# Structure Discovery in Sampled Spaces

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 Bring tools from Computational Geometry and Topology to the analysis and visualization of massive, distributed data sets

Perform global structure discovery on such data

- Produce meaningful topological and geometric maps over the data
- Extract structural similarities or structure preserving correspondences within and across data sets
- Exploit this discovered structure in enabling visual exploration and human interaction with the data

### **Understand Data via Maps**









## The Problem of Correspondences



### Some Tools

#### Heat Diffusion on Manifolds



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

▲ : Laplace-Beltrami Operator (div grad)

Persistence diagrams (barcodes)

Persistent Homology

$$H_k = Z_k / B_k$$

0	κ_+	 κ	κ <sub>0</sub>
0	- κ <sub>+</sub>	κ	$\kappa_0$ $\kappa_0$ $\kappa_0$

- $\beta_0$ : # components
- $\beta_1$ : # tunnels or loops

 $\beta_2$ : # voids

## **Three Quick Vignettes**

- I. Isometric Descriptors and Shape Correspondences
- II. Circular Coordinates for Data Sets
- **III. Interlinked Image Collections**



Topology

#### I. Isometric Descriptors and Shape Correspondences

[Ovsjanikov, Sun, G., SGP'08, Sun, Ovsjanikov, G., SGP'09]



## Extrinsic vs. Intrinsic

- Most multi-scale methods of geometric analysis, e.g. wavelets, require explicit parametrizations of the geometry, e.g. coordinate functions
- What if we have only metric, or distance information?
- And what if the distances are intrinsic, not extrinsic?





#### **Extrinsic vs. Intrinsic Symmetries**



**Extrinsic Symmetry** 

- Invariance under translation, rotation, reflection and scaling (Isometries of the ambient space)
- Break under isometric deformations of the shape



Intrinsic Symmetry

- Invariance of geodesic distances under selfmappings. For a homeomorphism  $T: O \rightarrow O$  $g(\mathbf{p}, \mathbf{q}) = g(T(\mathbf{p}), T(\mathbf{q})) \forall \mathbf{p}, \mathbf{q} \in O$
- Persist under isometric deformations

## Correspondences are Often Based on Descriptors



## **Shape Descriptors**

For shapes, there are many descriptors invariant to rigid motions:







Integral Invariants: Manay et al. '04 Pottmann et al. '09

Shape Contexts: Belongie et al. '00 Frome et al. '04

Spin Images: Johnson, Hebert '99

- Many tradeoffs among different descriptors ...
- But what about intrinsic descriptors? Heat kernel signatures

### 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?

## Background

• Heat equation on a Riemannian manifold: If u(x,t) is the amount of heat at point x at time t, then  $\partial u$ 

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



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

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

$$f(x,t) = e^{-t\Delta} f$$
$$H_t \text{ heat operator}$$



## Background

• 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 -- an integral over all paths from x to y

#### **Basic Properties**

• 
$$k_t(x,y) = k_t(y,x)$$

• 
$$k_{t+s}(x,y) = \int_M k_t(x,z)k_s(z,y)dz$$

• 
$$k_t(x,y) = \sum_{i=0} e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$
  
LB eigenvalues and eigenvectors

Invariant under isometric deformations

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

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

Conversely: it characterizes the shape up to isometry.
 If k<sub>t</sub>(x, y) = k<sub>t</sub> (T(x), T(y)) ∀ x, y, t then
 *M* is an isometry

This is because:

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

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

#### 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



truncation effect

#### Robustness:

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



Let k<sub>t</sub>(x, ·) 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

Let k<sub>t</sub>(x, ·) 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 of the kernel:

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

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

• Since HKS is a restriction of the heat kernel, it is:

- Robust
- Multiscale
- Question 1: How informative is it?

Related to Gaussian curvature for small t:



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



t = 0.004 t = 0.008 t = 0.02 t = 2

HKS computational aspects omitted in this talk

### **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  $T : X \to Y$  is an isometry if and only if, for all x

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

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

## **Applications of HKS**

Multi-scale matching, structure discovery



Feature extraction



• Two heuristics for making HKSs comparisons practical:

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

Compare using L2 norm of these HKS vectors

• Comparing points through their HKS signatures:









• Finding similar points – robustly:





Medium scale

Full scale

Armadillo

• 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:  $k_t(x, \cdot)$
- 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

Partial and approximate intrinsic symmetries can be detected this way

### **Informative Theorem**

#### • How general is the theorem?

• If there are repeated eigenvalues, it does not hold:



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

 Do not know if an "approximate" version of the theorem is true, but suspect so

## Intrinsic Measures of Shape Similarity

 Gromov-Hausdorff distance: a second order optimization over correspondences

$$egin{aligned} \Gamma_{X,Y}(x,y,x',y') &\coloneqq \left| d_X(x,x') - d_Y(y,y') 
ight| \ d_{\mathcal{GH}}(X,Y) &= rac{1}{2} \inf_R \| \Gamma_{X,Y} \|_{L^\infty(R imes R)} \end{aligned}$$

intrinsic distance distortion

evaluated via intrinsic distances



## Are There Perfect Signatures?

- To optimally align two shapes, is it sufficient to optimally align their point signatures, or certain features derived from these signatures?
- Optimal alignment can be defined in terms of certain intrinsic but hard-tocompute shape distances, such as Gromov-Hausdorff
- If this is so, then we only have a firstorder optimization problem to solve ...
- Of course this can fail if there are symmetries ...

[data sets: Stanford 3D Scanning Repository / Carsten Stoll]


# **Key Points and Issues**

- Heat kernel signatures (HKS) provide a powerful tool for describing shape neighborhoods. They are
  - Robust
  - Multiscale
  - Informative. Related to curvature and geodesics
  - Easily computable
- They can be used to
  - Provide point signature for multiscale matching
  - Extract shape features
  - Discover intrinsic symmetries
  - Study a formal spectral metric between shapes

#### II. Circular Coordinates for Data Sets

[de Silva, Morozov, Vejdemo-Johansson, SoCG'09]



### **Circular Structures**

- Circular structures are often present in data
- Classically
  - Linear coordinatization: find linear transformations from X to R<sup>d</sup>
  - Principal component analysis, projection pursuit

#### Recently

- Non-linear methods: drop the expectation of linearity for the transformation
- MDS, kernel methods, locally linear methods



#### **Problematic Cases**

- Some shapes take up too many coordinates
- Circle locally 1dimensional, globally needs 2 coordinates
- Torus locally 2dimensional, globally needs 3, or even 4 coordinates



### How Can We Fix This?

#### Circle-valued coordinates

- Use  $S^1 = [0,1]/(0 \sim 1)$  as an additional coordinate space
- Fixes the circle
- Fixes the torus
- Occurs naturally:
  - Phase coordinates for waves
  - Angle coordinates for directions



## Approach

#### Exploit canonical isomorphism

#### $H^1(X;Z)\cong [X,S^1]$

- Use persistent cohomology to pick out features
  - Compute over  $Z_p$ , for several p
- Use least-squares smoothing to generate nice circlevalued functions from cocycles
- Cohomology is calculated with variant on the persistence algorithm: coboundaries are computed and matched for consecutive simplices

### **Double Torus Correlation Plots**



## **Key Points and Issues**

- Circular structures are very common in real data
- Linear structures can also be discovered this way, by appropriate identification of endpoints
- The need for such parametrizations arises in many other problems
- The cohomology persistence algorithm is very lightweight and fast (faster than regular persistence)

#### **III. Interlinked Image Collections**

[Heath, Gelfand, Ovsjanikov, Aanjenaya, G., '09]













LGORITHMS

#### Image Match Links



### Paths Through Image Collections



### Homotopy Classes



# Large Scale Image Acquisition

- Acquiring, storing, and sharing large image collections is becoming easier and easier
  - Ubiquitous cell phone cameras
  - Inexpensive storage
  - Wireless networking
- Photo sharing sites (e.g., Flickr, Picasa)
- Systematic commercial acquisition projects (e.g., Google Streets)
- Camera sensor networks





### Image Webs



- The idea of Image Webs is to interlink images through a variety of link types, based on both content and image metadata (GPS, time)
- The same way that the WWW of documents has proved useful, the hope is that interlinked webs of signals will also be valuable for propagating, extracting, and filtering information – and the web types two can crosslink and cross-fertilize





## Image Webs Agenda

- Understand the local and global structure of image webs, aiming at a softer, more topological understanding
- Develop efficient construction algorithms
- Explore applications (image browsing, annotation transfer, social networks, etc.)



[Zheng et. al., CVPR 2009]

## The Space of All Images

- If we frieze time, the local structure of the space of images is well understood: it that of a low dimensional manifold – the manifold of views
- This is also the local structure of an image web based on match links
- But at larger scales the structure is more complex
  - because of moving objects
  - because of repeated similar objects
- For us this is exactly the structure that is of interest



#### **Non-Local Links**





### Proximity Through Mobility: Home to Office









## Proximity Through Mobility on the Stanford Campus



# Getting Down to It: Building Image Webs

 Feature Extraction: interest points, associated with a region and summarized by a descriptor



## Getting Rid of False Feature Matches



#### raw matches

#### after geometric verification

## Symmetries and Repetitions: Link Aliasing



#### **Overlap and Pivot Links**



Basic element of a Web is a pair (patch, image)

## Links and Their Decorations

Link decoration:

- Match (M)-links
- Overlap (O)-links
- Pivot (P)-links

(quality of match, transform attributes)

(degree of overlap)

(patch distance, visual attributes)





### **Image Webs Pipeline**



# Gaining Efficiency: Pruning Pairs by CBIR Filtering

- Content-Based Image Retrieval (CBIR) via "Bag of Words" models:
  - cluster and quantize descriptors into vocabulary trees
  - use document information retrieval type indices





 Used to retrieve "visually similar" images – in our case possible Web neighbors for which match links exist

## **Computation Times (w. a Cluster)**

- Image matching steps (VGA image size)
  - Feature extraction (~ 4 sec per image)
  - CBIR indexing (~ 30 sec per image)
  - Cosegmentation operation (~ 1.5 sec per image pair)
- Image Web construction times\*
  - Car (70 images ~ 1 minute)
  - Art museum (1200 images ~ 52 minutes)
  - Stanford campus (4200 images ~ 3 hours)

\*just cosegmentation stage using up to 500 compute nodes

## Scaling Up Web Construction

- We want to build Image Webs with millions of images -- and understand how they are connected
- We cannot afford to try cosegmentation on all image pairs
- CBIR is a useful filter, but …
- Vital connectivity information may reside in sparser areas of the Web



## Getting an Unknown Graph to Reveal Itself ...

- Testing for the presence of links is expensive
- Which images pairs should we try to connect?
- We seek a sparser graph which captures the connectivity of the unknown Web
  - On the one hand, the CBIR filter favors image pairs where links are likely to exist
  - But how can we tell is a particular link improves connectivity?
  - What should be our ultimate measure of Web utility?
- Spectral graph theory and harmonic analysis to the rescue

## **Algebraic Connectivity Measures**

Connectivity of a graph based on heat diffusion notions

Second smallest eigenvalue of the graph Laplacian

$$L_{i,j} = \begin{cases} d(i) & \text{if } i = j \\ -1 & \text{if } i \sim j \\ 0 & \text{otherwise} \end{cases}$$

- Smallest eigenvalue of L is always 0 and has a constant eigenvector
- Multiplicity of 0: number of connected components





## **Algebraic Connectivity**

 Connectivity Measure: Second smallest eigenvalue of the graph Laplacian



- Related to the diameter D of a graph with n nodes, random walk convergence, diffusion distances, and many other measures of graph connectivity
- The eigenvector corresponding to λ<sub>2</sub> is the Fiedler vector, and is often used to partition the graph

## Building a "Good" Graph

#### • Objective:

- Build a "well connected" graph in minimal time
- Difficulty:
  - Given a graph, finding the k extra edges which maximally increase algebraic connectivity is NPhard
- Use a greedy strategy:
  - For every potential new connection, test its EdgeRank *R* – how much it will increase connectivity

## Building a "Good" Graph

#### Use a strategy from graph cuts



Assign to each node its value in the Fiedler vector

• Add an edge (*i*, *j*) to maximize connectivity score:

$$R(i,j) = \max_{i \not\sim j} |\phi_2(i) - \phi_2(j)|$$

## Building a "Good" Graph

#### Practical considerations



- Update the Fiedler vector after each new edge
- Can use the old estimate as a guess
- Use a *power iteration* to update the Fiedler vector
# Building a "Good" Graph

Power Iteration

$$u_{i+1} = (2nI - L)u_i$$
$$u_{i+2}(j) = u_{i+1}(j) - \frac{1}{n} \sum_{k=1}^n u_{i+1}(k) \ \forall \ j$$
$$u_{i+3} = \frac{1}{\|u_{i+2}\|} u_{i+2}$$

- Converges to the Fiedler vector
- Convergence is fast if have a good estimate. We don't expect the Fiedler vector to change drastically
- Small overhead: only 1 vector in memory

#### **Results on Real Data Sets**









(a) Edge Rank

(b) Query Expansion

# Applications: An Image Webs Browser

- How can we navigate through large Image Webs effectively?
- How do we mitigate the effects of wrong links?
- How do we extract "persistent" global structure



# Computing a `Summary Graph'



A global map makes navigation easy

# Persistent Local Homology

- Image Webs are often stratified spaces because of the acquisition process – understanding the strata structure helps
- Use some algebraic topology: image webs as combinatorial complexes
- Rips-Vietoris complex on images, based on distances coming from the links (affine maps)
- Exploit filtered complexes and persistence ideas





# Persistent Local Homology

Different types of nodes in an Image Web:



#### **Persistent Local Homology**



### Summarizing Image Webs



### Parametrizing Edges/Loops



### Web Navigation: Video 1



# **Other Applications**

- Object models as subwebs: focus and context
- Annotation transfer
- Linking people through their images
- Mobile webs: photoguided navigation, collaborative exploration



# **Key Points and Issues**

- Interlinked images and other signals contain a wealth of information not apparent in any one image or signal alone
- Such signal webs form networks of maps; maps can be used to carry to transport information and arrive at a global understanding of both the sensed environment and the acquisition process

• The information is in paths induced by the maps

# Mapper Application: Breast Cancer Study

This flare consists entirely of patients which survive. This is a new piece of the taxonomy of breast cancer, not identified before, and which cannot be recognized by clustering.



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# The Information is in the Maps

We understand data by studying maps or self-maps among the data, and networks of such maps





