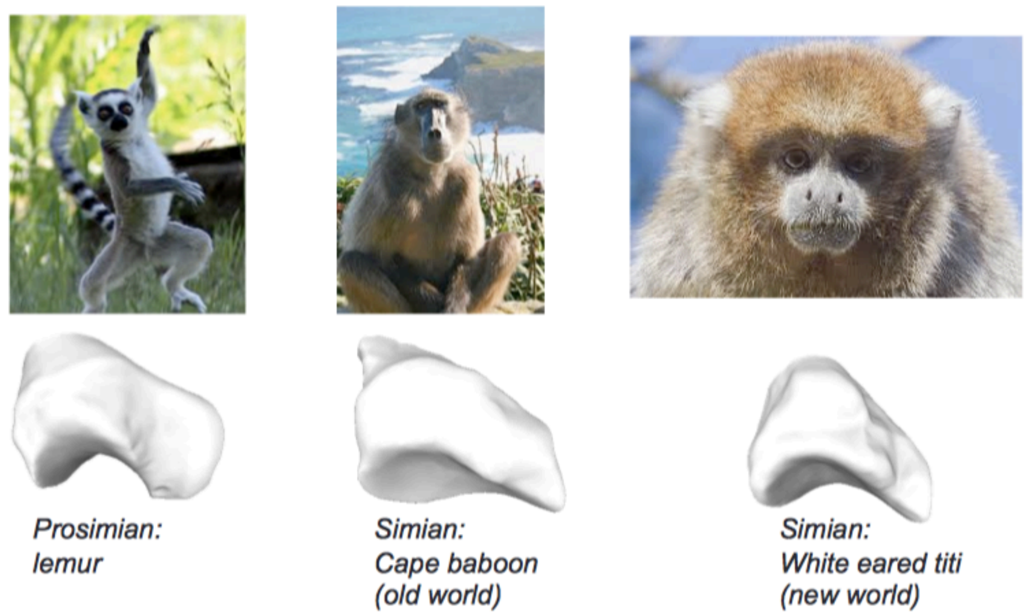
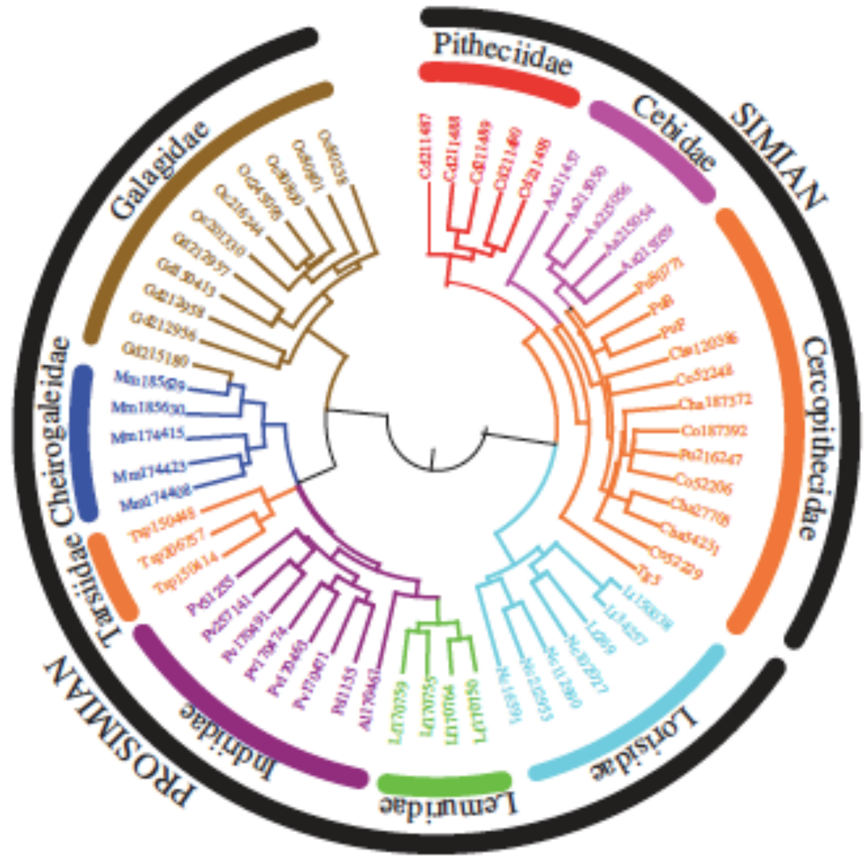


Method: Compute distances between all pairs of bones (1830 distances). This was done purely by shape, without using any human expertise.

Application



This evolutionary tree was reconstructed from a collection of simian and prosimian metatarsal bones, using only the shapes and a distance between shapes. No human input, no biological knowledge was used.

Application

This evolutionary tree was reconstructed using only metatarsal bone shapes and a distance between shapes.

The Centrality of Surface Comparison

1. Everything we see is a surface.

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2. Scanning will be everywhere.
Cell phones can already digitize surfaces.

How can we use this digitized data?

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Some potential applications:

Diagnose disease or bone fracture - Radiologists

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Recognize bones and fossils	Human experts

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Morph two images	Disney

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Drug design	~~Drug companies~~
Recognize bones and fossils	~~Human experts~~
Compare teeth	~~Dentists~~
Morph two images	~~Disney~~

The Centrality of Surface Comparison

Even More potential applications:

Parts replacement

The Centrality of Surface Comparison

Even More potential applications:

Parts replacement ~~Inventory Managers~~

The Centrality of Surface Comparison

Even More potential applications:

Parts replacement
Rorschach test

~~Inventory Managers~~




The Centrality of Surface Comparison

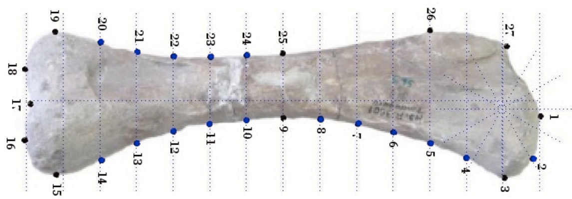
Even More potential applications:

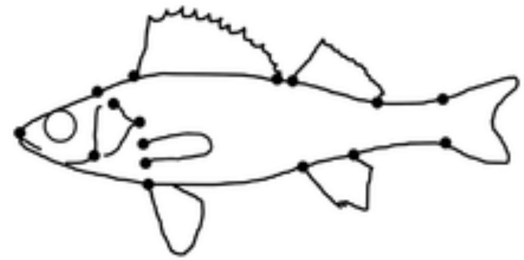
Parts replacement ~~Inventory Managers~~
Rorschach test ~~Psychologists~~

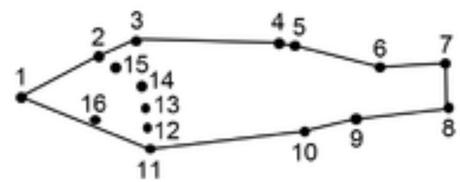
   

Morphometrics

A traditional approach to comparing bones.

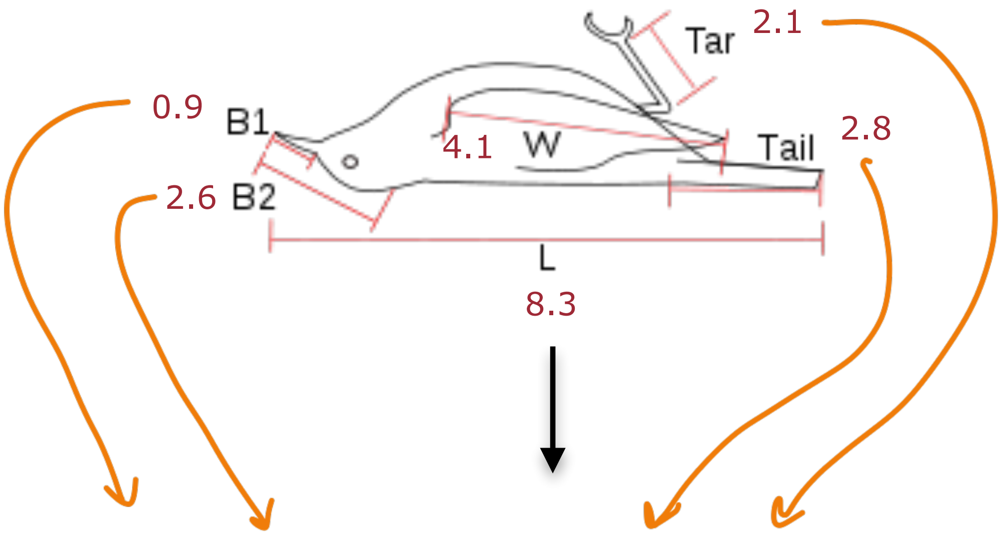






Shape ⟶ “Feature Vector”

Morphometrics

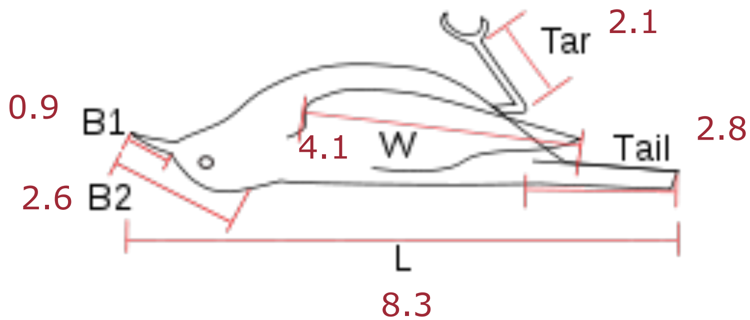


Shape

$(0.9, 2.6, 8.3, 2.8, 2.1, 4.1)$ Feature Vector

The distance between shapes is the distance in $\mathbb{R}^6$

Morphometrics



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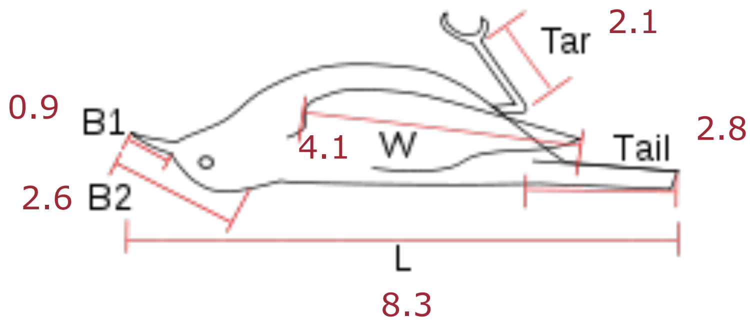
Can work quite well, but:

1. Requires human expertise.

Morphometrics



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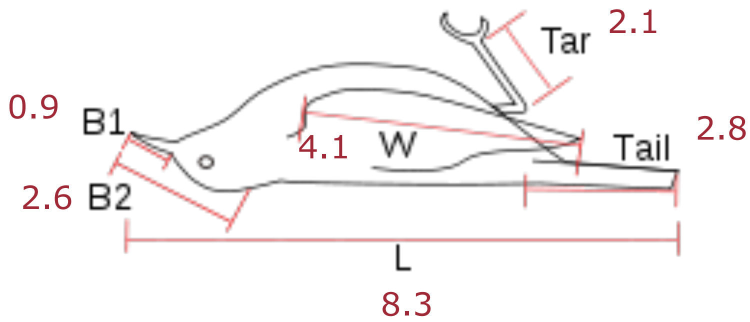
2. Expensive and slow and error prone.

Morphometrics



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Can work quite well, but:

1. Requires human expertise.
2. Expensive and slow and error prone.

(3. Not a metric)

Machine Learning Approach

Dog or Cat?

Machine learning approach

https://www.imageidentify.com

Machine learning approach

https://www.imageidentify.com

Works well for: Dog or Cat

But

Dog or Muffin?

Cat or Ice Cream?

Dog or Bagel?

Dog or Fried Chicken?

Dog or Mop?

Comparing surfaces with geometry

1. What is the distance between a pair of surfaces?

Which two of these three are most alike?

Comparing surfaces with geometry

1. What is the *distance* between a pair of surfaces?



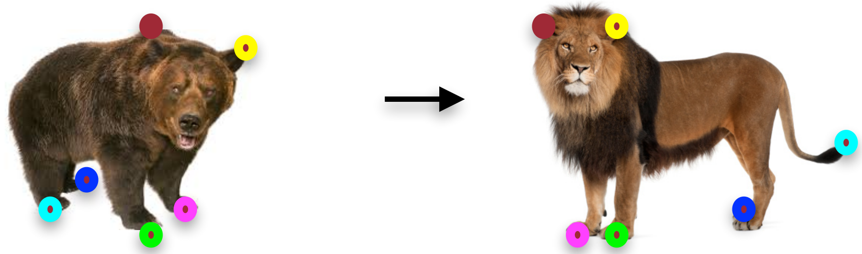
Which two of these three are most alike?

When $d(S_1, S_2)$ is small, we also want a "good" correspondence $f\colon S_1 \rightarrow S_2$

2. What is a good *alignment* between two surfaces?

Two approaches to alignment

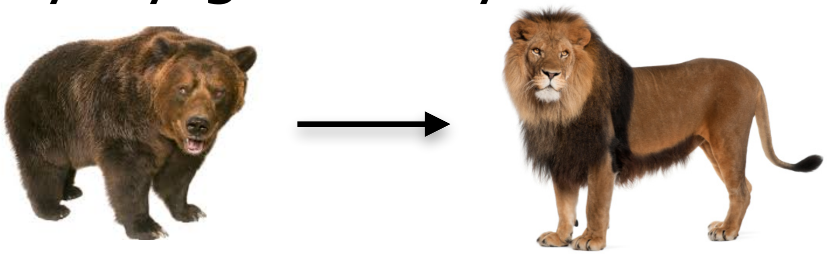
Landmark based: Key feature points are chosen and used to align.



Problem: Choosing landmarks can be hard and expensive and is error prone.

We look at *landmark free* methods.

Landmark free: Alignment determined completely by geometry.

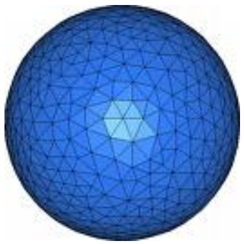


The space of shapes to a geometric topologist

genus 0 genus 1 genus 2 genus 3 genus *k* ...

Need to make precise: *Shape, distance, alignment*.
Appropriate definitions will vary.

GOAL 1: A *metric* on Genus-Zero surfaces




1. $d(C_1, C_2) = 0 \Longleftrightarrow C_1$ is the same as C_2 (Isometry)

2. $d(C_1, C_2) = d(C_2, C_2)$ (Symmetry)

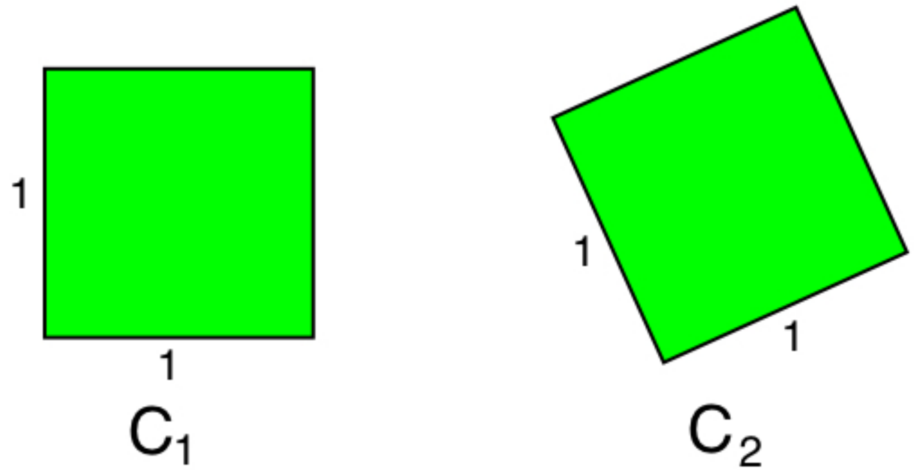
3. $d(C_1, C_3) \leq d(C_1, C_2) + d(C_2, C_3)$ (Triangle inequality)

Why do we want these three properties?

Each plays an important role in applications

Isometry: $d(C_1, C_2) = 0 \Longleftrightarrow C_1$ *is isometric to* C_2

Allows for identifying different views of the same object.



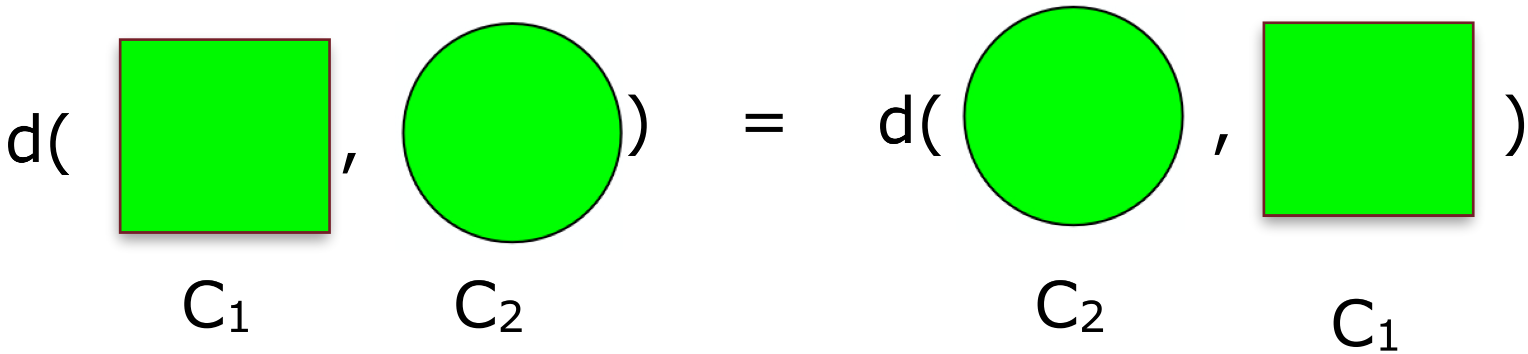
We probably want to consider these to be the same object.

If so, our distance measure should not change if one shape is moved by a rigid motion.

It should not depend on a parametrization.

Symmetry: $d(C_1, C_2) = d(C_2, C_2)$

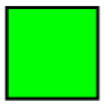
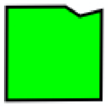
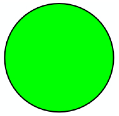
The distance between two objects does not depend on the order in which we find them.

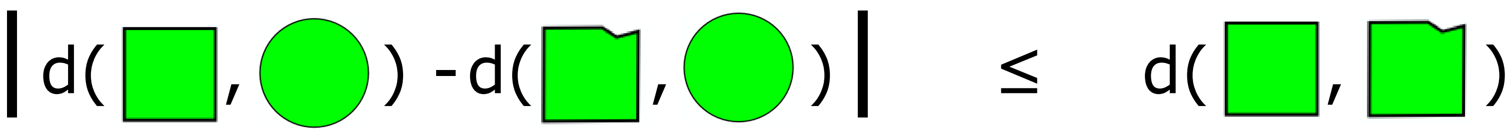


Triangle inequality: $d(C_1, C_3) \leq d(C_1, C_2) + d(C_2, C_3)$

Measurements should be stable under small errors.

$$| d(C_1, C_3) - d(C_2, C_3) | \leq d(C_1, C_2)$$

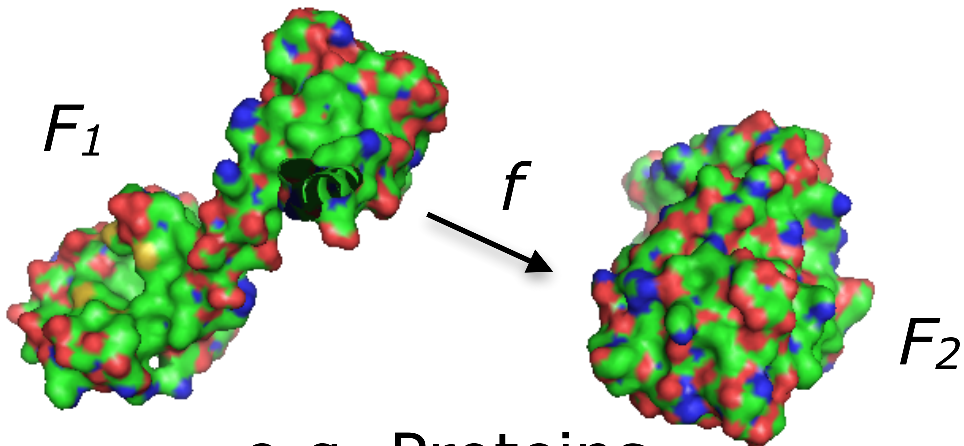
When C_1  *and C_2*  *are close, so that $d(C_1, C_2)$ is small, then the distance of C_1 or C_2 to a third shape C_3*  *is about the same.*



Noise, or small measurement error, does not affect distance measurement very much.

We use *intrinsic* geometry

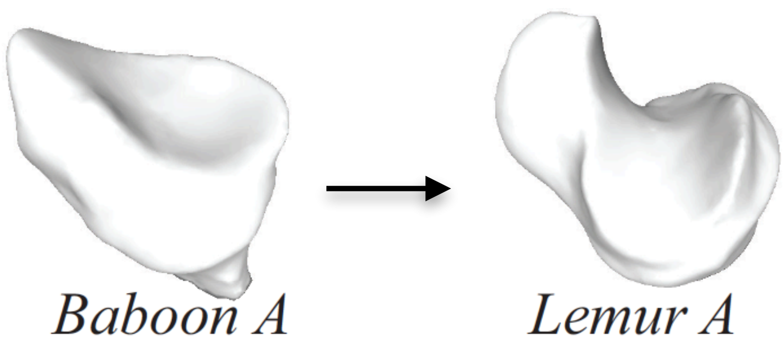
1. Captures similarity between flexible surfaces.



e.g. Proteins

2. As well as between rigid surfaces:

metatarsal bones



Searching among diffeomorphisms

Our technique is to compare two shapes by measuring how much energy it takes to stretch one over the other.

$$S_1 \xrightarrow{f} S_2$$

Searching among diffeomorphisms

We search the space of diffeomorphisms for a map closest to an isometry.

Choosing the best $f: S_1 \rightarrow S_2$ from this infinite-dimensional space is difficult.

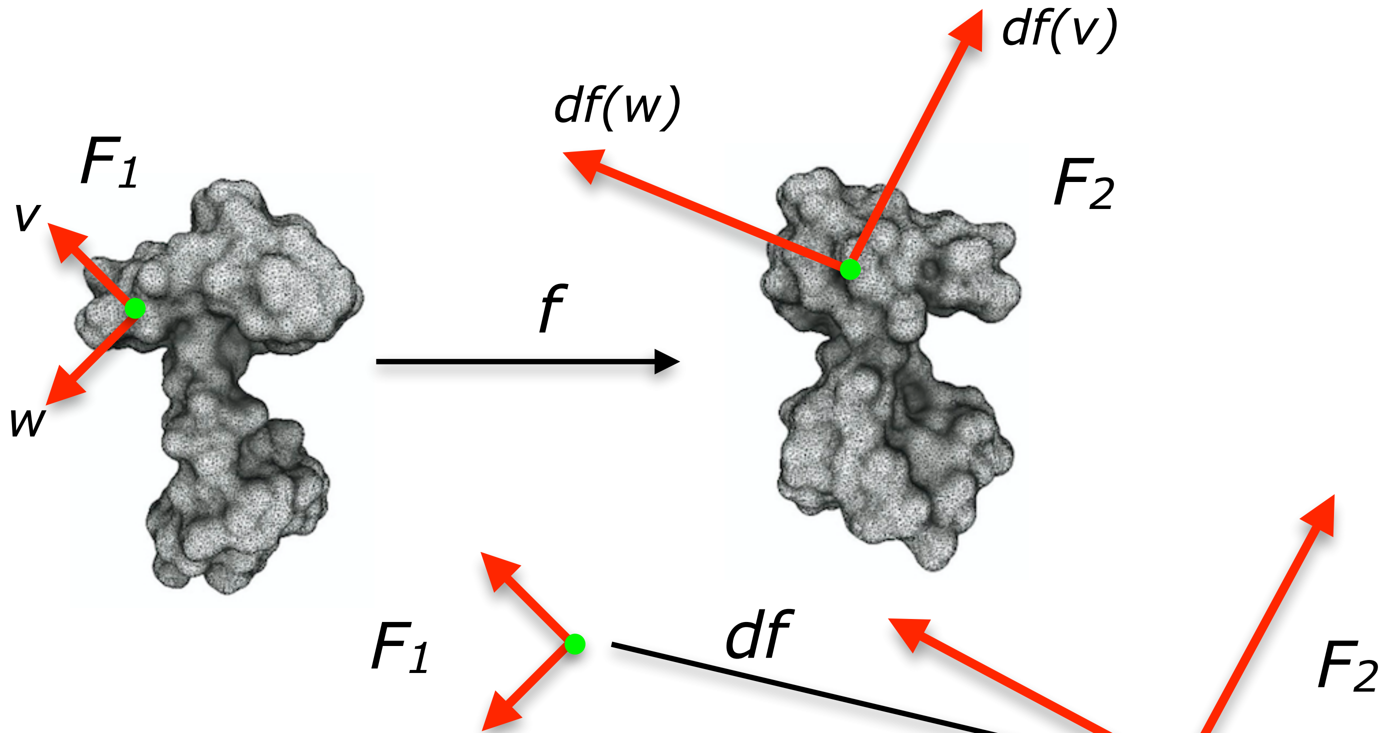
Idea: Restrict the search to *conformal* maps

$$C: S_1 \rightarrow S_2$$

C is chosen from the much smaller space of conformal maps. This is still a big space, but not too big to work with.

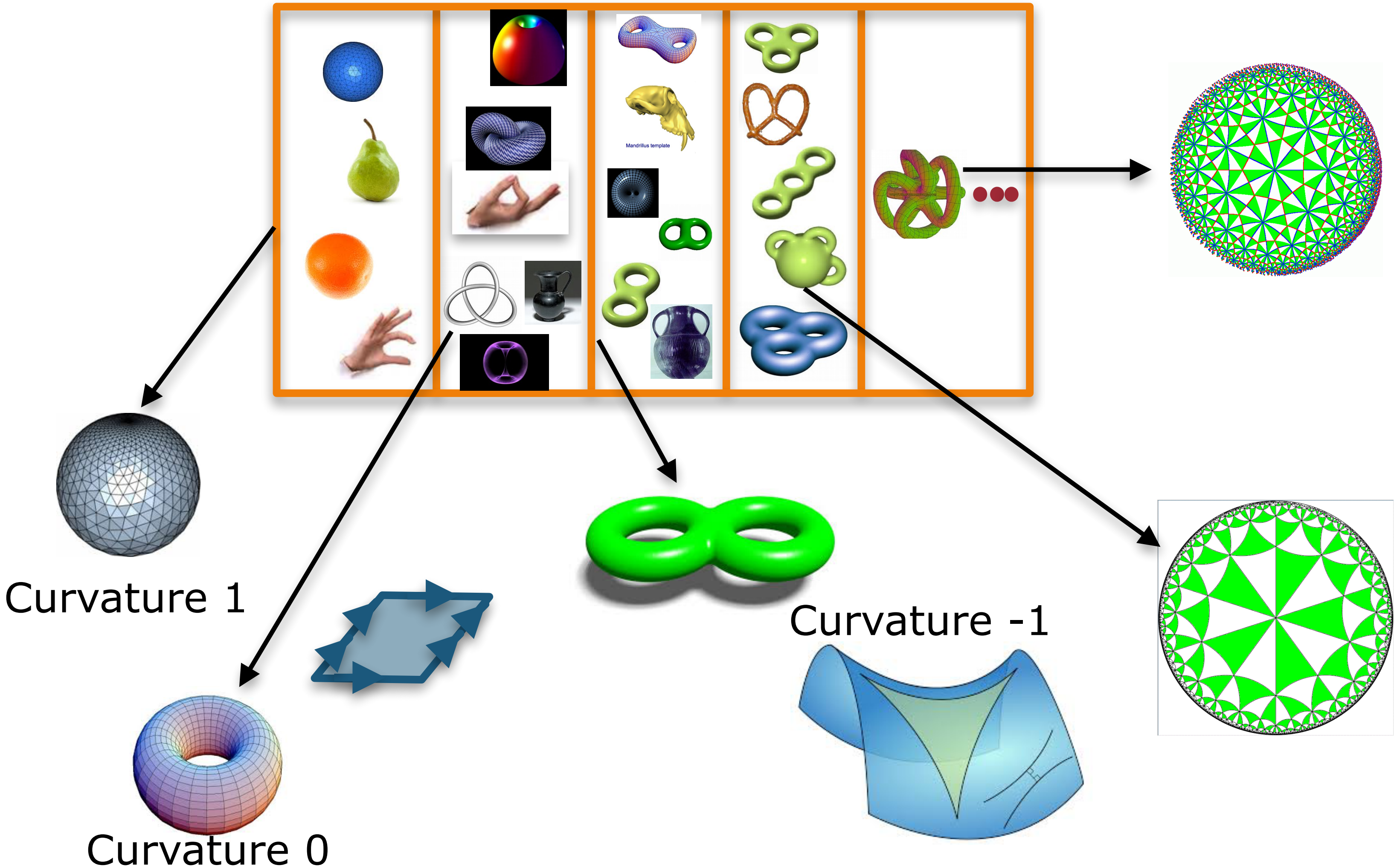
What is a conformal map?

A conformal map f: $F_1 \longrightarrow F_2$ preserves angles.



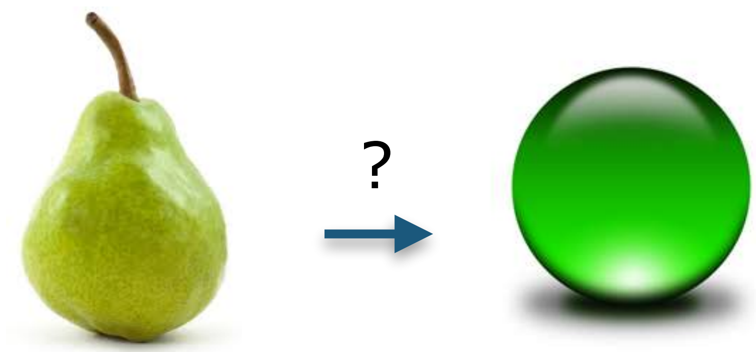
Are there any conformal maps?
What is the *best* conformal map?

Uniformization: Conformal maps exist



These maps are ***conformal***, *or angle preserving.*

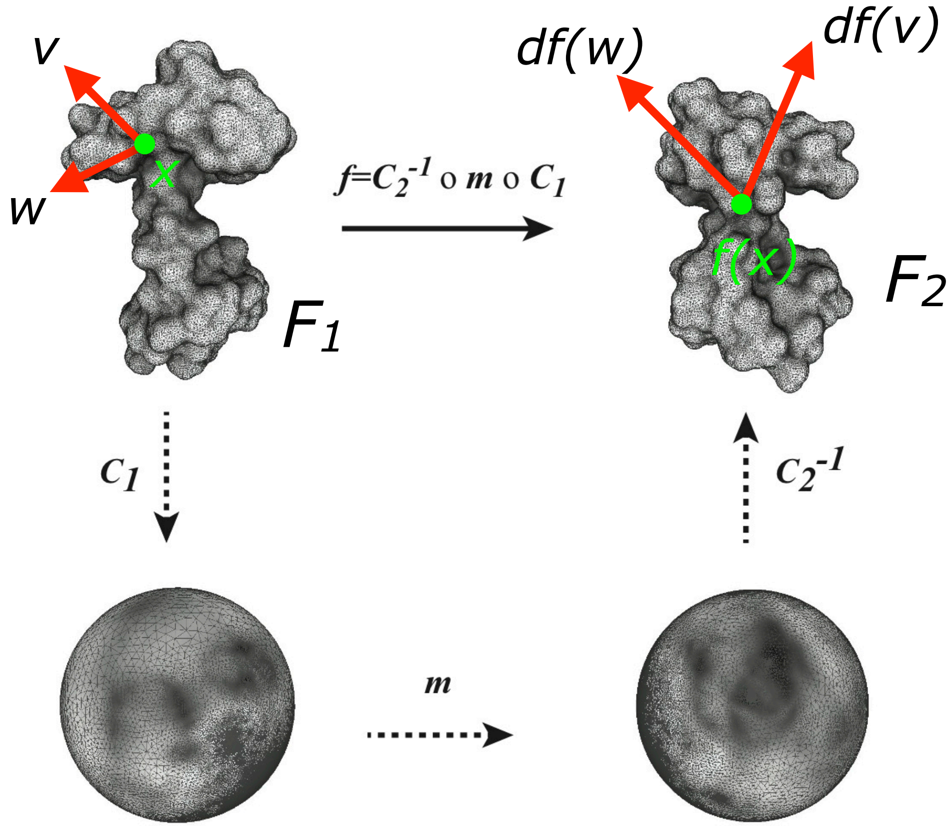
Conformal maps exist in genus 0



For genus zero surfaces, we can *always* find a map that preserves angles.

In fact, we can find many such maps:
a six dimensional family.

What is the *best* conformal map?



How can we choose m to make f closest to an isometry?

f is conformal. At each point x of F_1, f stretches lengths by a conformal factor $\lambda_f(x)$. If $\lambda_f(x)=1$ then f is an isometry. Idea: measure how $\lambda_f(x)$ differs from 1.

Define a measure of stretching

$$\xrightarrow{f}$$

$$E_{sd}(f) = \sqrt{\int_{F_1} (\lambda_f(z) - 1)^2 \, dA_1}$$

Symmetric Distortion Energy

Define a new measure of stretching

Symmetric Distortion energy:

$$E_{sd}(f) \;=\; \sqrt{\int_{F_1} (\lambda_f(z) - 1)^2 \, dA_1}$$

The smallest value among all conformal maps from F_1 to F_2 defines a distance:

Symmetric Distortion distance:

$$d_{sd}(F_1, F_2) := \inf_{f \in \mathcal{C}} E_{sd}(f)$$

A new way of measuring distance between surfaces

$$d_{sd}(F_1, F_2) = \inf_{\text{conformal} f} \{E_{sd}(f) | f : F_1 \to F_2\}$$

Theorem (H-Koehl)

Given two genus-zero surfaces F_1, F_2,

1. There is a conformal diffeomorphism $f : F_1 \to F_2$ with $E_{sd}(f) = d_{sd}$.

2. d_{sd} gives a metric on the space of Riemannian genus-zero surfaces.

Idea of proof: Show that E_{sd} is a proper map on the space of conformal diffeomorphisms ($PSL(2, \mathbb{C})$).

Question: What does d_{sd} tell us about the resemblance of two shapes?
The hope: Sensitive to change in shape. Not sensitive to noise.

A new way of measuring Distance between surfaces

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How useful is d_{sd} for real applications?

From smooth to discrete

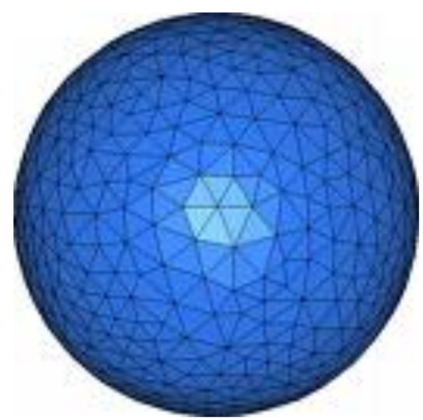
The theory of conformal maps is well developed for *smooth* surfaces.

?

A conformal map exists.

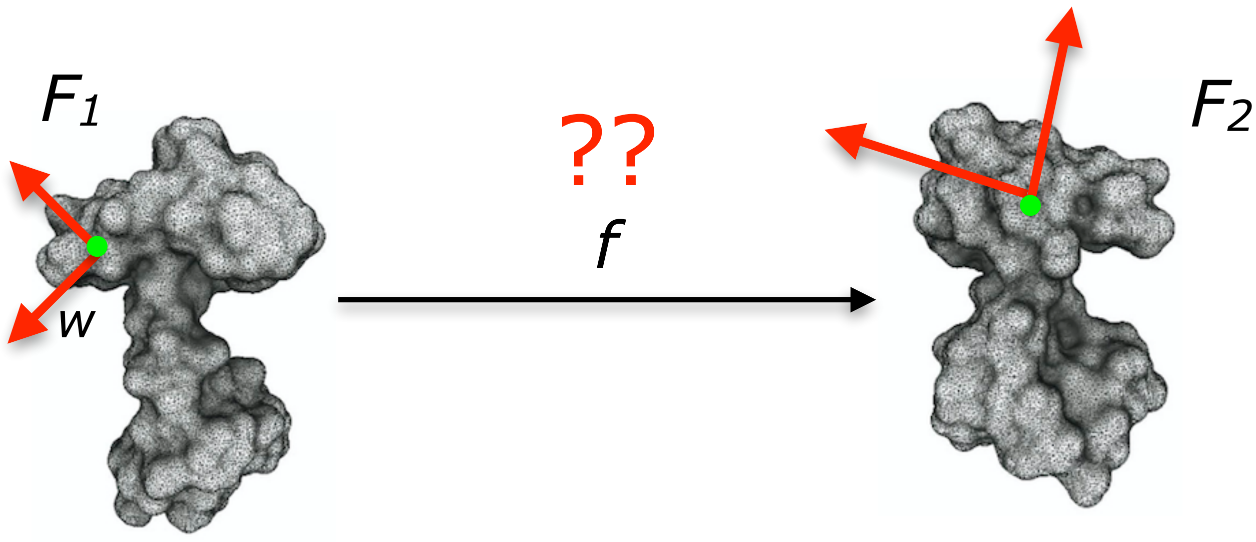
In applications we work with *discrete* surfaces

?



Computing a conformal map

Finding a discrete conformal map $f\colon F_1 \longrightarrow F_2$



What does it mean to say that a map $f\colon F_1 \longrightarrow F_2$ is conformal when the surfaces are triangulated rather than smooth?

How do we compute f?

How unique is f?

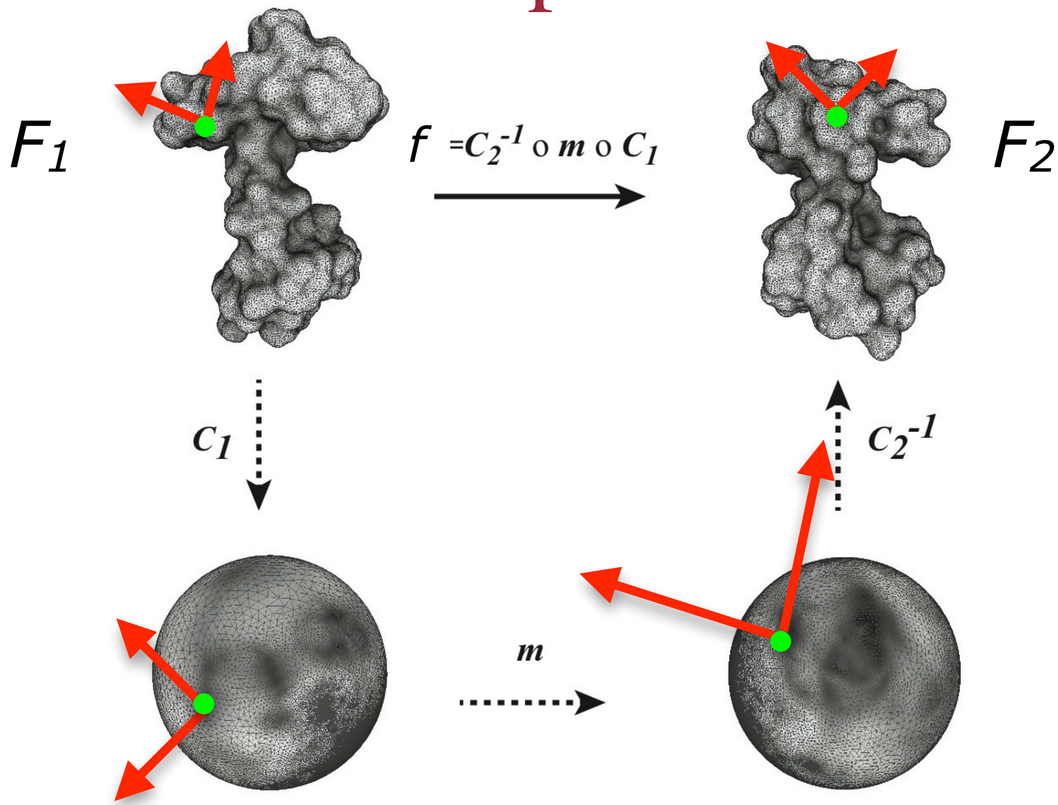
What is a discrete conformal map?

Many definitions and methods exist

1. Discrete Ricci Flow
2. Discrete Yamabe Flow
3. Conformal Mean Curvature Flow
4. Harmonic Maps
5. Finite Elements
6. Optimize a cost function
7. Wilmore Flow
8. Circle Packings

We use definitions and algorithms based on work of Feng Luo, Bobenko, Pinkall, Springborn

How to compute all conformal maps



a. Compute (discrete) conformal maps to the round sphere.
b. Choose a Mobius transformation *m*.
c. Take $f = c_2^{-1}\, m\, c_1$

This gives *all possible* conformal maps. A 6 dimensional family.

Implementing Uniformization

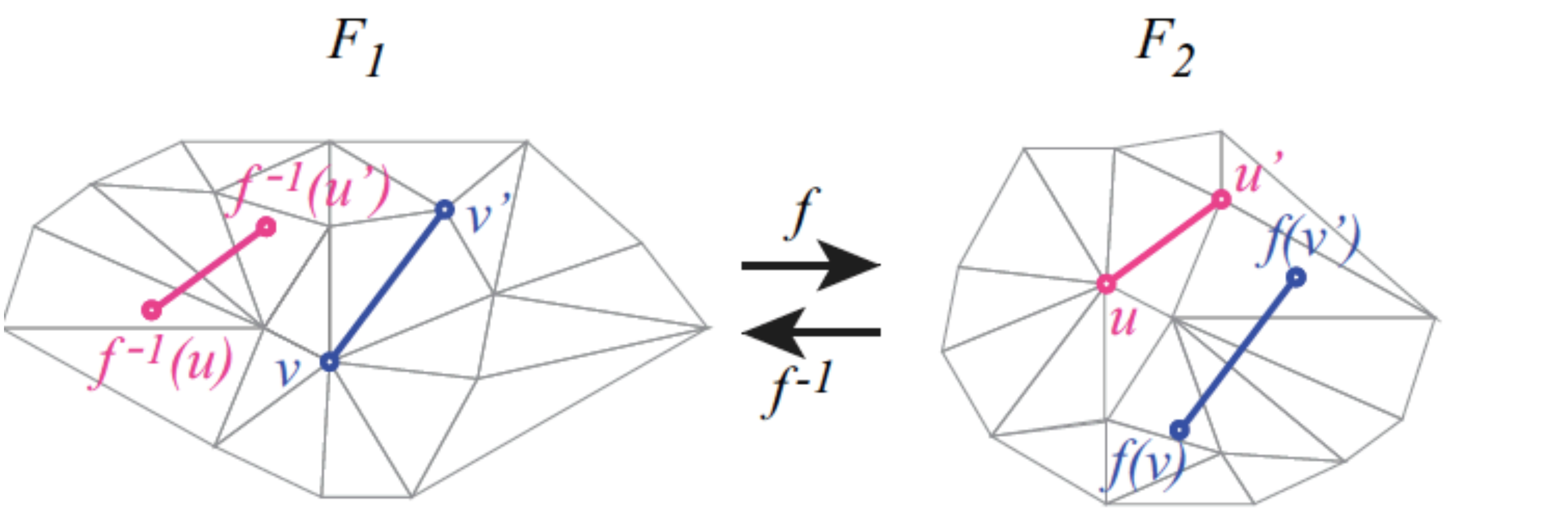
Uniformization: Any genus-zero surface can be mapped conformally to a round sphere.

A variety of discrete conformal mapping algorithms exist.
(Circle packing, Ricci flow, energy minimization …)

Conformal map of a cow (Keenan Crane)

Discrete Version

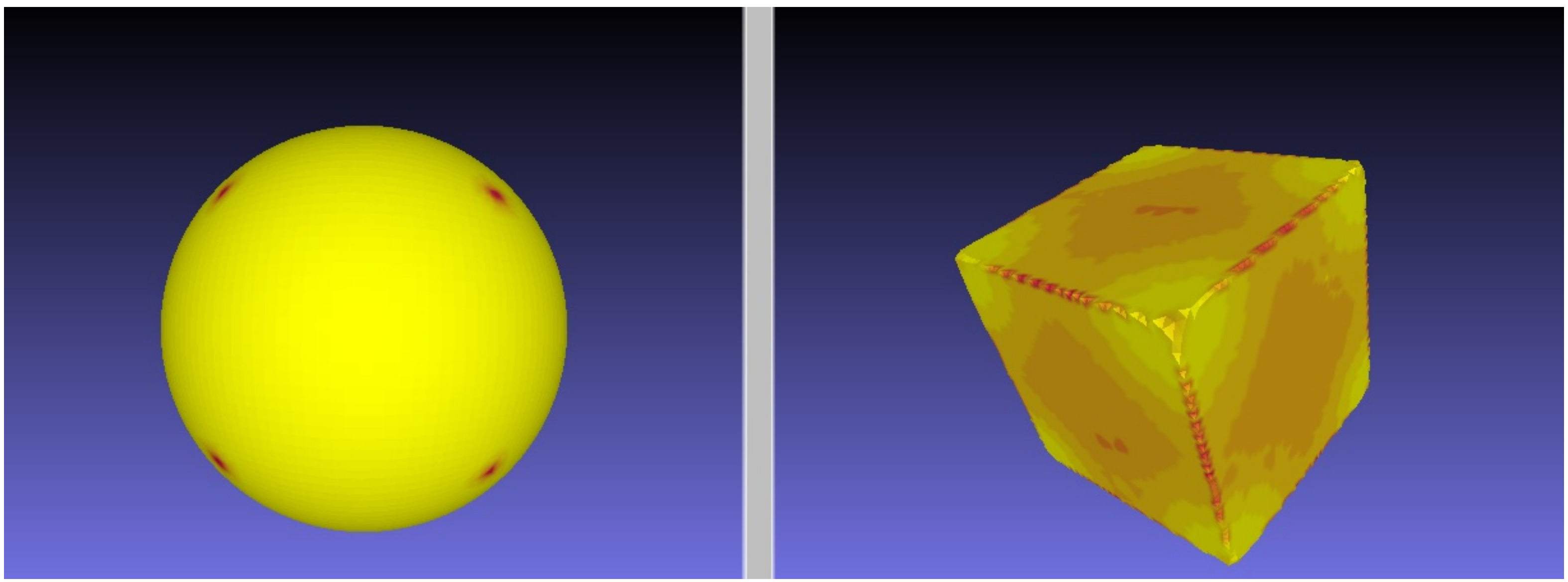
Optimizing the conformal map



$$E_{sd}(f)=\sqrt{\sum_{(v,v')\in F_1}\frac{A_{vv'}}{3}\left(\frac{l\left(f(v),f(v')\right)}{l(v,v')}-1\right)^2}+\sqrt{\sum_{(u,u')\in F_1}\frac{A_{uu'}}{3}\left(\frac{l\left(f^{-1}(u),f^{-1}(u')\right)}{l(u,u')}-1\right)^2}$$

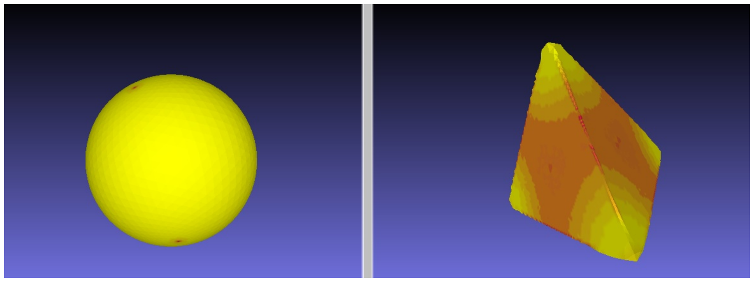
Practice Problem: How Round is an object?

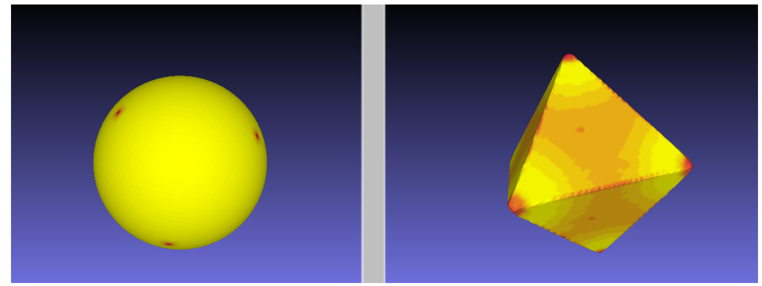
Perhaps the simplest shape question:
How round is an object?
or
How close is an object to a round sphere.

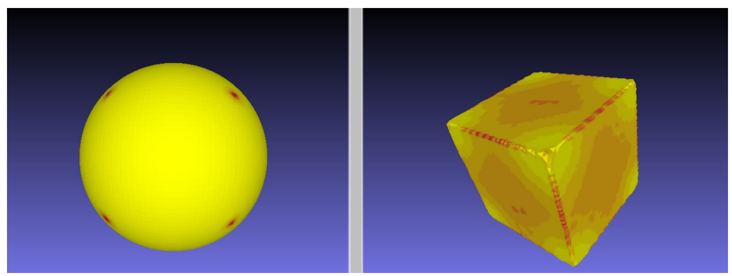


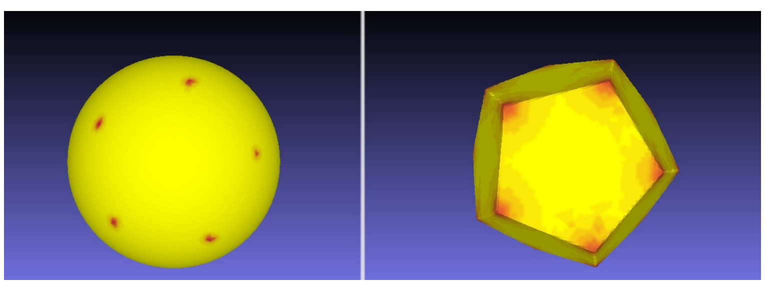
We measure the distance from objects to the round sphere.

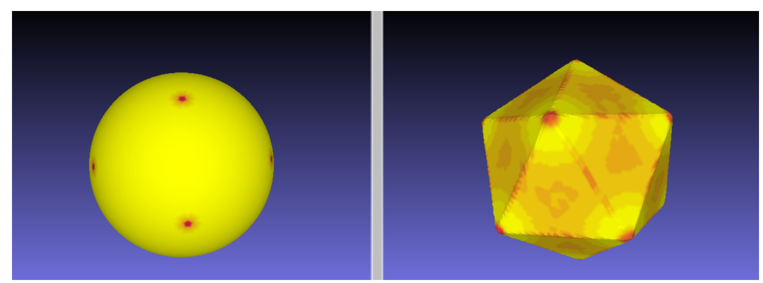
How Round is a Platonic Solid?



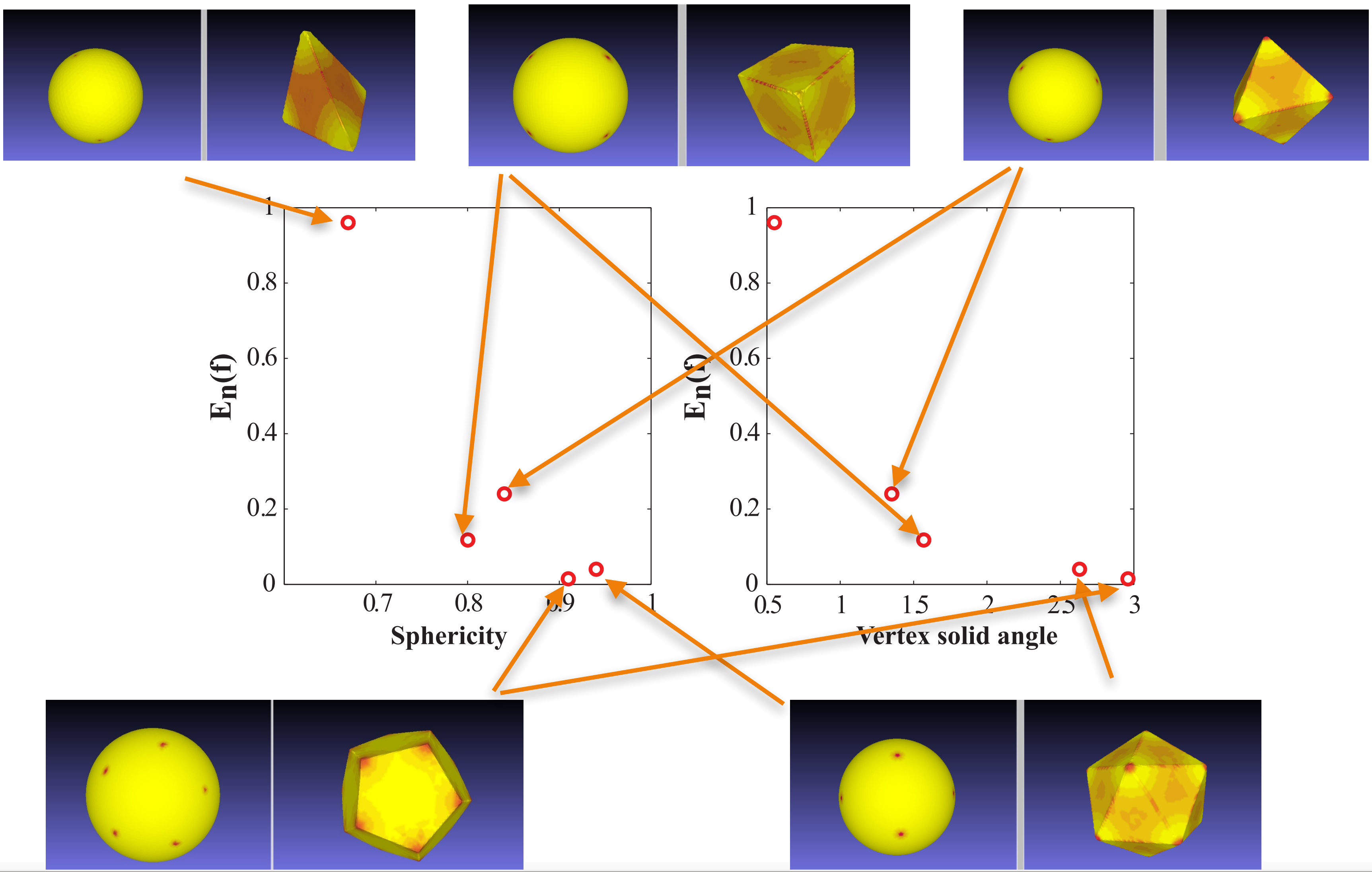




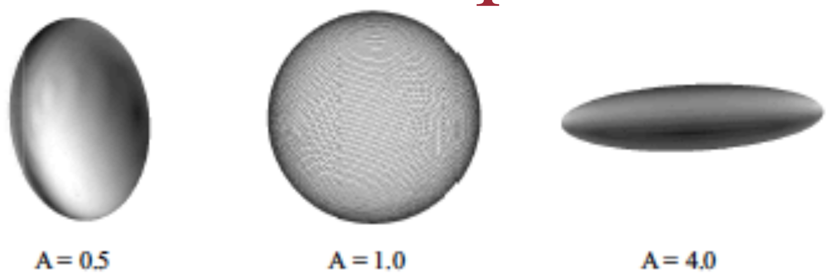




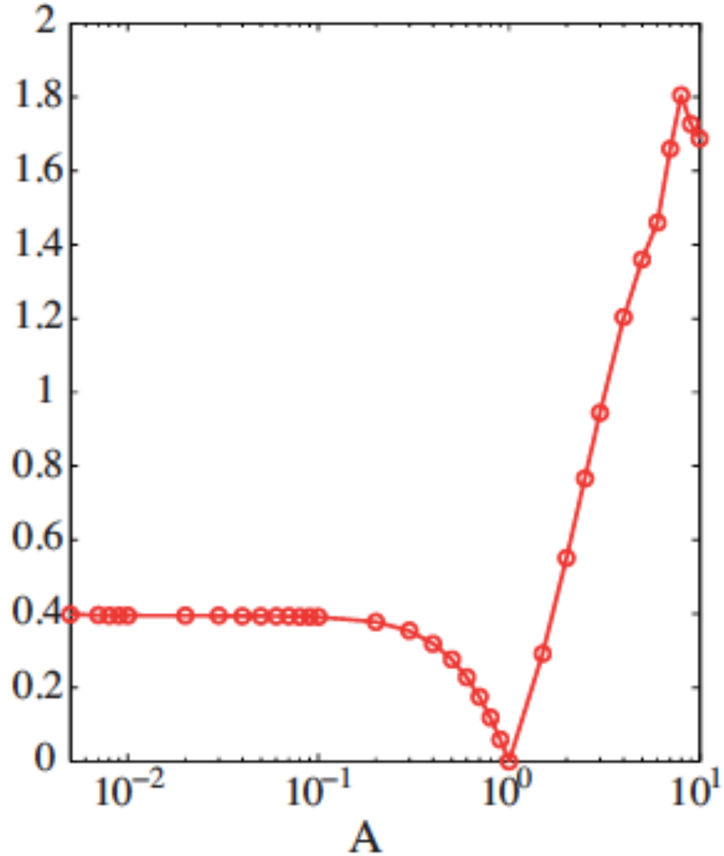
How round are the Platonic Solids?



Experiment: Ellipsoids



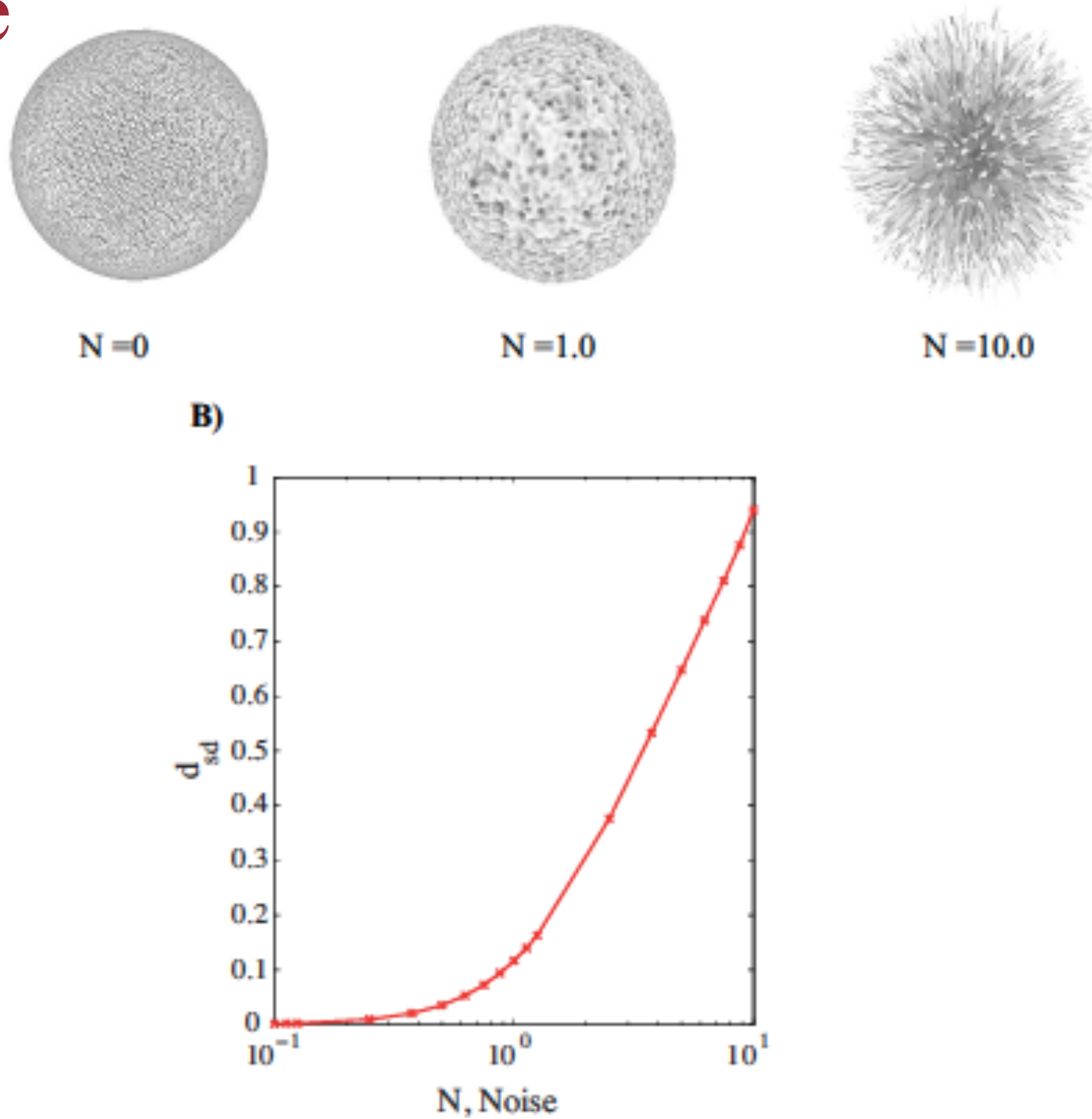
Distance d_{sd}



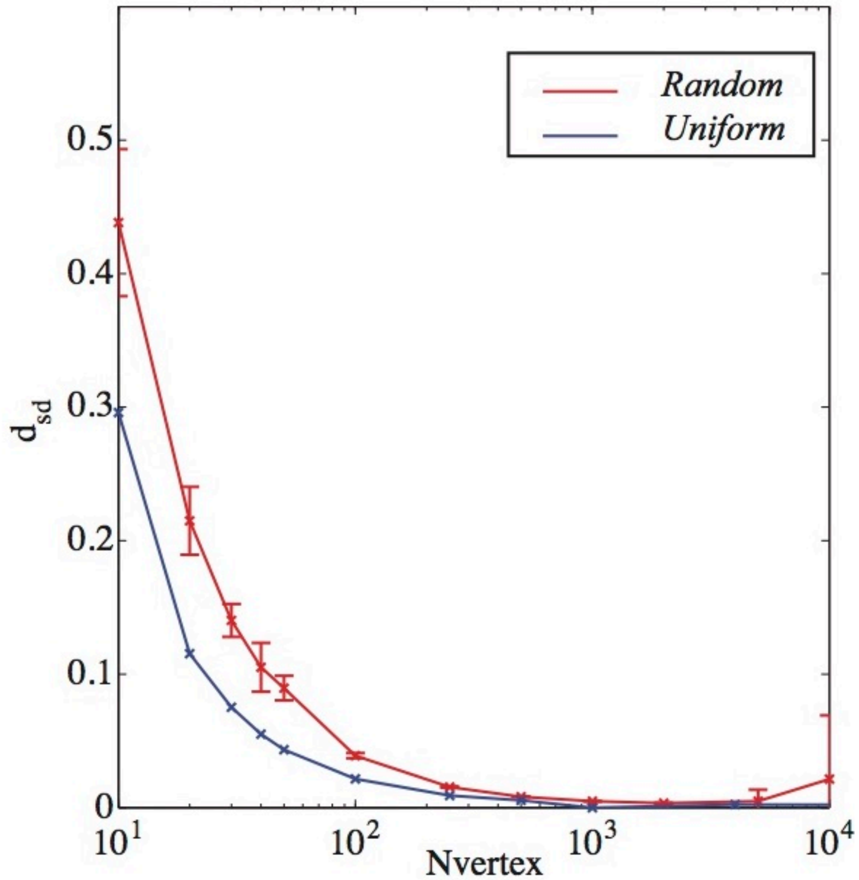
Ellipsoids scaled to have area = 1

A = principle axis

Noise



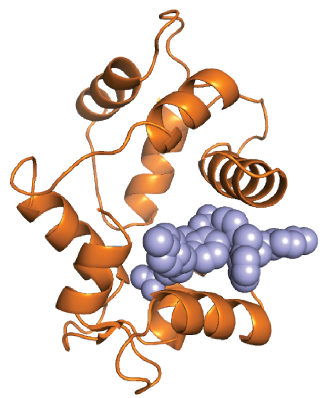
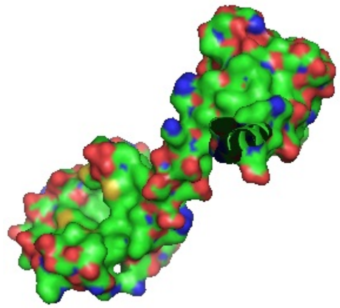
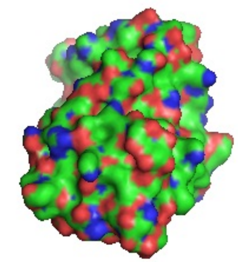
Remeshing - changing triangulations



Distance $d(S_1,S_2)$ where S_1 is a sphere with 1000 uniformly distributed points and S_2 has N vertices, distributed uniformly (blue) or randomly (red).

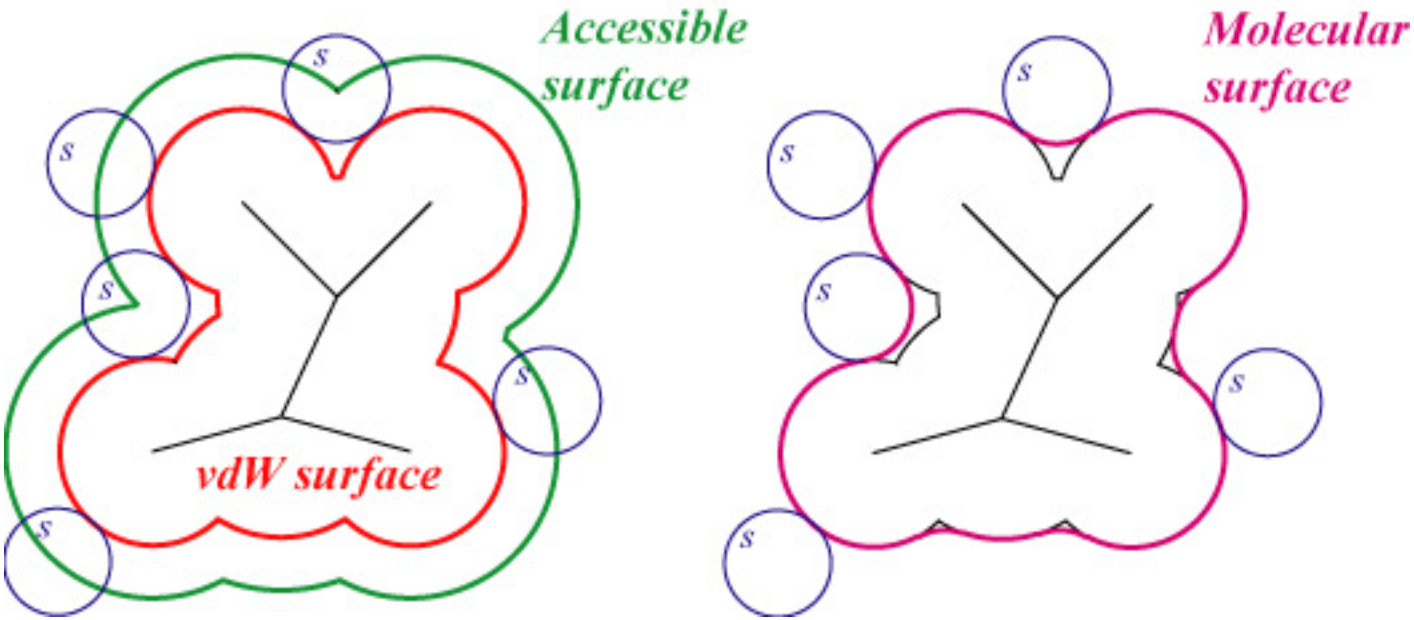
Protein Surfaces

Proteins are complex molecules whose function in biology is largely determined by their shape.

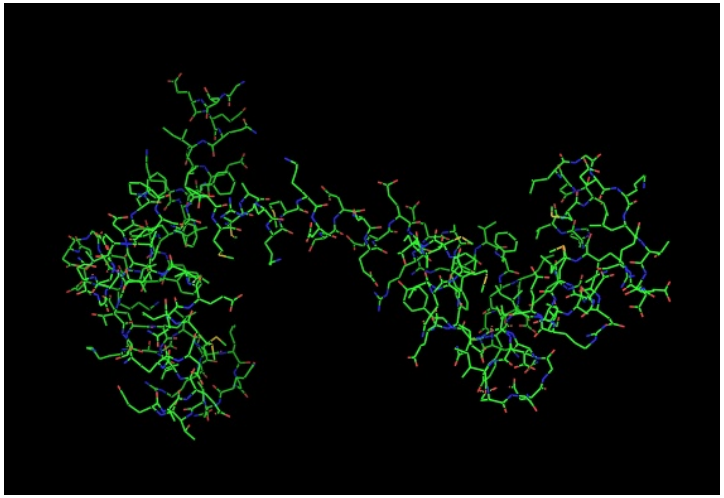
Proteins can be flexible, like the calmodulin protein above. We would like to compare the "surfaces" of two proteins.

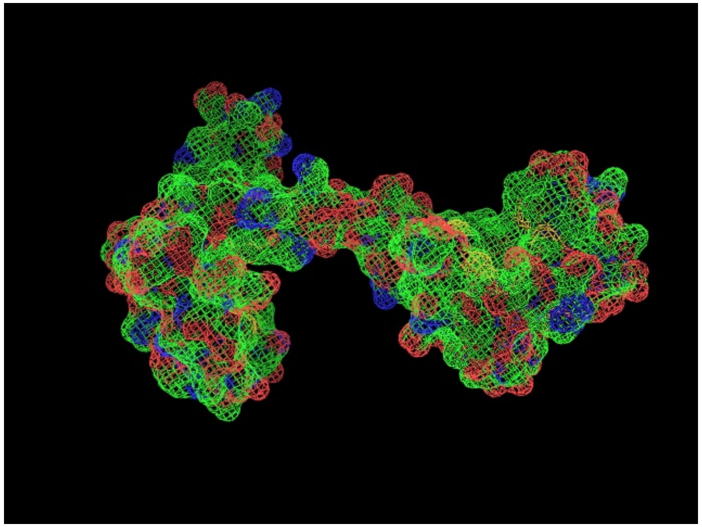
From Protein to Surface



Define a surface that envelops the protein.

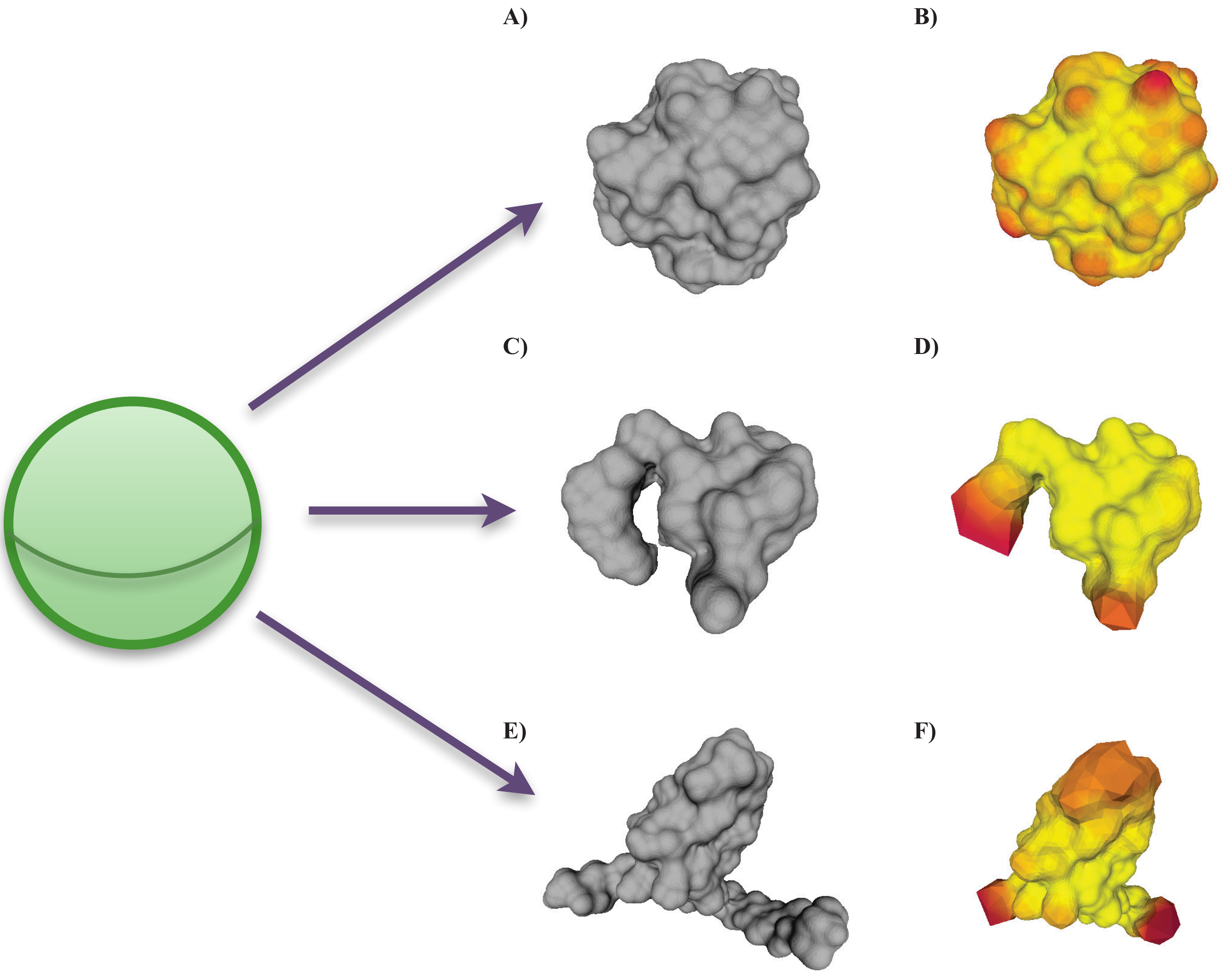
Triangulated Surface from Protein



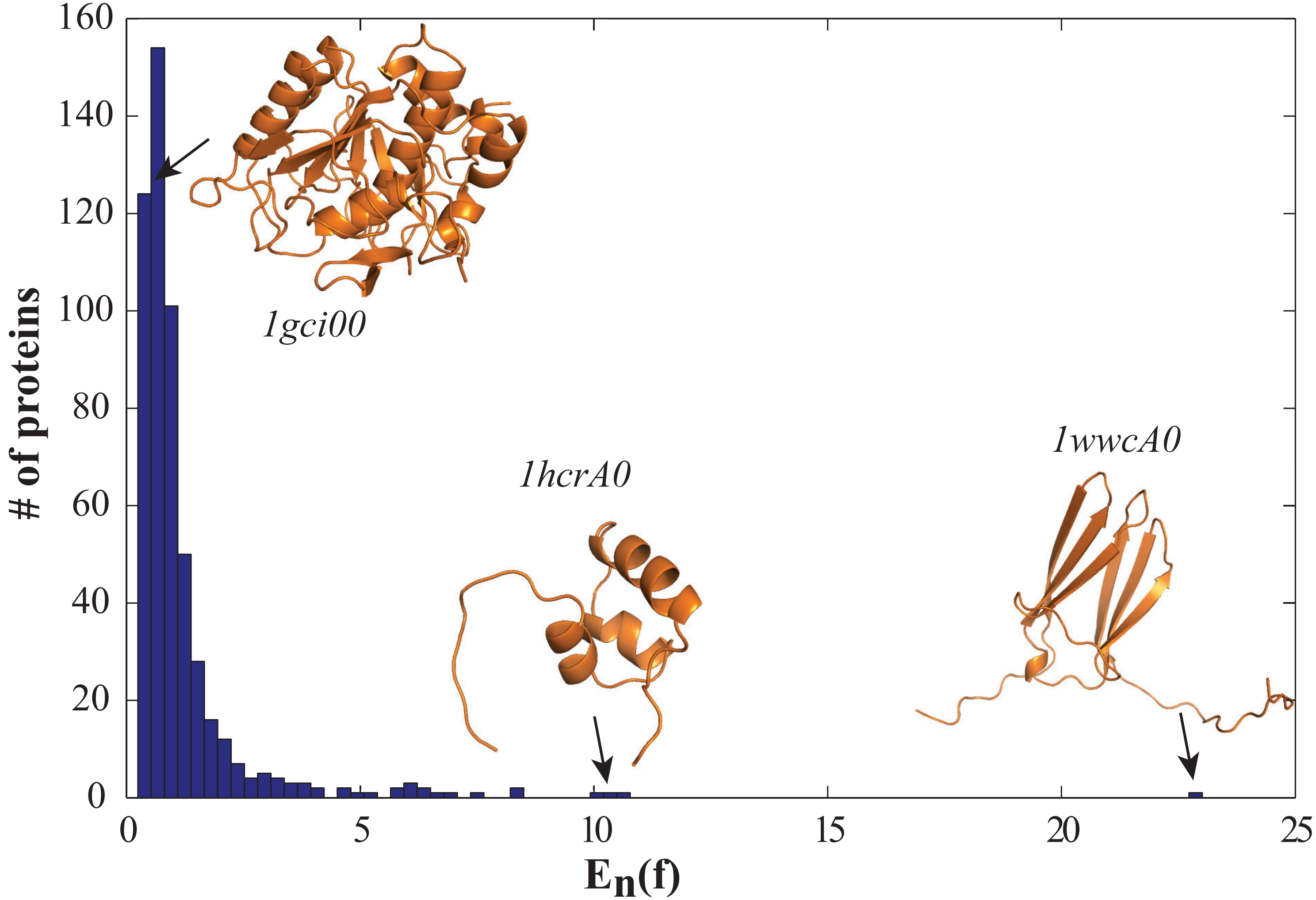


Two representations of a protein, a stick model and a molecular surface model.

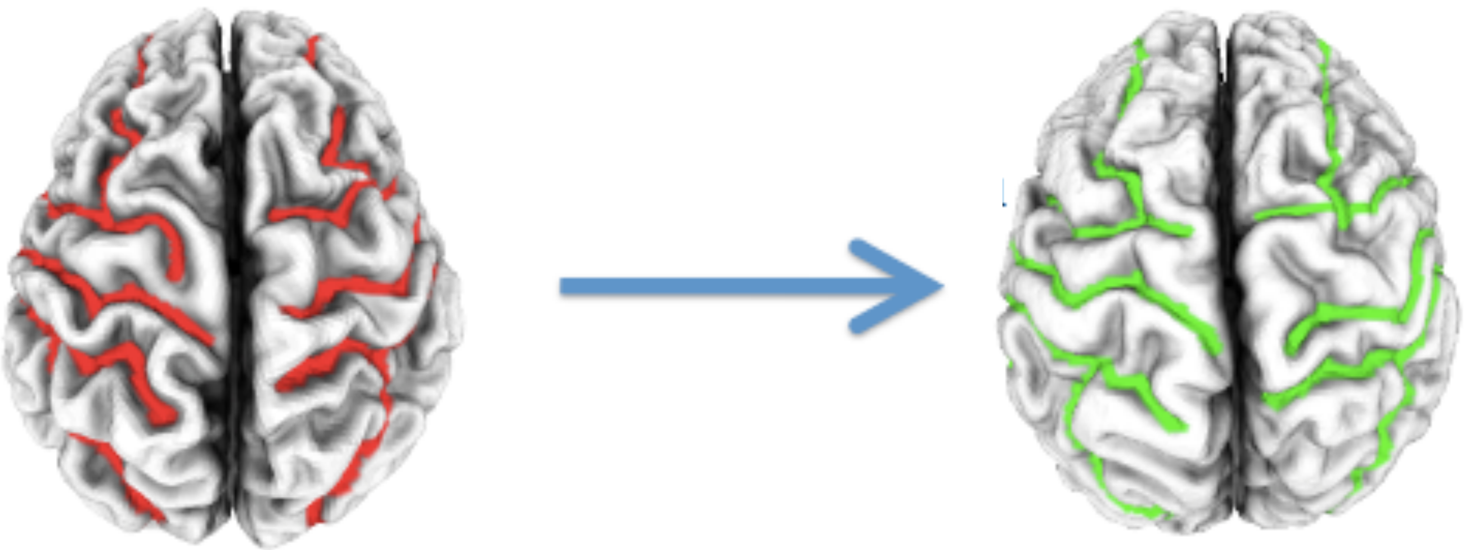
Experiment: How round is a Protein?



Roundness of 533 Proteins

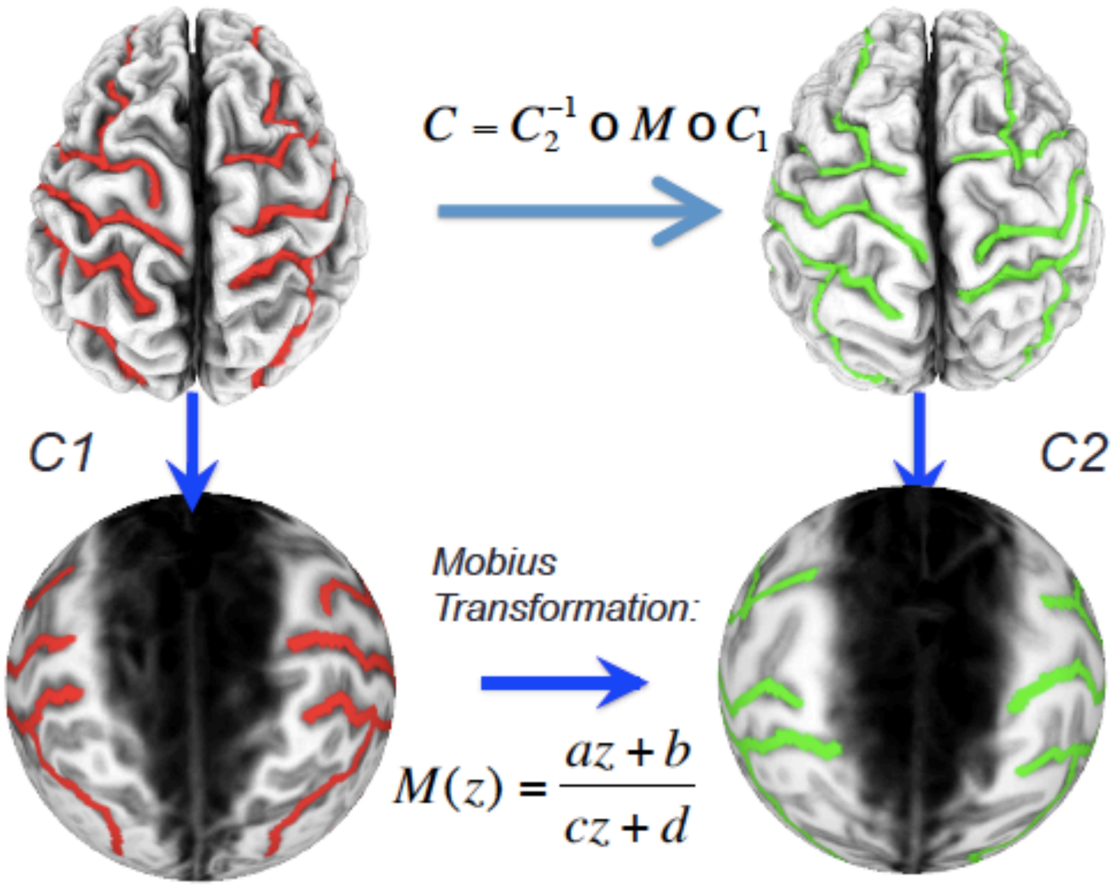


Alignment of a Brain Cortex



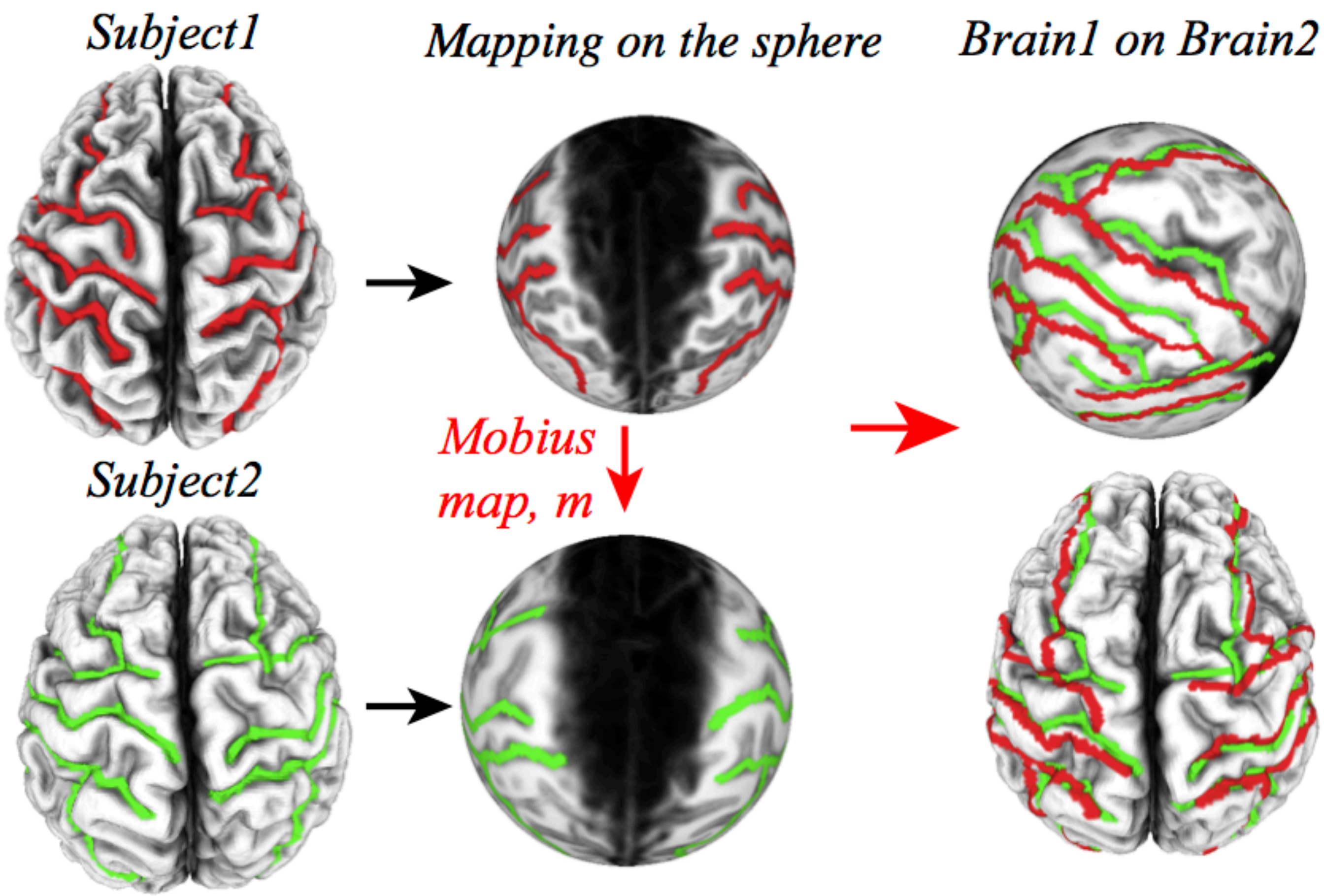
Neuroscientists need to align pairs of brain surfaces, or cortices.

Computing distance between Brain Cortices



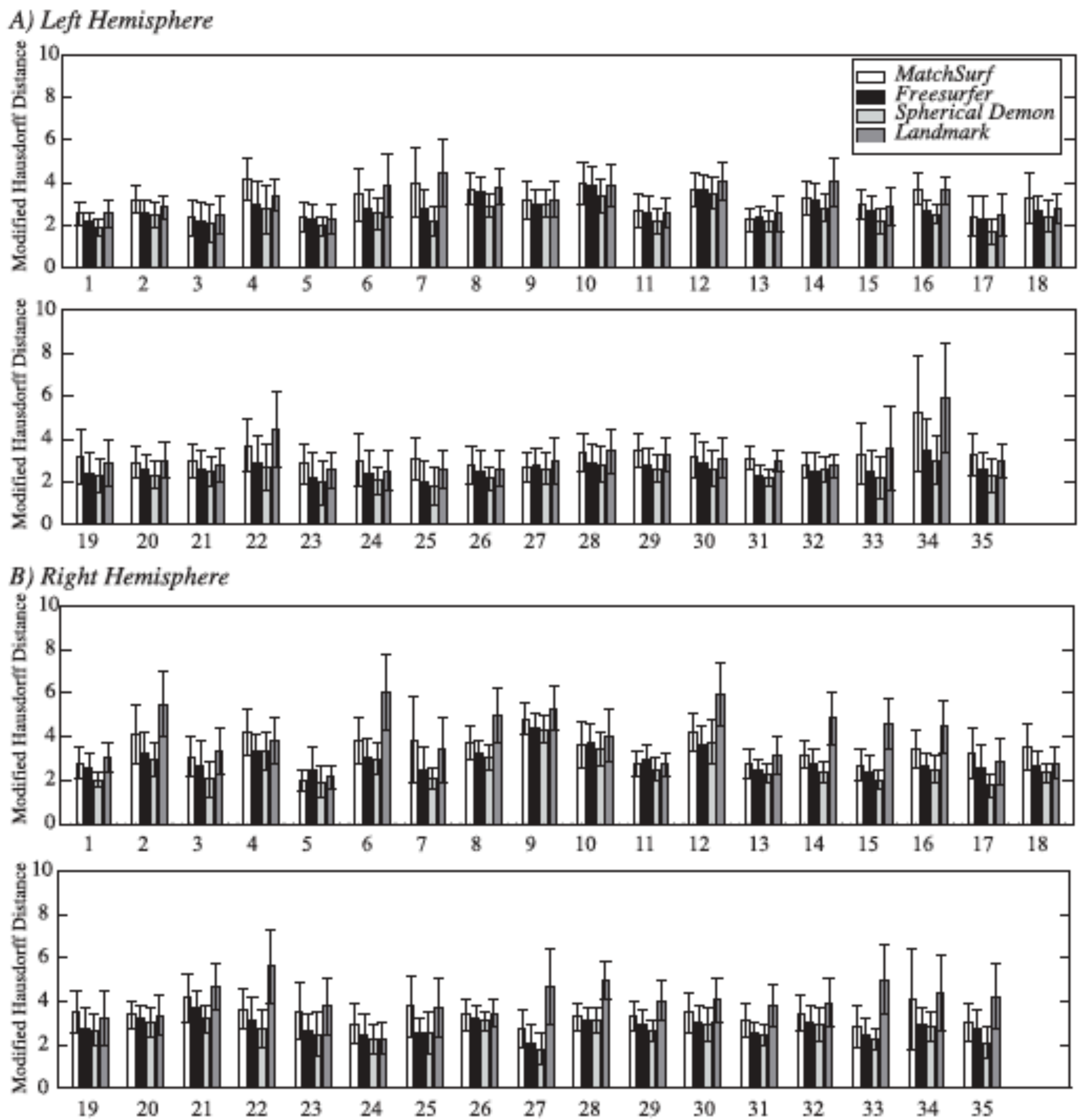
Chose *M* so that *C* minimizes distortion energy among all conformal maps.

How well does this work?



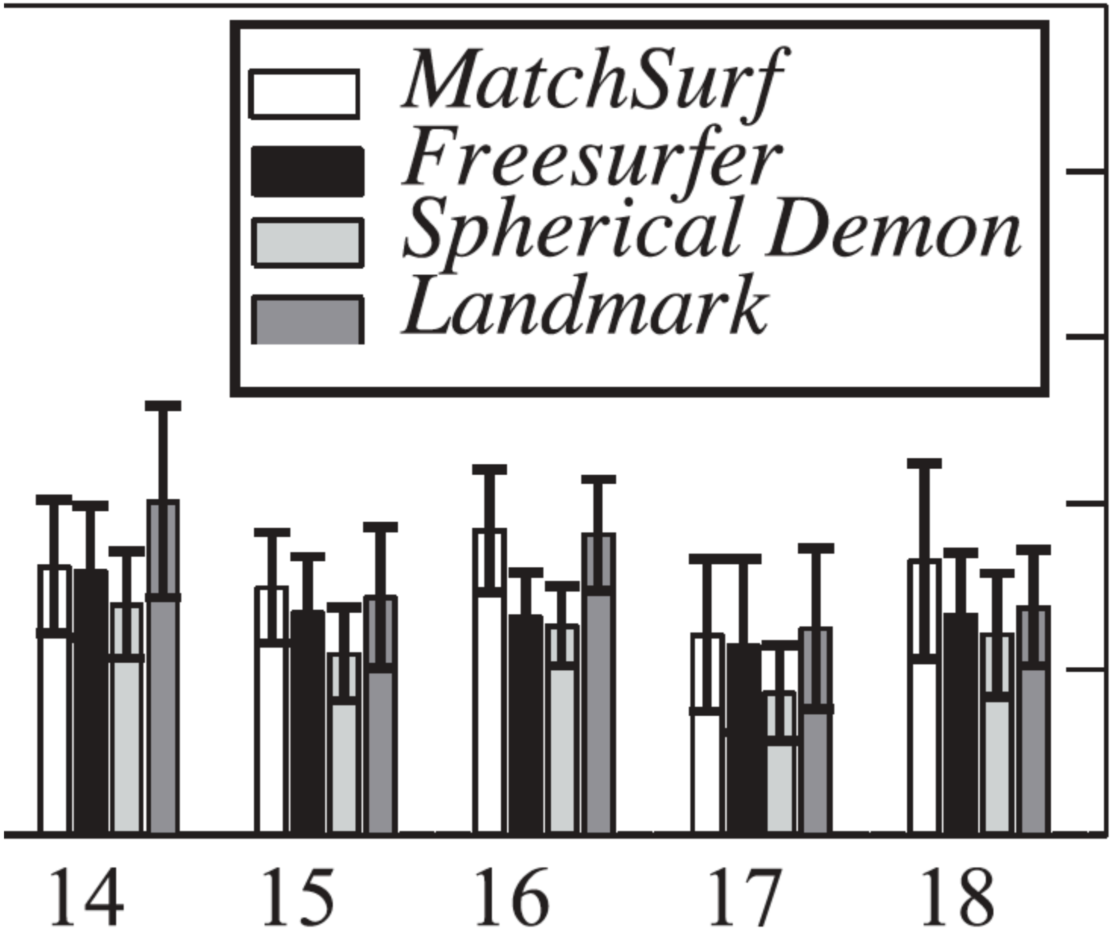
We compute an alignment that minimizes E_{sd}.
It was produced with no human input.

Results



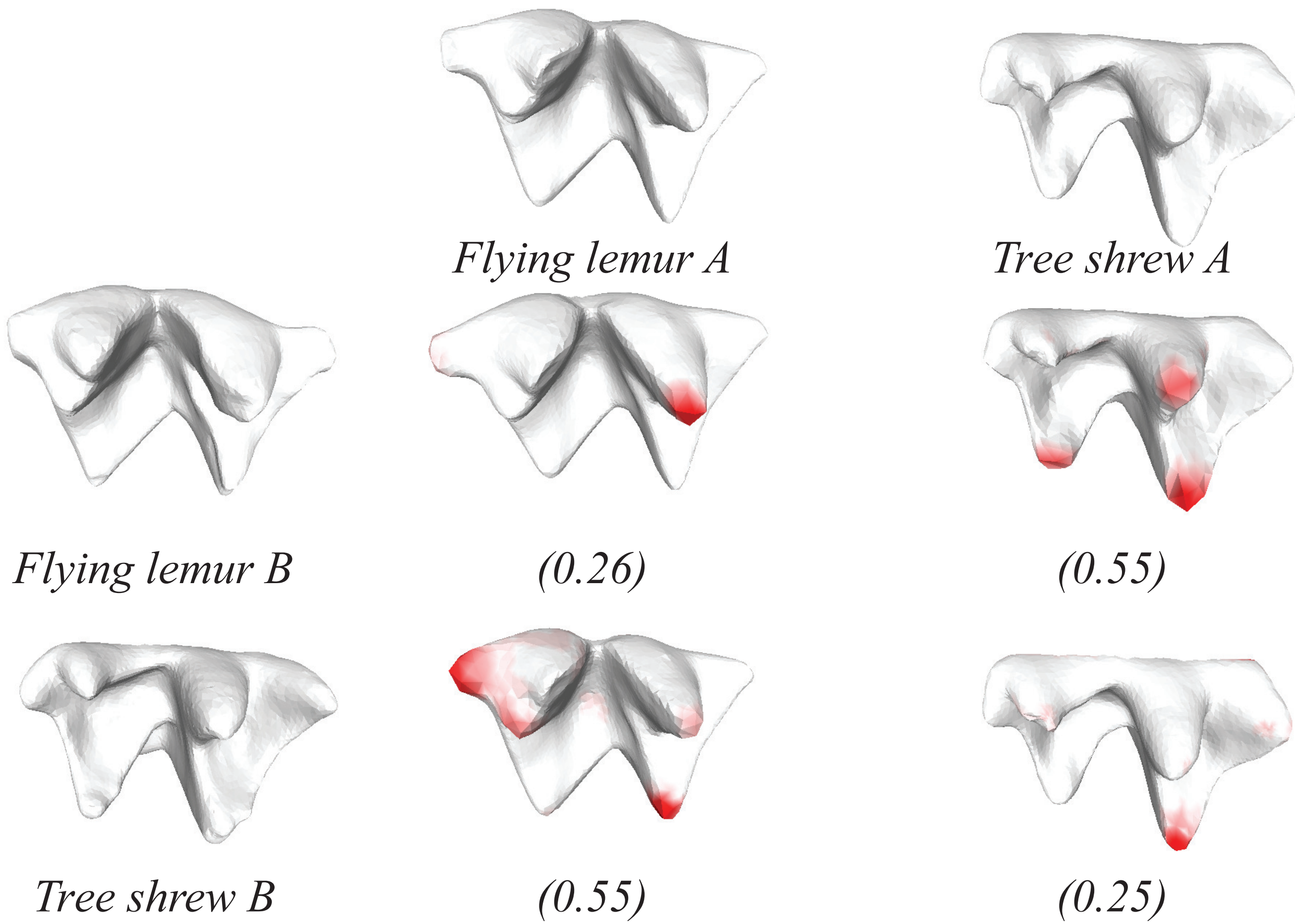
A) Left Hemisphere
B) Right Hemisphere
Modified Hausdorff Distance
MatchSurf
Freesurfer
Spherical Demon
Landmark

Results

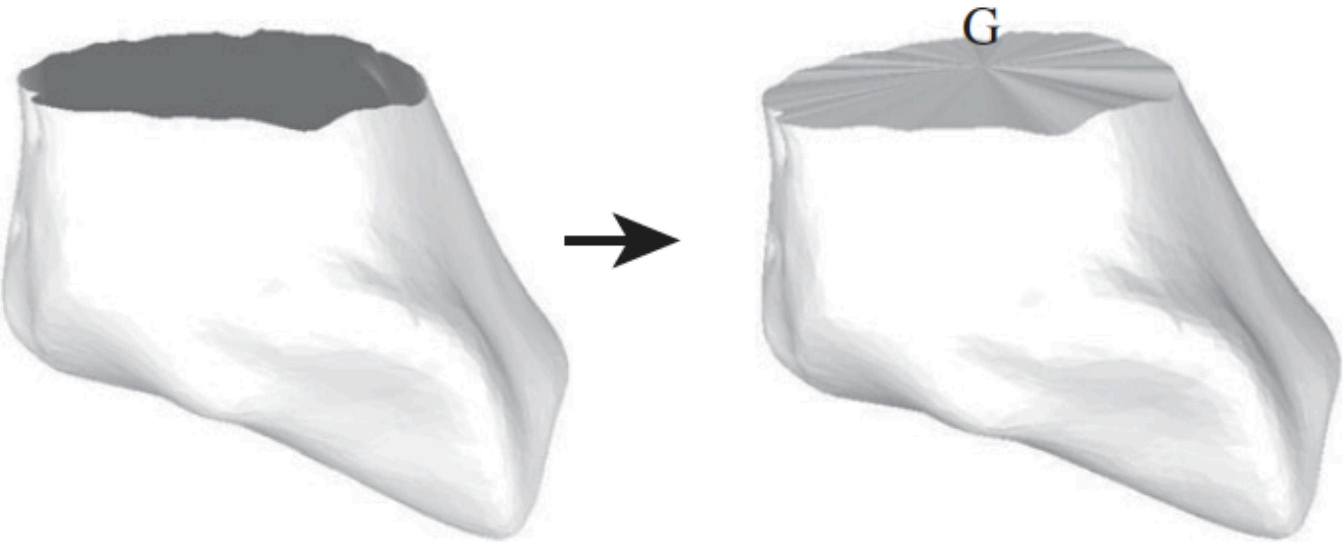


MatchSurf uses no landmarks or human input.
It produces conformal alignments.
Other methods use landmarks and generate non-conformal alignments.

Distance between Teeth

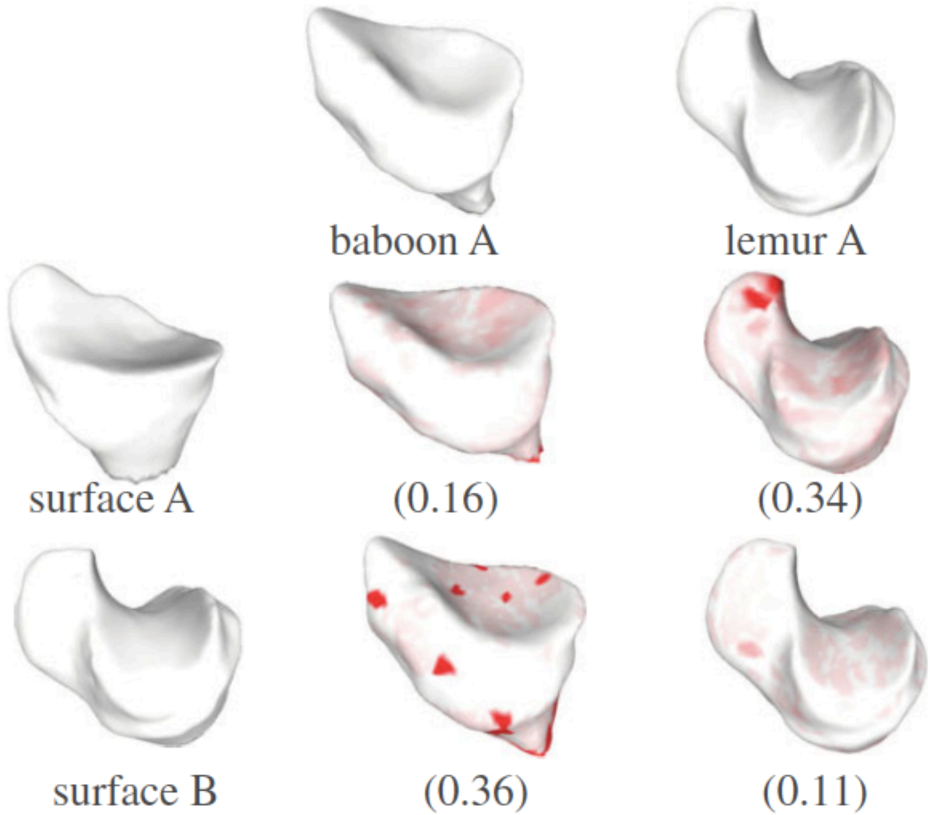


Distance between Arm Bones



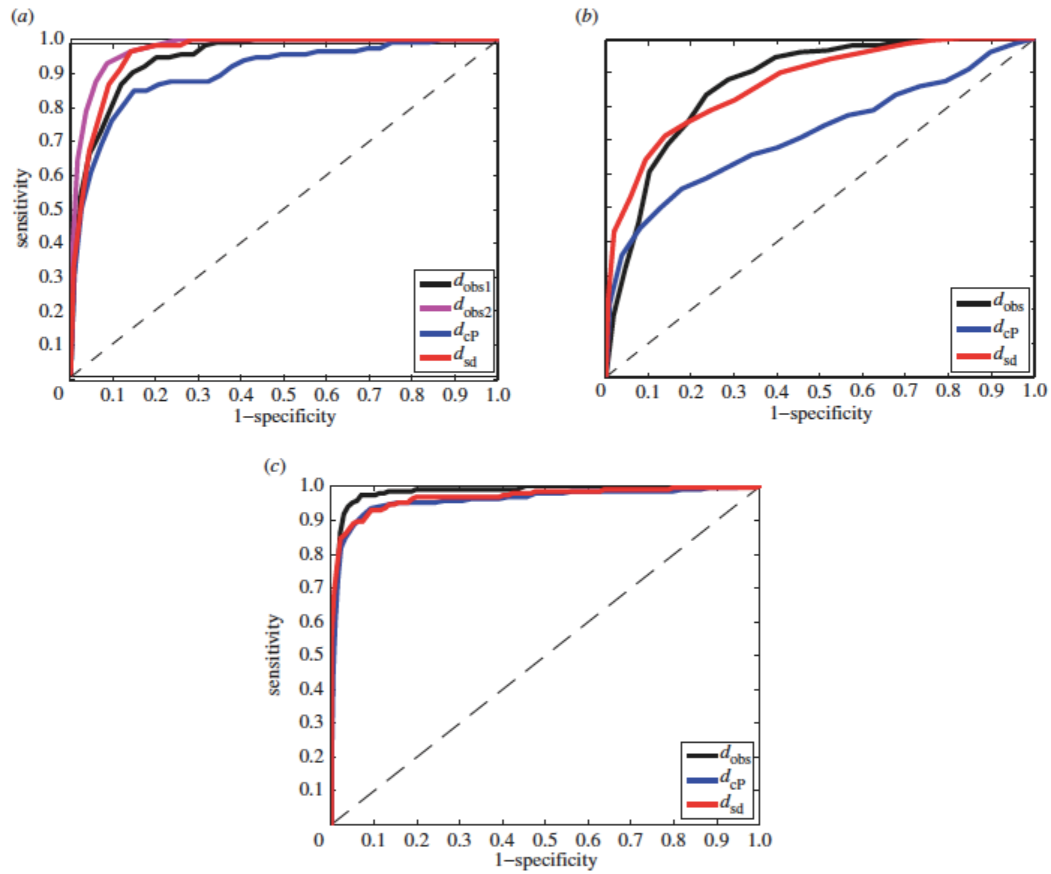
Proximal radius turned from a disk to a sphere.

Distance between Toe Bones



Metatarsal bones of primates

Comparing results

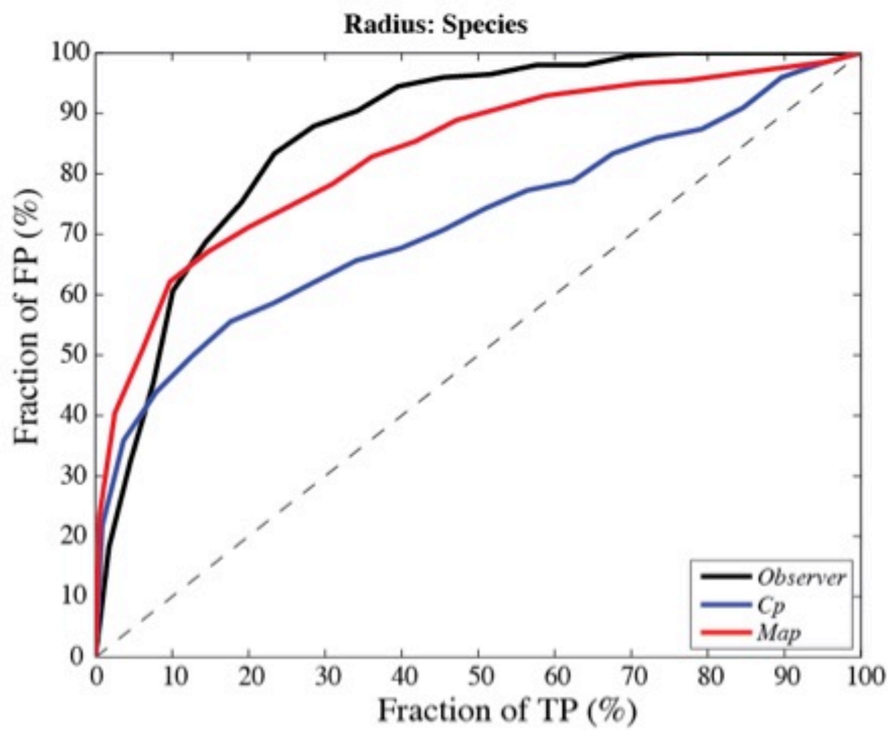


ROC tests on 61 metatarsals, 45 radius surfaces, 99 teeth.
Red is distortion distance, Blue is optimal transport,
Black and Purple are expert observers.

Distal radius

Analysis of anatomical data

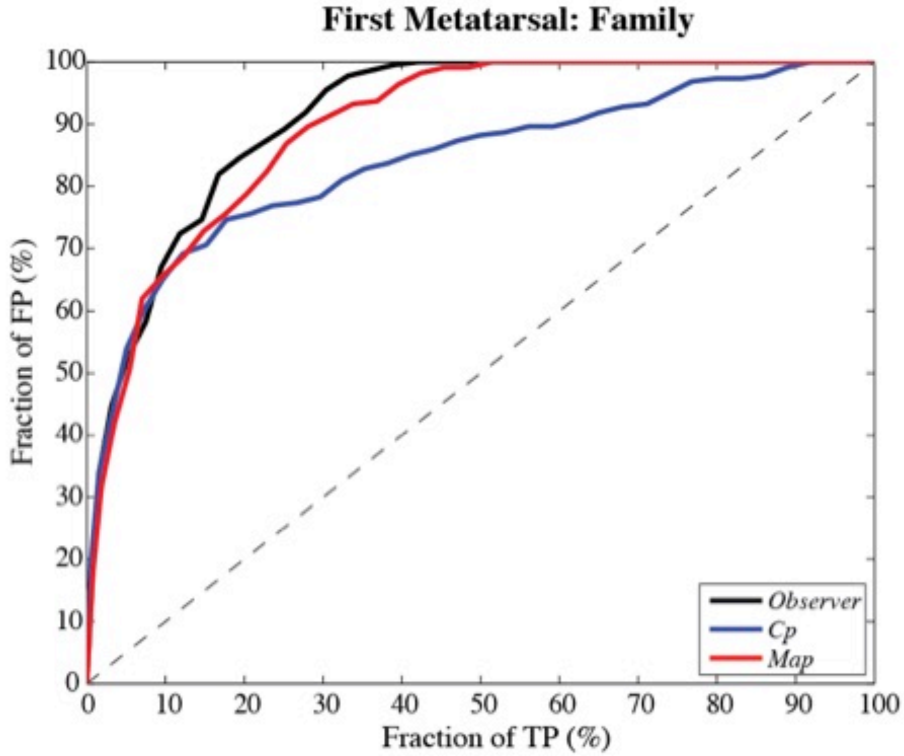
ROC (Receiver Operating Characteristic) Analysis



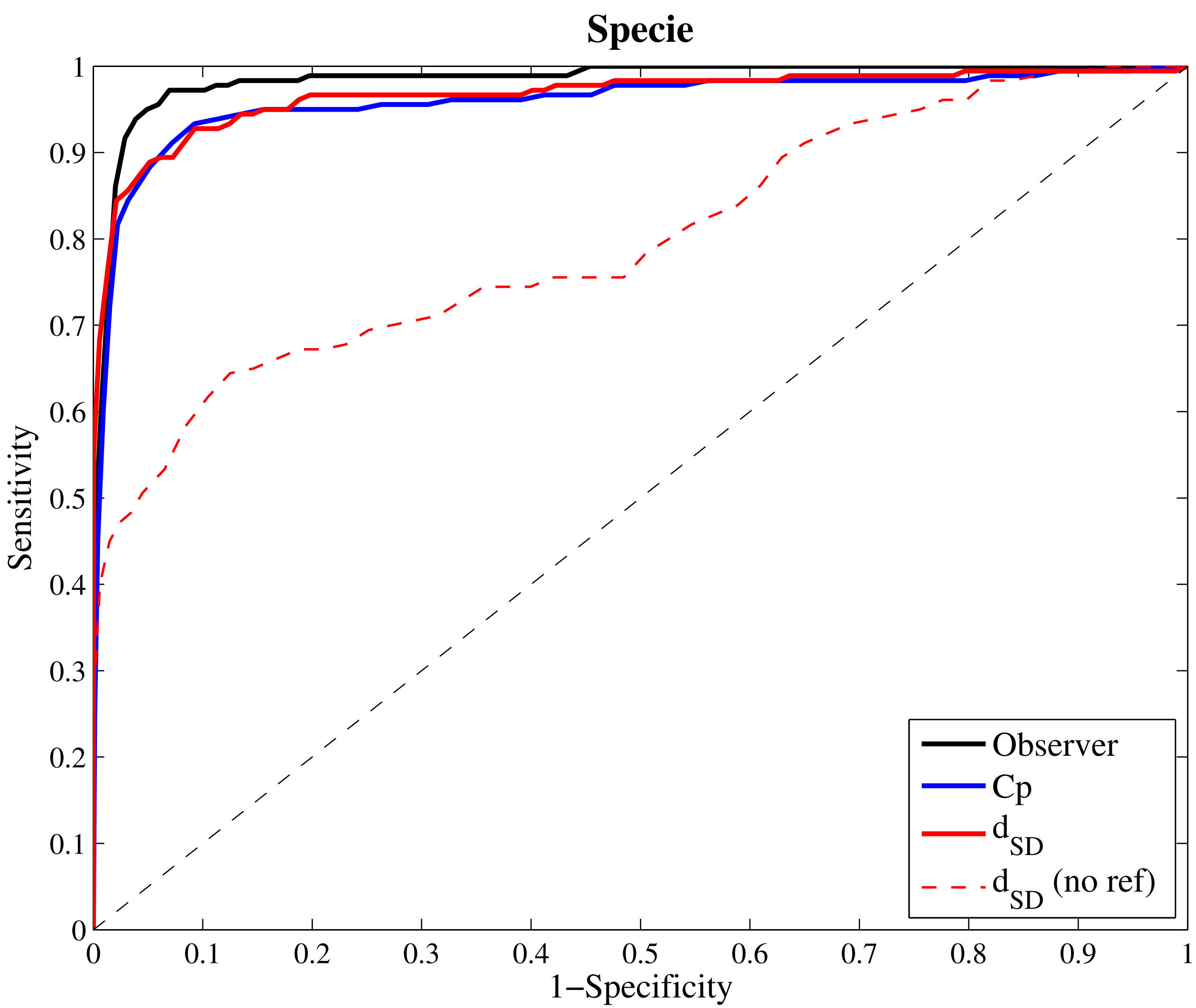
Metatarsal

Analysis of anatomical data

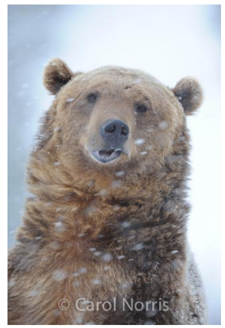
ROC (Receiver Operating Characteristic) Analysis



Teeth


Specie
Sensitivity
1−Specificity
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Observer
Cp
d_{SD}
d_{SD} (no ref)

Thanks for coming!



1. P. Koehl and J. Hass, *Landmark-free geometric methods in biological shape analysis,* J. Royal Society Interface (2015).
2. J. Hass and P. Koehl, *Comparing shapes of genus-zero surfaces,* J. Applied and Computational Topology (2017).

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