Why Compare Surfaces?

1. Every object we see is a surface (almost).

2. Cell phone software can already digitize surfaces. Scanners soon to be built in.

3. Can we recognize this digitized data?

4. Countless applications:
 Diagnose disease or fracture Radiologists
 Drug design Pharmaceutical costs
 Recognize bones and fossils Anthropologists

Today

- 1. Look at one surface comparison algorithm.
- 2. Apply it to some biological data.



3. Analyze how well it does compared to human experts.



Comparing Surfaces

Problem: How to compare two surfaces?

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

2. What is a good alignment between two surfaces?

Find a good diffeomorphism $f:S_1 \longrightarrow S_2$



Optimal Diffeomorphisms

We want to compare two surfaces by finding an *optimal diffeomorphism* between them.



If the surfaces have identical geometry then the optimal diffeomorphism is given by an isometry.

But what if they have different geometries? What map is *closest* to being an isometry?

Optimal Diffeomorphisms

Optimal diffeomorphisms do more than give a distance. They also give a *correspondence*.



Riemannian metrics

In the smooth setting, a geometry on a surface *S* is described by a Riemannian metric *g*.

This is an inner product on vectors at each point of *S*. The inner product is used to describe lengths of paths, angles between vectors, and distance between points.

g: TS x TS \longrightarrow R is a Riemannian metric $\langle v, w \rangle = g(v,w)$

Discrete metrics

In the PL setting, a geometry on a surface *S* is described by a triangulation with an edge length function. A PL metric assigns lengths to each edge of a triangulation.



Isometries

Two surfaces are "the same" if there is an isometry between them.



f is an isometry

How can we find a good correspondence when the surfaces are *not* isometric?



h is not an isometry

Intrinsic versus Extrinsic Isometries preserve *intrinsic* geometry



These 9 surfaces have the same intrinsic geometry.

Approximating Isometries

Neither of these maps is an isometry. Can we deform them to become isometries?



If not, can we deform them to something having some properties of an isometry?

Diffeomorphisms Diffeomorphisms are maps *f* such that *f* and *f*⁻¹ are smooth.



Each of these surfaces is diffeomorphic to a sphere. Four of these five surfaces are isometric.

To align or compare surfaces, we search for a near isometry in the space of diffeomorphisms. "Near" refers to how much stretching is needed to fit one surface over another.

The space of diffeomorphisms There are many ways to map a surface to another surface by a diffeomorphism. Too many!!



How can we search this vast space for a map closest to an isometry?

Isometries

Isometries have two key properties:

They preserve angles (conformal)
 They preserve area (area preserving)

Lemma

 $f:S_1 \rightarrow S_2$

f is an isometry \longleftrightarrow *f* preserves angles *and* area



Searching among diffeomorphisms

How can we search the vast space of diffeomorphisms for a map closest to an isometry?

Choosing the best $f:S_1 \rightarrow S_2$ from an infinite-dimensional spaces is hard.

Idea: Restrict our 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.

Conformal maps

A Conformal Map has some of the properties of an isometry.

A *Conformal Map* is a map between two smooth surfaces that preserves angles.



Conformal maps

The angle between two vectors is the same as the angle between their images.

Take two unit vectors at any point. The angle between them is the same as the angle between their images under *f*.

 $<V, W>_1 = <df(V), df(W)>_2$

They are stretched equally.



Riemann Mapping Theorem



There is a conformal map from any planar disk region to the round unit disk.

Conformal mapping





Mercartor projection

Mobius Transformations

The conformal maps from the entire complex plane, or Riemann sphere, to itself are called *Mobius Transformations*.





ad-bc = 1

Coincides with the group $PSL(2,C)=SL(2,C)/\{ \pm Id \}$

This is a six dimensional space.

A path of Mobius Transformations













Higher genus surfaces

Can we always find a conformal diffeomorphism between two surfaces?



Not always.

Conformal maps exist in genus 0 We can't always find an isometry between S_1 and S_2 .

But for genus zero surfaces S_1 and S_2 , we can *always* find a map that preserves angles.



Conformal maps don't always exist in genus > 0



A close to conformal map of genus-two surfaces. (Amenta)

From smooth to discrete

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

Yes



What can we say about discrete surfaces?



PL metrics

In the discrete setting, a geometry on a triangulated surface S is described by a PL metric that assigns a length to each edge of the triangulation.

 $I(e_{kj})$

Two surfaces with *PL metrics*







What does it mean for a map between two discrete surfaces to be conformal?

What is a discrete conformal map?

Many definitions and algorithms 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. Discrete Differential Equation
- 8. Wilmore Flow
- 9. Circle Packings

Good and Bad triangulations

Warning: Working with discrete surfaces often requires special types of "nice" triangulations. eg Delaunay triangualtions.



Bad triangulation

Good triangulations

How to compute a conformal map Finding a conformal map $c: S_1 \rightarrow S_2$



Question: What does it mean to say that a map $c: S_1 \rightarrow S_2$ is conformal when the surfaces are triangulated rather than smooth?

Conformal maps preserve angles

Conformal maps stretch, rotate or both



Circle to circle maps also preserve angles These maps can change radius and rotate a circle. But angles are preserved.



Map of circles is f(z) = Az, simplest conformal map.



How can we find a (roughly) conformal map? Pack circles



Discrete Conformal Maps by Circle Packing S_1 ? S_2

How can we find a (roughly) conformal map?



Circle Packing

A *circle packing* is a collection of tangent circles whose bounded complementary regions are "triangular".



Each circle packing has a corresponding triangulation. For each vertex there is a circle, for each edge a tangency and for each triangular face a triple of circles.



Discrete Analytic Map

Theorem. (Thurston-Andreev-Koebe) For any triangulation T of a surface, there exists a collection of radii that produce a circle packing corresponding to T.

Thurston gave a simple algorithm for finding these radii. This gives one way to compute a discrete conformal map.





Just need to find these radii.

Smooth and Discrete Conformal Maps

In a smooth surface S, a conformal change scales a Riemannian metric at each point.

A metric g changes to a new metric g^* . A function $u: S \longrightarrow R$ gives the scaling factor at each point.

$$g^{*} = e^{u}g$$

$$g^{*}(v,w) = e^{u}g(v,w)$$

1 4 /

Angles between vectors are the same in g and in g^* . If u(p) = 10, then a vector at p is stretched by a factor of ???
Discrete Conformal map

The corresponding idea for a map between two triangulated surfaces is called a *Discrete Conformal Map*. What is this?



 $l^{*}(e_{ij}) = e^{u(i)+u(j)}l(e_{ij})$

Formula for a discrete conformal map $PL metric l: E \longrightarrow R_+$ Vertex scaling function $u: V \longrightarrow R$ New PL metric l^*



Two Notions of Conformality

S Smooth Riem. metric g Conformal map

 $u: S \longrightarrow R$

 $g \longrightarrow g^*$

 $g^* = e^u g$

Uniformization Theorem

 S_1 and S_2 smooth genus-zero Riemannian surfaces. There is a conformal map

 $c: S_1 \longrightarrow S_2$

S Discrete PL metric $l: E \longrightarrow R_+$ Discrete Conformal map $u: V \longrightarrow R$ $l \longrightarrow l^*$ $l^*(e_{ij}) = e^{u(e_1)+u(e_2)} l(e_{ij})$

Discrete Uniformization Theorem: S₁ and S₂ discrete genus-zero surfaces with PL metrics and "*nice"* triangulations. There is a discrete conformal map

$$c: S_1 \longrightarrow S_2$$

Implementing Conformal Mappings Any genus-zero surface can be mapped conformally to a round sphere.





From Conformal Map to Shape Distance

The space of diffeomorphisms is too big to work with directly. So we don't try to find a minimal stretching energy among all possible diffeomorphism correspondences.

Instead, we minimize stretching energy over all conformal maps.

The resulting minimal energy required to stretch one surface over a second surface gives a distance between the two surfaces.

Smooth Stretching Energy

Definition. The Symmetric Distortion Energy of a conformal diffeomorphism $f : F_1 \to F_2$ with dilation λ_f is

$$E_{sd}(f) = \sqrt{\int_{F_1} (1 - \lambda_f(z))^2 \, dA_1} + \sqrt{\int_{F_2} (1 - \lambda_{f^{-1}}(z))^2 \, dA_2}.$$
 (1)

 $d_{sd}(F_1, F_2) = \mathcal{I} = \inf\{E_{sd}(f)|f: F_1 \to F_2 \text{ is a conformal diffeomorphism}\}.$



Discrete Stretching Energy

A Metric on Shapes

We can use this measure of stretching of conformal maps to define the distance between two shapes (of genus zero).

The distance between two surfaces is equal to the sum of the energies needed to stretch each over the other.

 $d_{sd}(F_1, F_2) = \mathcal{I} = \inf\{E_{sd}(f)|f: F_1 \to F_2 \text{ is a conformal diffeomorphism}\}.$

Where do biological surfaces come from? Proteins

Brain surfaces

Bones

Teeth

.... many more

Example - 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.

Protein Surfaces



Two surfaces generated from two prion proteins

Triangulated Surface from Protein





Two representations of a protein, a stick model and an accessible surface.

From Protein to Surface



Define a surface that envelops the protein.

Triangulated Surfaces from Brains



² Gray matter mesh (extracted from MRI with BrainVisa)

Triangulated Surfaces from Bones



Metatarsal (toe) bones from 23 old and new world monkeys and 38 prosimians.

Phylogenetic Tree from Toe Bones



This tree is generated from a distance between metatarsal bones.



Noise







N=0







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 rounds sphere.

How Round is a Platonic Solid?











How round are the Platonic Solids?



How round is a Protein?



Experiment - Roundness of 533 Proteins



Experiment - A non-rigid Protein



Distance between Teeth



Teeth have orientations



Distance between Arm Bones



Morphometrices

A traditional approach to measuring distance between shapes.





Requires human expertise. Expensive and slow.

Comparing results



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

Distance between Toe Bones



Comparing results

Evolutionary tree based only on metatarsal bone shapes.



Distance between Brain Cortices





Step 1: Brain Cortex to Sphere



Computing distance between Brain Cortices





Find conformal maps to the sphere for each cortex

Computing distance between Brain Cortices



Chose *M* so that *C* minimizes stretching energy among all conformal maps.
Computing distance between Brain Cortices



The energy of *C* measures how much stretching is required to stretch the red cortex over the green one. This gives a distance between the two brain surfaces.

How well does this work?









THANK YOU FOR COMING!

