Laplace Operator and Heat Kernel

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Outline

- manifold Laplacian (Laplace-Beltrami operator)
  - detection of intrinsic symmetry [Ovsjanikov, S., Guibas, 2008]
    - transforming theorem
  - heat kernel signature [S., Ovsjanikov, Guibas, 2009]
    - informative theorem
- graph Laplacian
  - graph partition
    - Cheeger inequality
  - application on clustering biomolecule conformations
    [Huang, et al, 2010], [S. et al submitted]
- relation between manifold Laplacian and graph Laplacian

Laplace Operator

- on $\mathbb{R}^k$, the standard Laplace operator:
  - $\Delta_{\mathbb{R}^k} f := \frac{\partial^2 f}{\partial x_1^2} + \cdots + \frac{\partial^2 f}{\partial x_k^2}$

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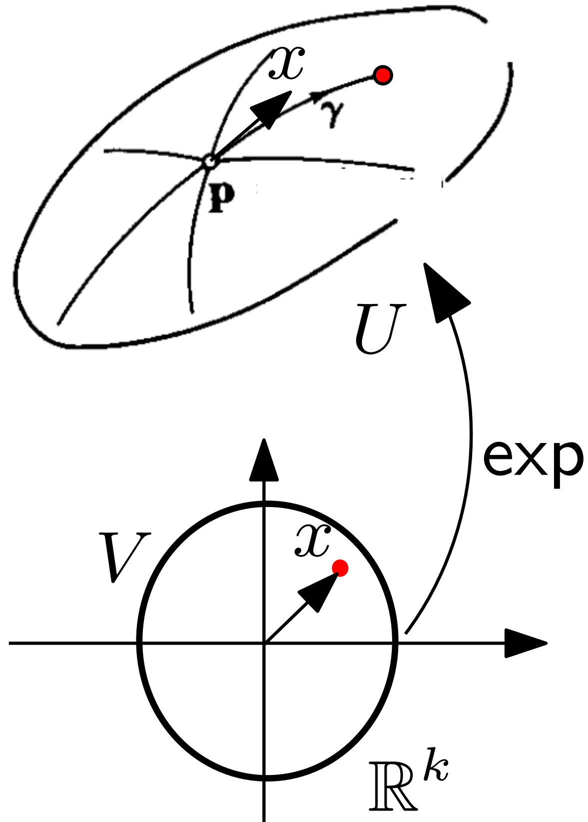
- on a Riemannian manifold, Laplace-Beltrami operator:
  - Exponential map: exp : $V \subset \mathbb{R}^k \to U$ by $\exp(x) = \gamma(p, x, 1)$



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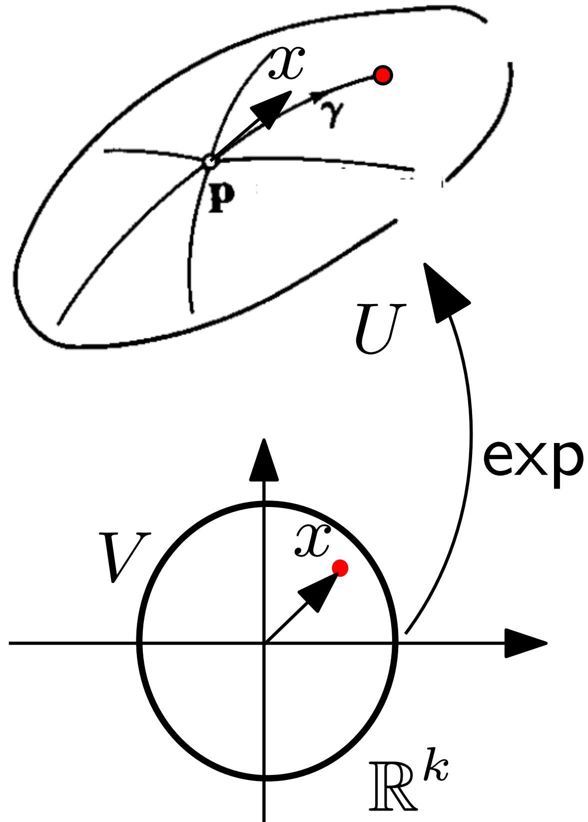

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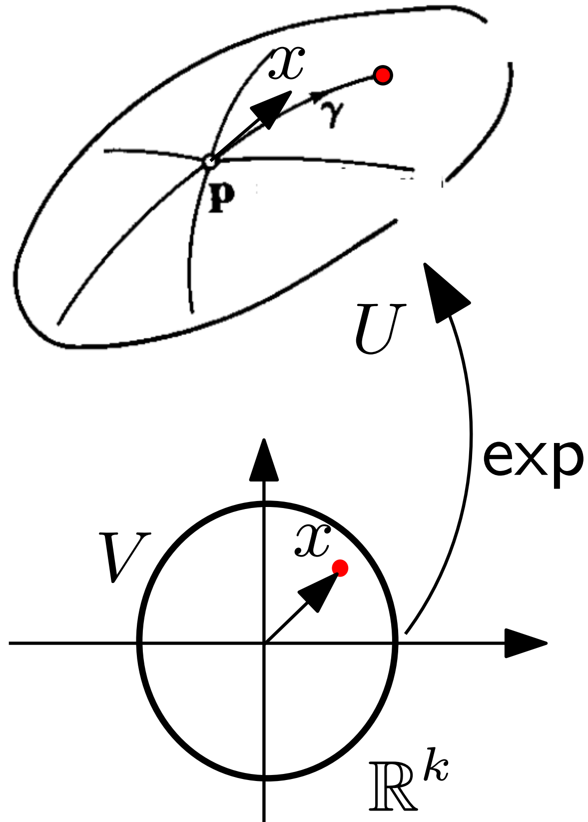
  - Laplace-Beltrami operator is invariant under the map preserving geodesics



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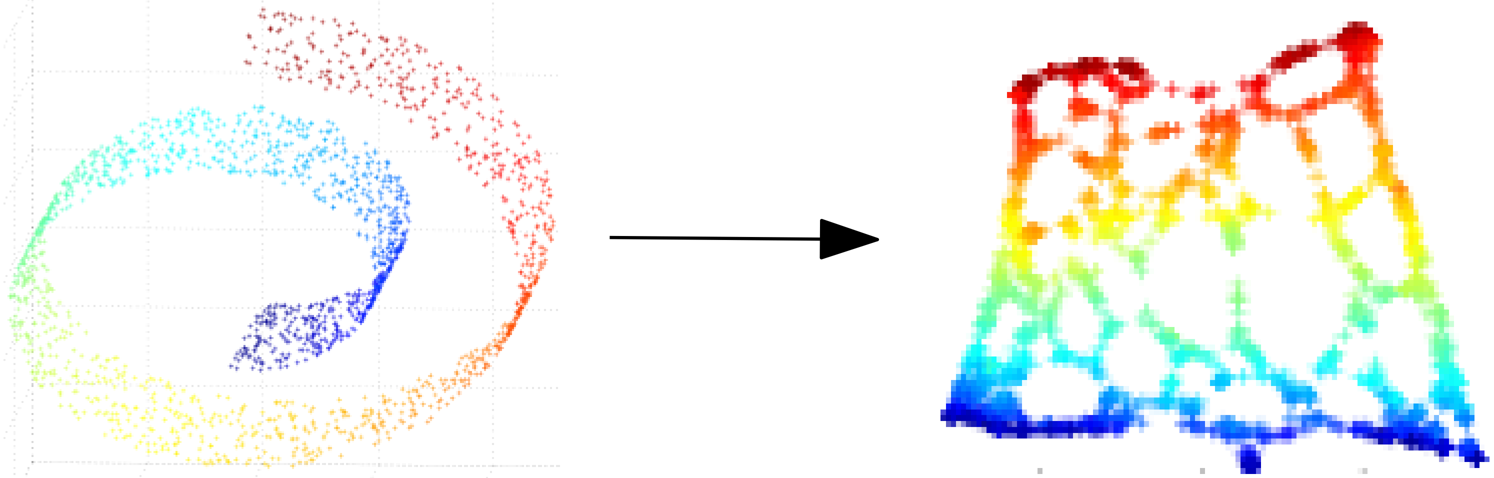

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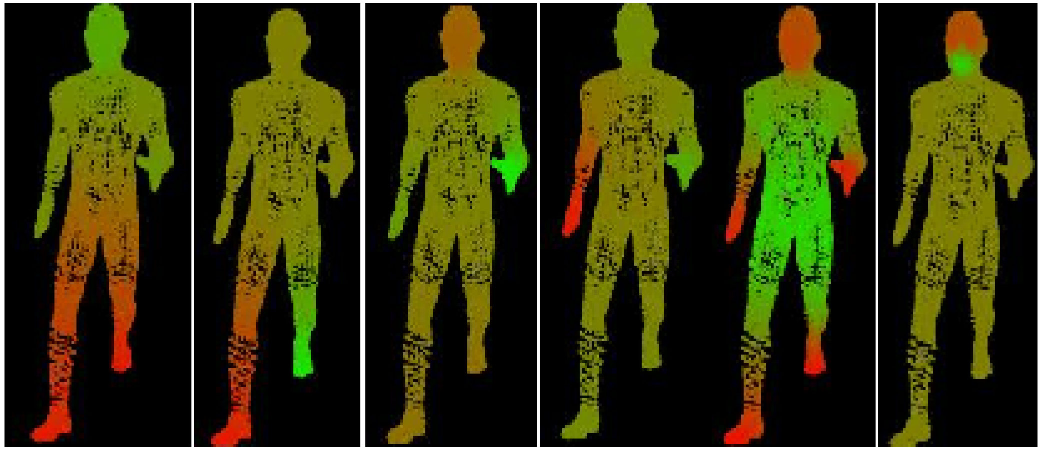

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  - analogous to Fourier harmonics in Euclidean space.
  - dimensionality reduction [Belkin and Niyogi 03]
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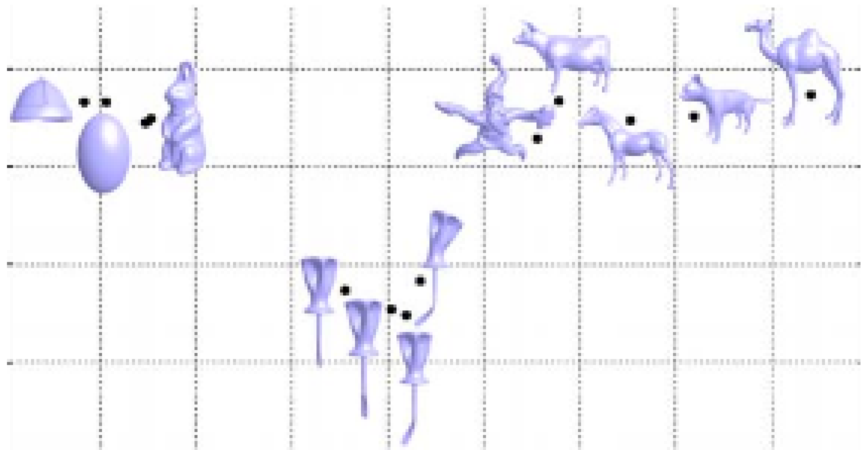
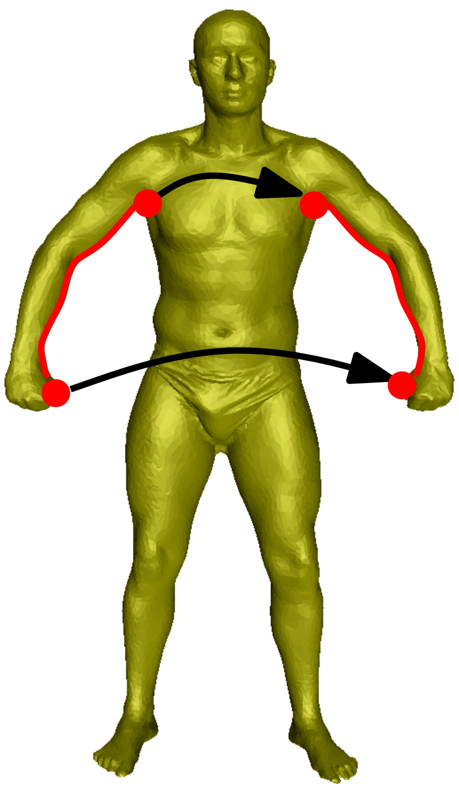
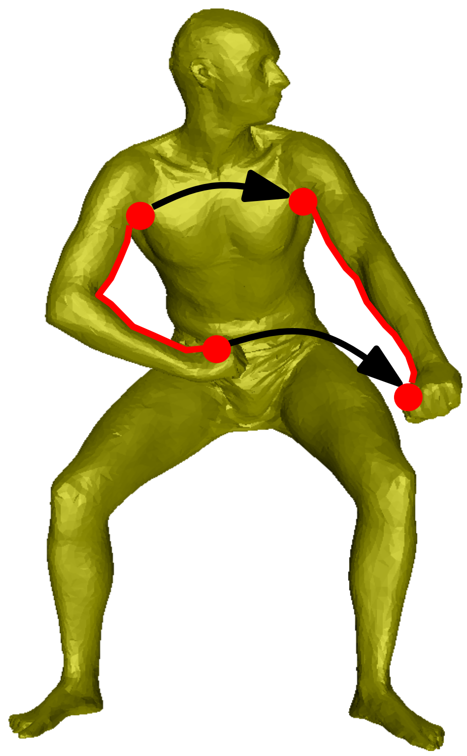
- eigenvalues form the spectrum of a manifold
  - spectral invariant: dimension, volume, scalar curvature, etc.
  - Shape-DNA: shape matching and indexing [Reuter et al. 05]



Intrinsic Symmetry

- intrinsic symmetry: a self map preserving geodesic distances





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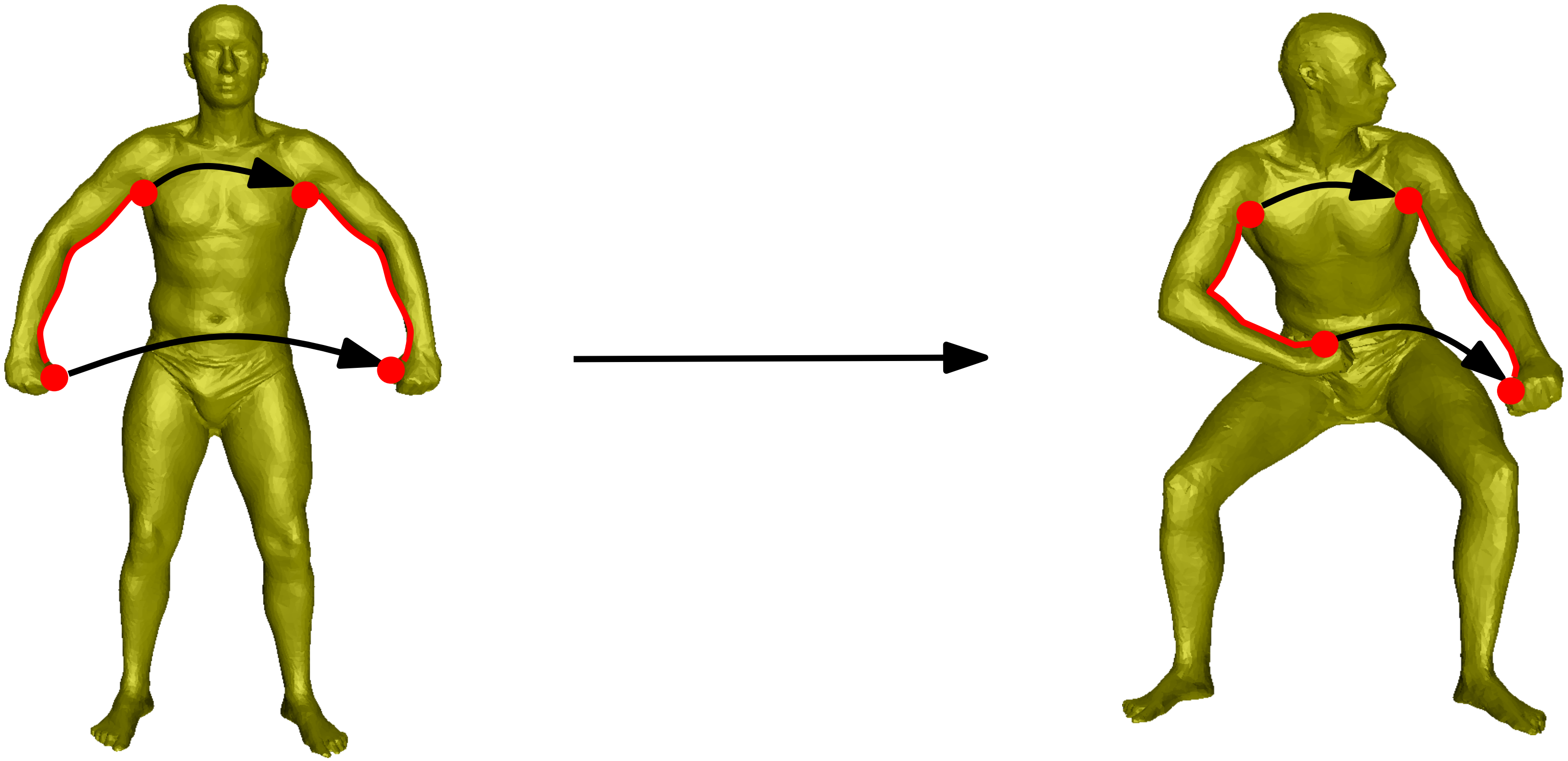
  - invariant under non-rigid transformations



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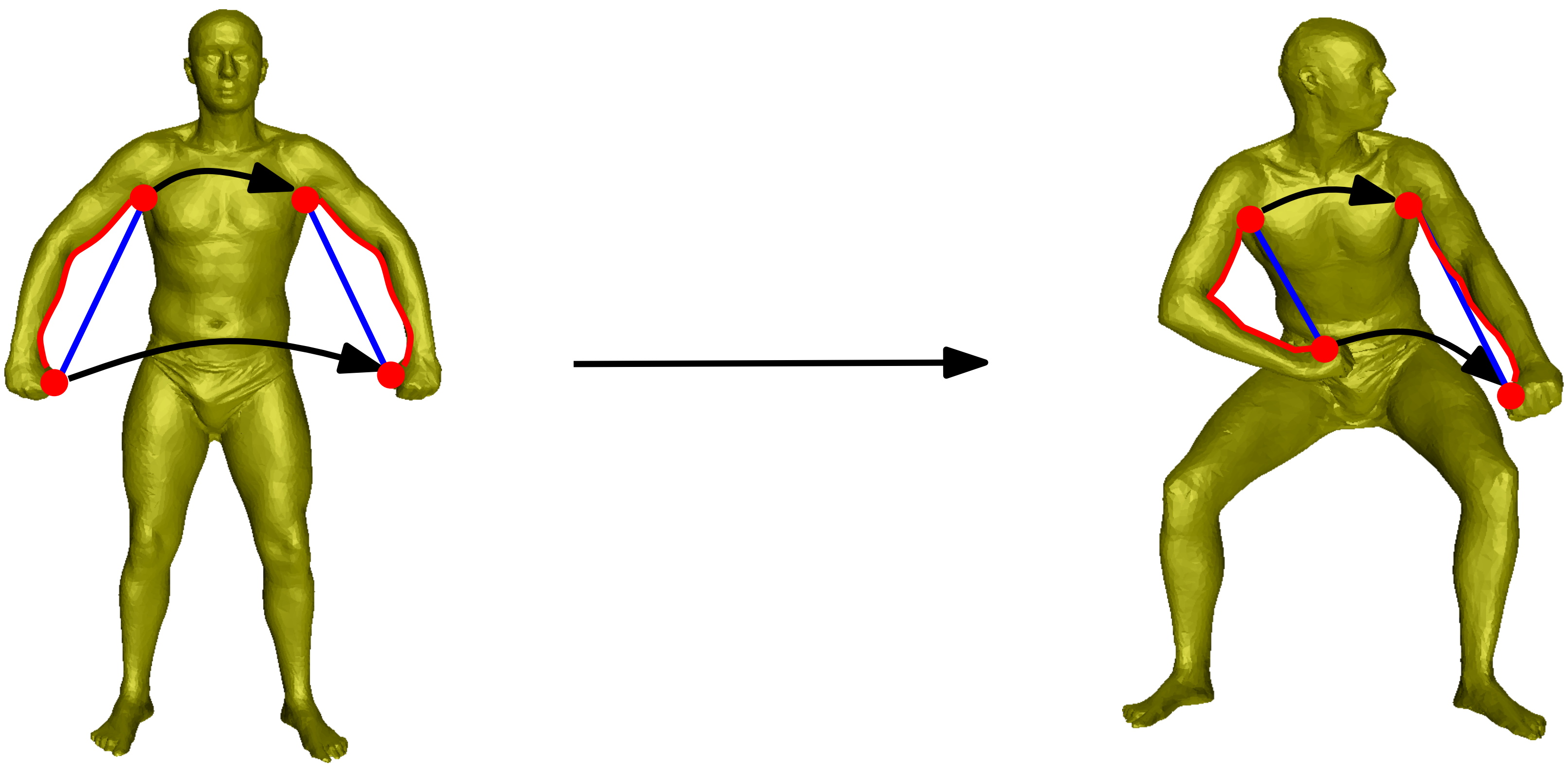
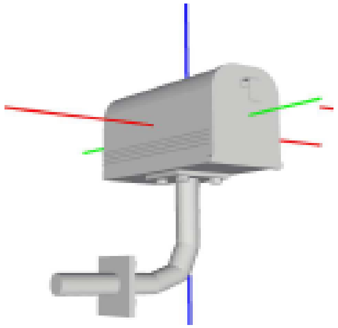


- extrinsic symmetry: rotation and reflection
  - preserve Euclidean distances
  - invariant only under rigid transformations

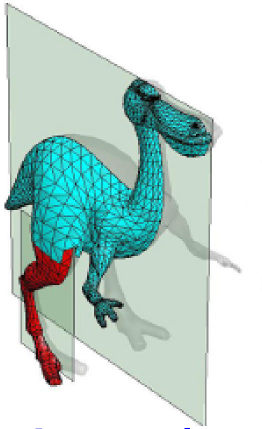
Related Work

- extrinsic symmetry

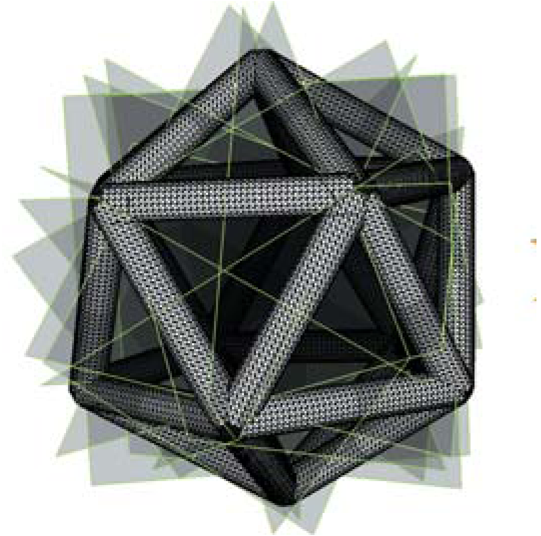


[Podolak et al. 06]

[Mitra et al. 06]



[Shimari et al. 06]



[Martinet et al. 07]

- intrinsic symmetry
  - difficulty: no simple characterization

Global Point Signature

- our strategy: reduce intrinsic to extrinsic
- our tool: eigenfunctions ϕ_i and eigenvalues λ_i of Δ_M

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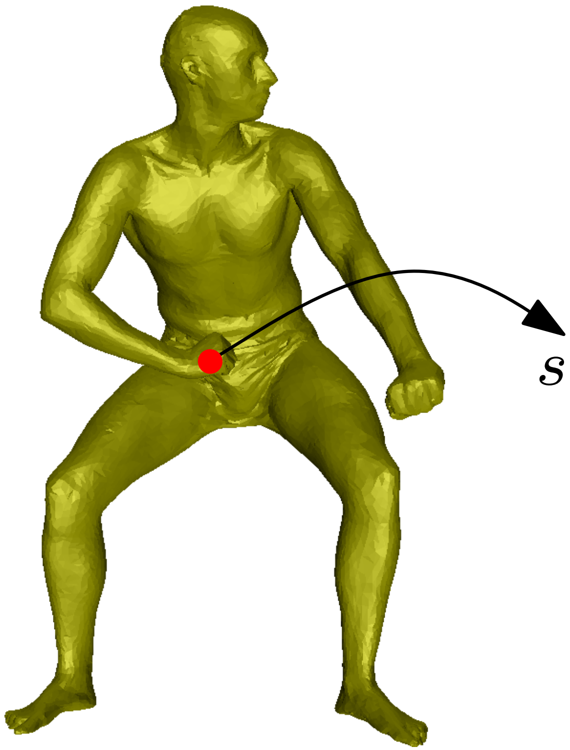
- for each point p on M, its GPS [Rustamov 07]



$$s(p) = \begin{pmatrix} \frac{\phi_1(p)}{\sqrt{\lambda_1}} \\ \frac{\phi_2(p)}{\sqrt{\lambda_2}} \\ \vdots \\ \frac{\phi_i(p)}{\sqrt{\lambda_i}} \\ \vdots \end{pmatrix}$$

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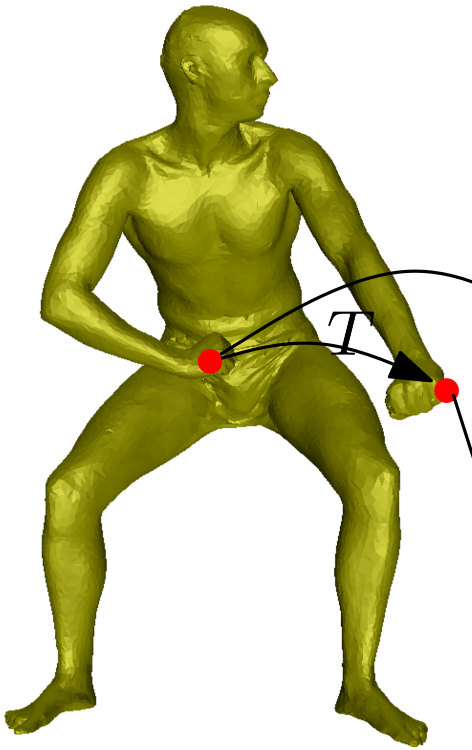

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  - relation between $s(p)$ and $s(T(p))$?

Transforming Theorem

Theorem: For a compact manifold M, T is an intrinsic symmetry if and only if there is a transformation R such that $R(s(p)) = s(T(p))$ for each point $p \in M$ and R restricting to any eigenspace is a rigid transformation.

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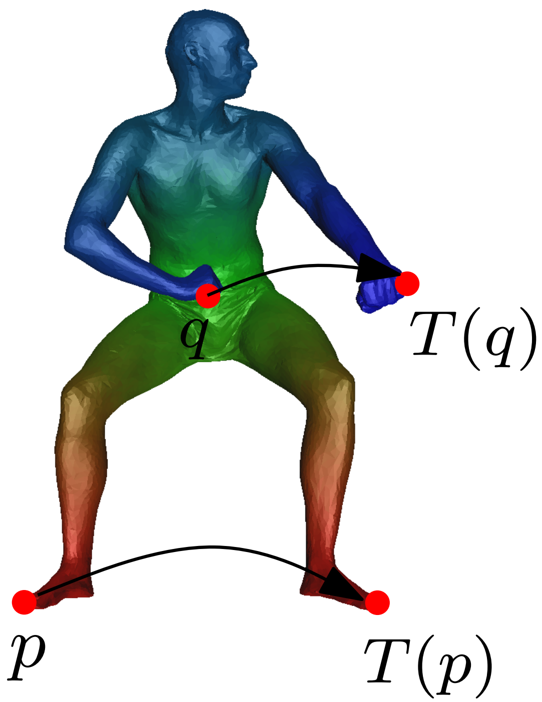
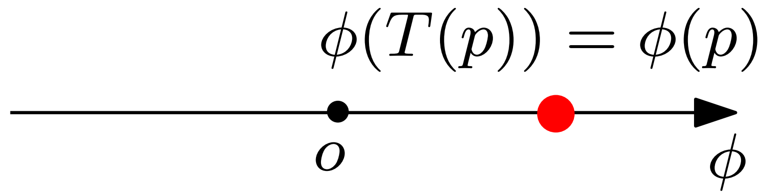
- "only if" part

Eigenfunctions and Intrinsic Symmetry

1. $\phi = \phi \circ T$: **positive** eigenfunction
2. $\phi = -\phi \circ T$: **negative** eigenfunction
3. λ is a repeated eigenvalue





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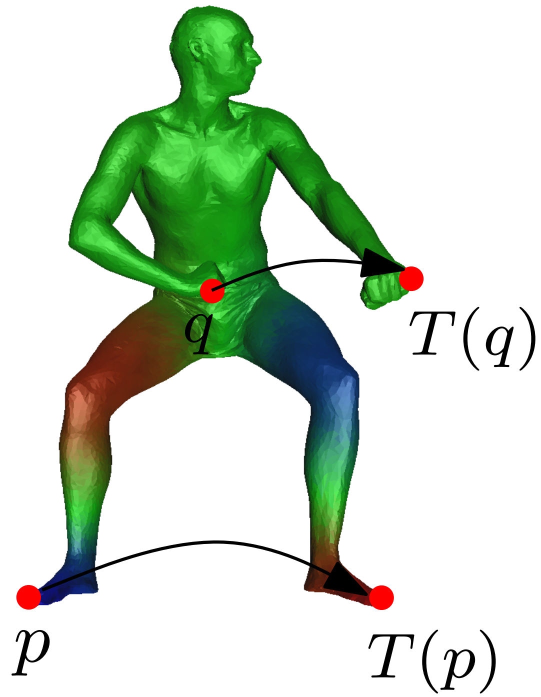

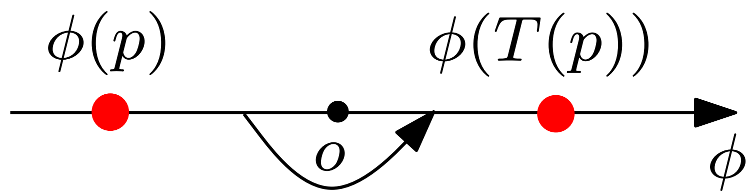

reflection

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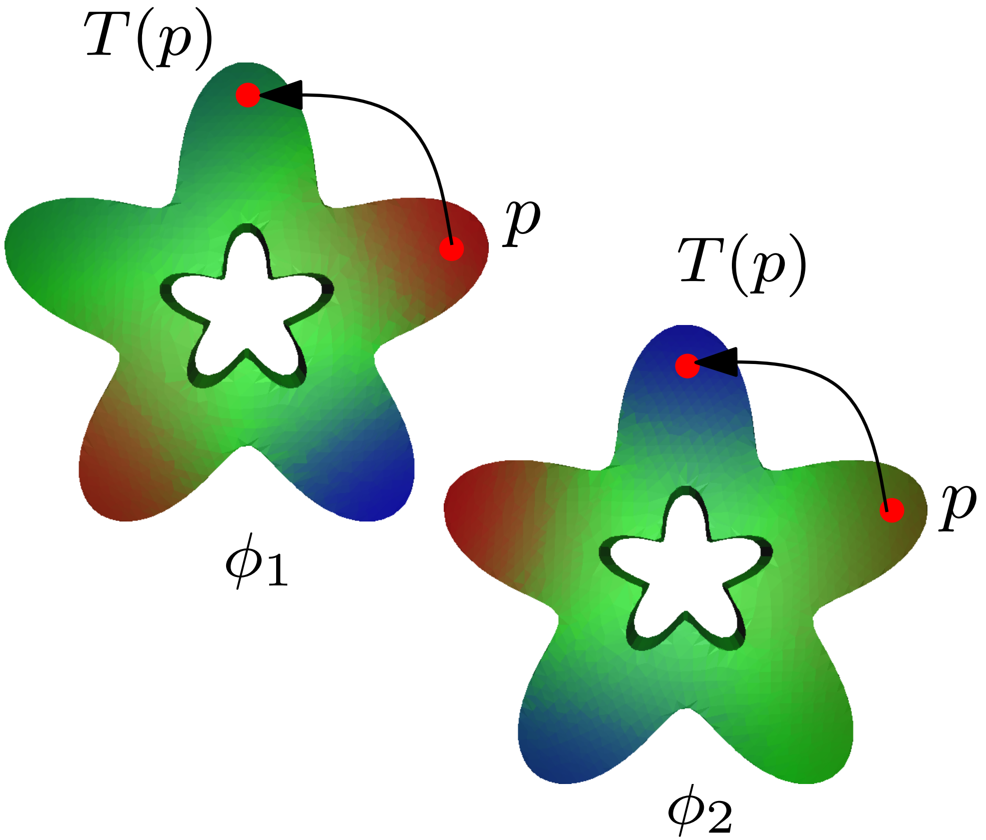

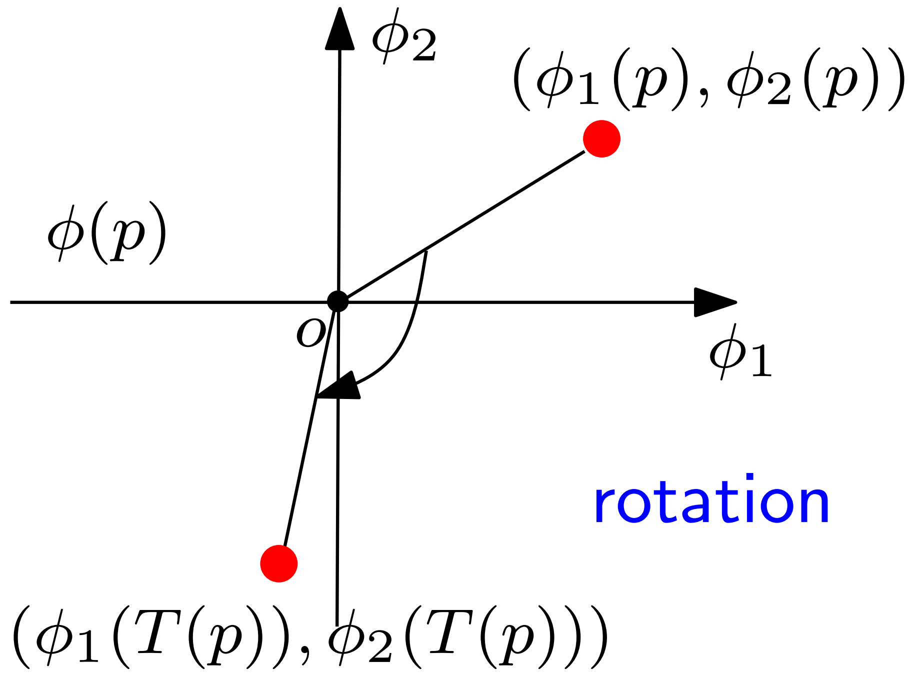

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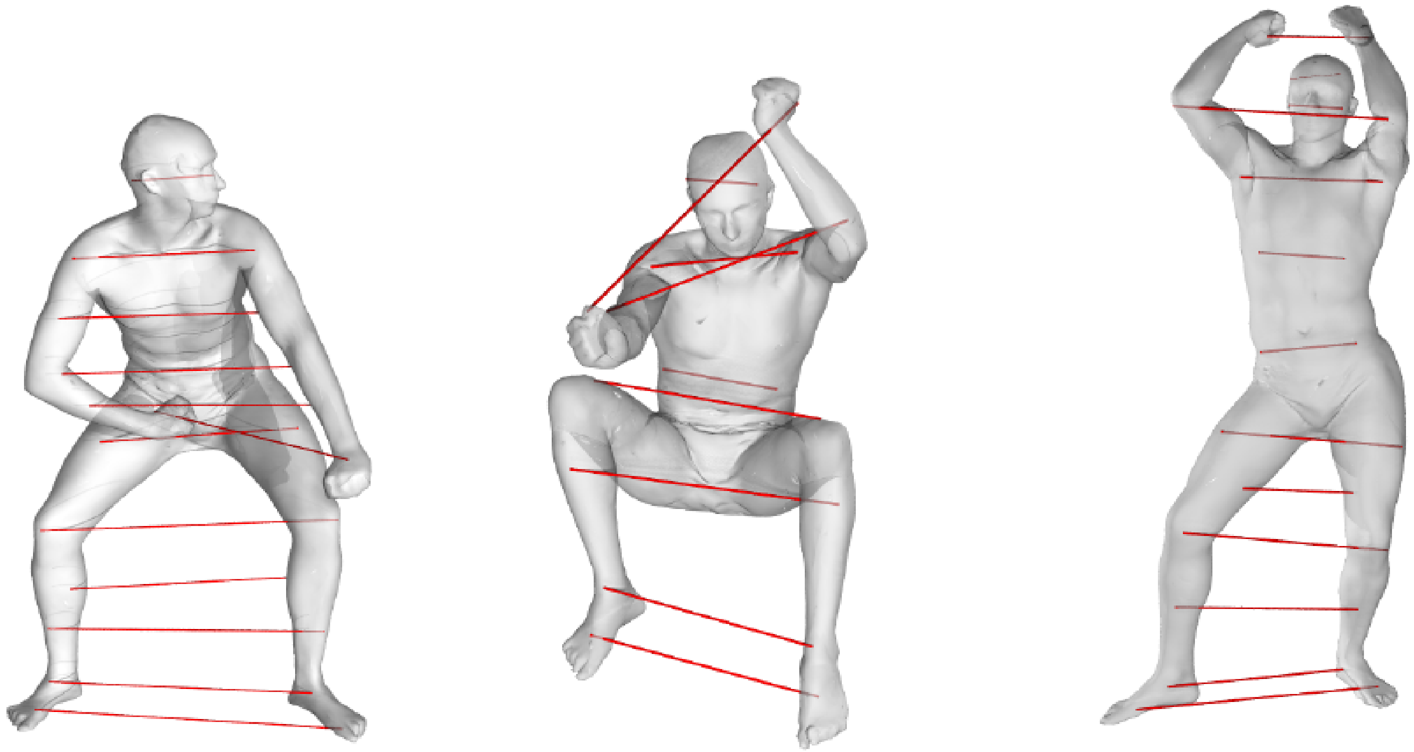
- one to one correspondence between T and R
  - T is an identity $\Leftrightarrow$ R is an identity
- detection of intrinsic symmetry reduced to that of extrinsic rigid transformation
  - detection of extrinsic symmetry
    [Rus07, PSG06, MGP06, MSHS06]

Results



(a) (b) (c)

scans of a real person
(SCAPE dataset)

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- manifold Laplacian (Laplace-Beltrami operator)
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    - transforming theorem
  - heat kernel signature
    - informative theorem
- graph Laplacian
  - graph partition
    - Cheeger inequality
  - application on clustering biomolecule conformations
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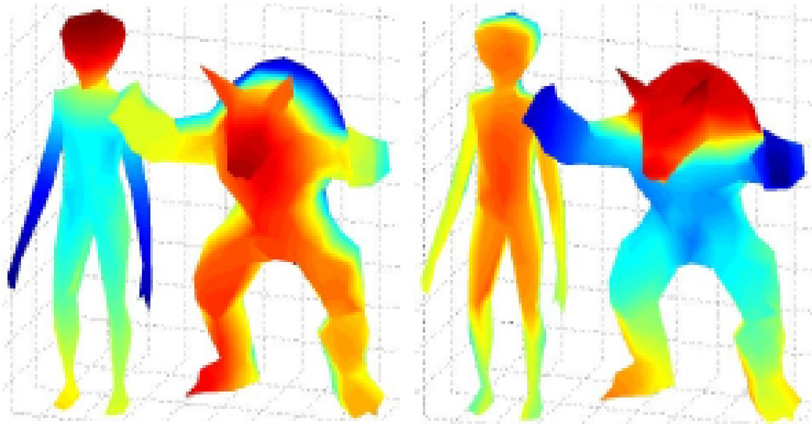
Limitation of Global Point Signature

- For any x, its GPS [Rus07]:

$$\mathrm{GPS}_x = \left(\phi_1(x)/\sqrt{\lambda_1}, \phi_2(x)/\sqrt{\lambda_2}, \cdots, \phi_i(x)/\sqrt{\lambda_i}, \cdots\right)$$

  - global
  - not unique
    - orthonormal transformation within eigenspace
    - eigenfunction switching [GVL96]



courtesy of Jain and Zhang

Heat Kernel Signature

- define HKS for any point x as a function on $\mathbb{R}^+$:
  - $\text{HKS}_x : \mathbb{R}^+ \to \mathbb{R}^+$

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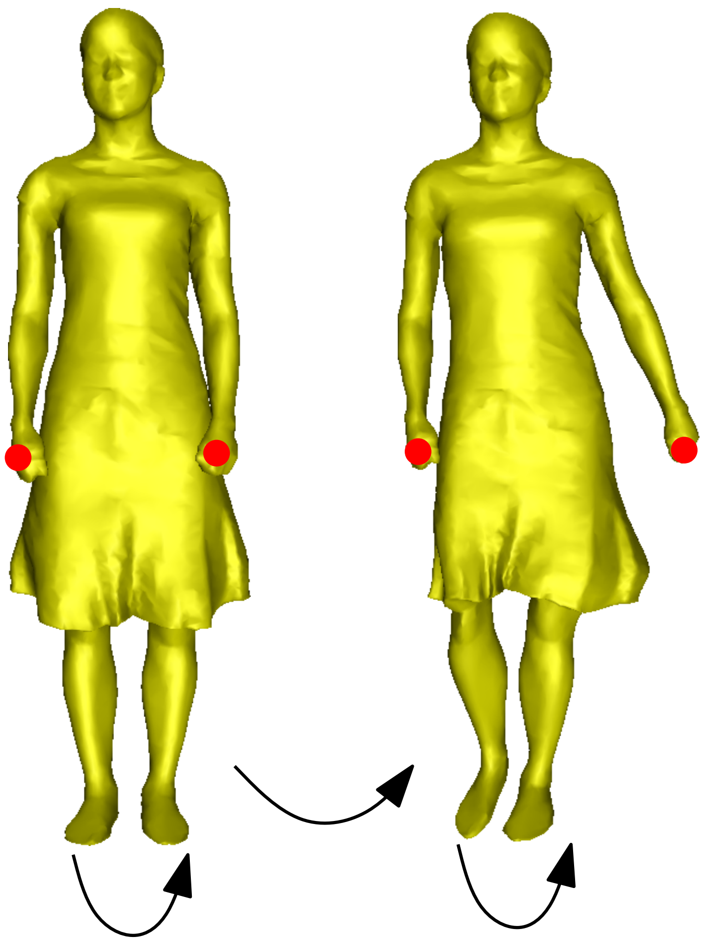

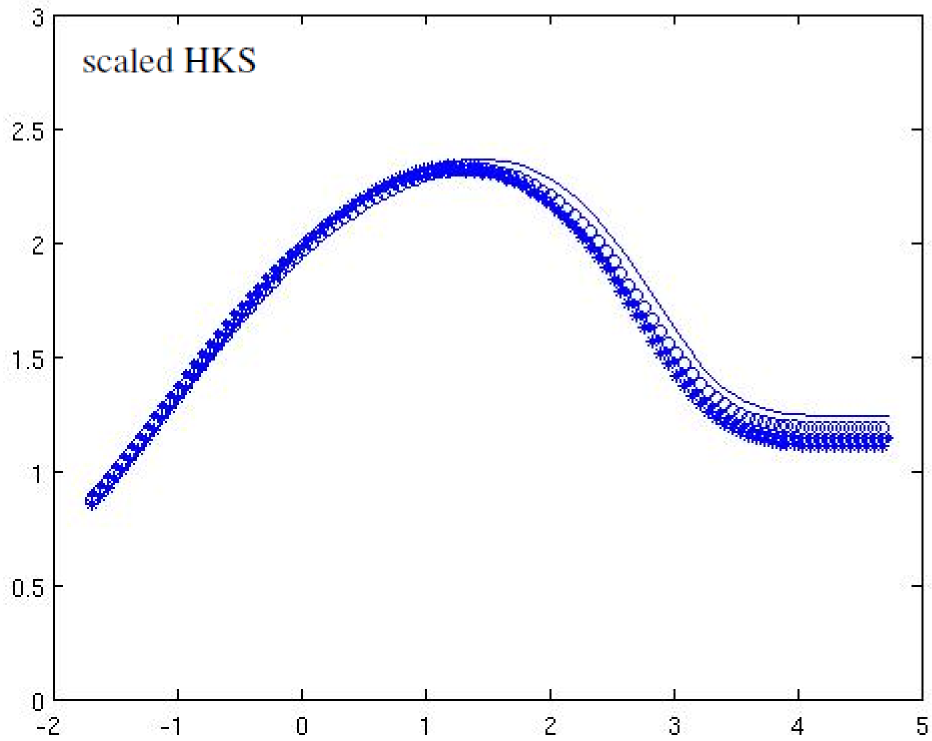

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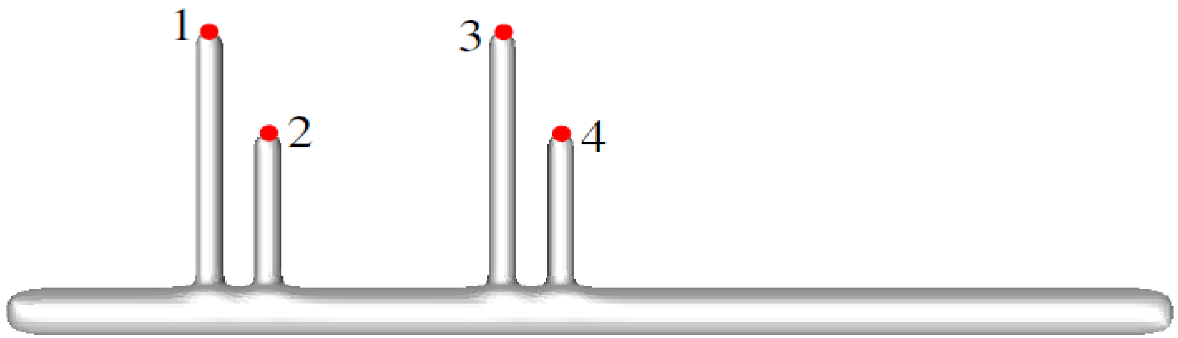

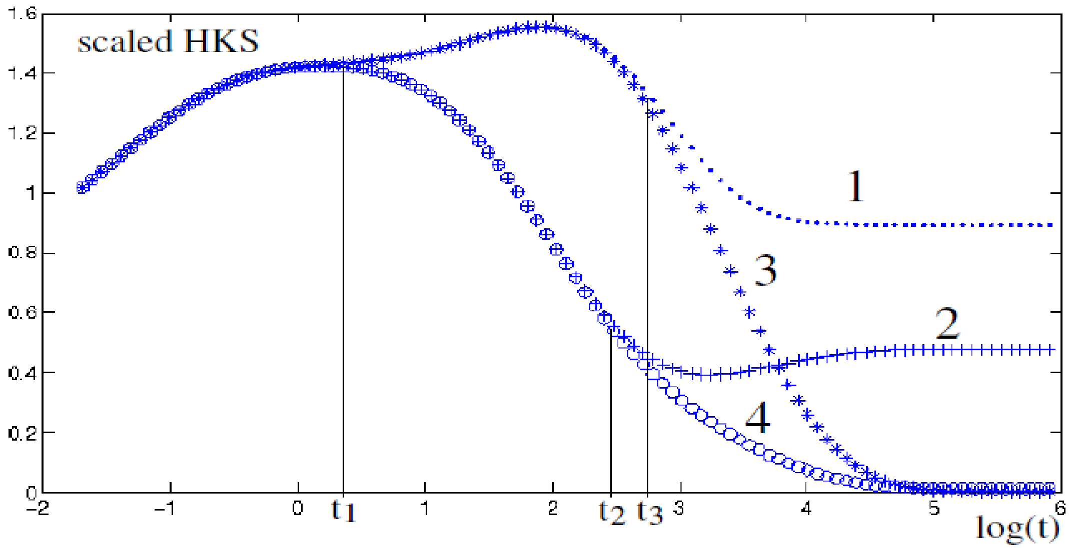

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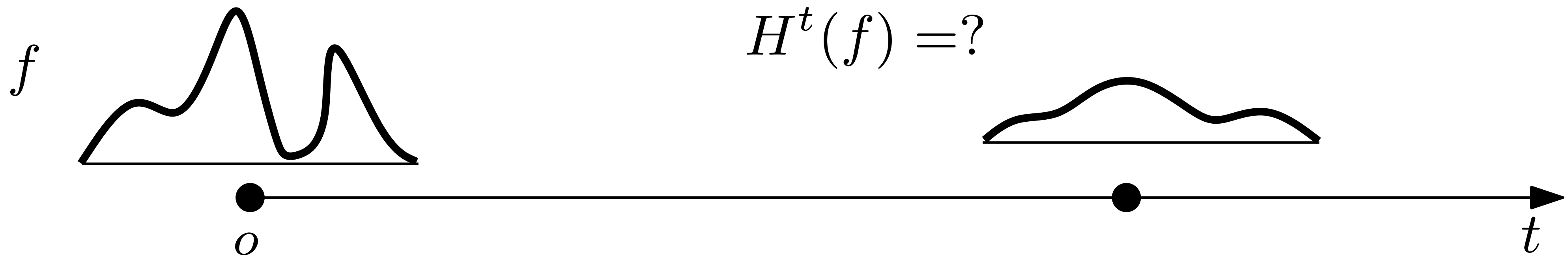
  - $\mathsf{HKS}_x : \mathbb{R}^+ \to \mathbb{R}^+$
- isometric invariant
- multi-scale
- informative
  - $\{HKS_x\}_{x \in M}$ characterizes almost all shapes up to isometry.

Heat Diffusion Process

- how heat diffuses over time



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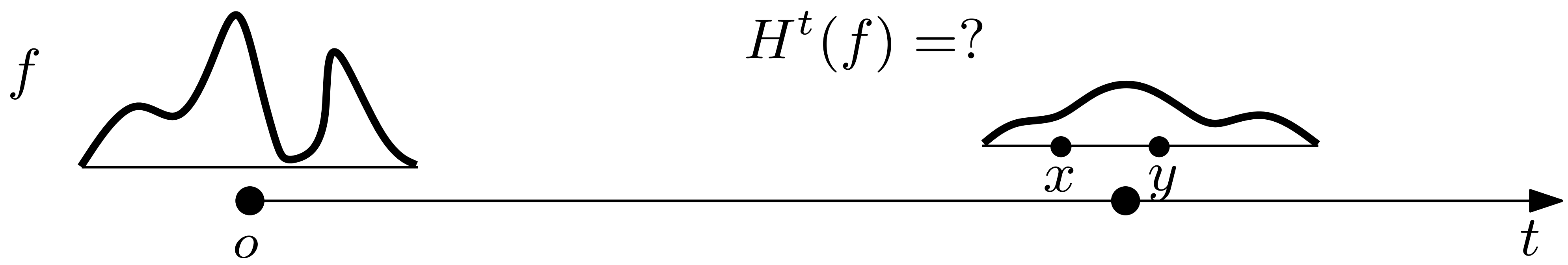


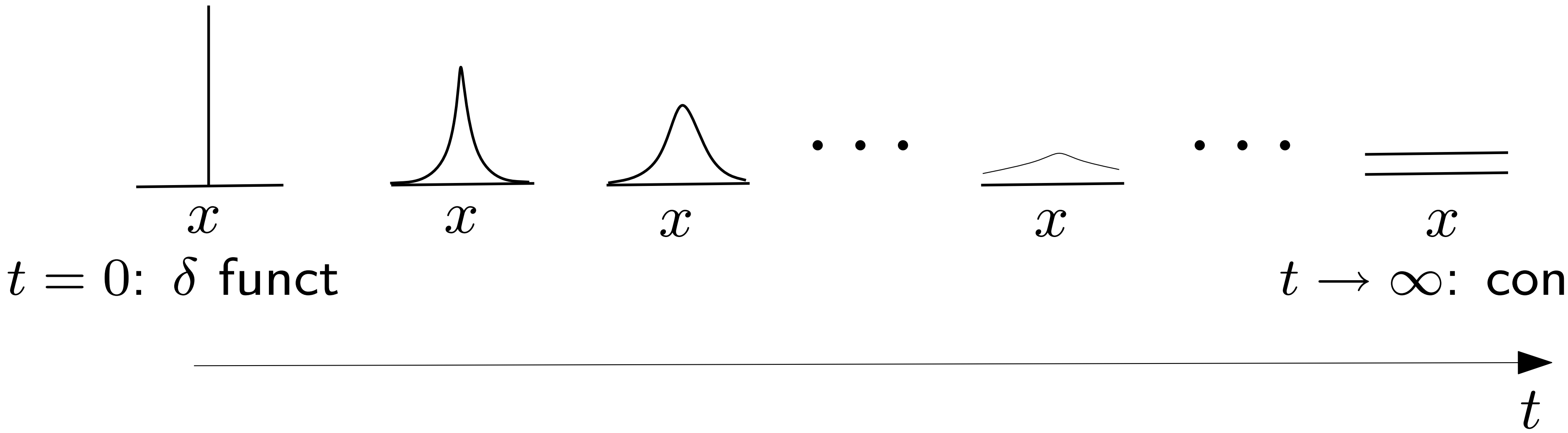
- heat kernel $k_t(x, y) : \mathbb{R}^+ \times M \times M \to \mathbb{R}^+$
  - heat transferred from y to x in time t
  - $H^t f(x) = \int_M k_t(x, y) f(y) dy$

Heat Kernel

- characterize shape up to isometry
  - $T : M \to N$ is isometric iff $k_t(x, y) = k_t(T(x), T(y))$.
  - heat kernel recovers geodesic distances.
    - $d_M^2(x, y) = -4 \lim_{t \to 0} t \log k_t(x, y)$
  - heat diffusion process governed by heat equation.
    - $\Delta_M u(t, x) = -\frac{\partial u(t,x)}{\partial t}$
- generate Brownian motion on a manifold.

Heat Kernel

- multi-scale
  - for any x, a family of functions $\{k_t(x, \cdot)\}_t$



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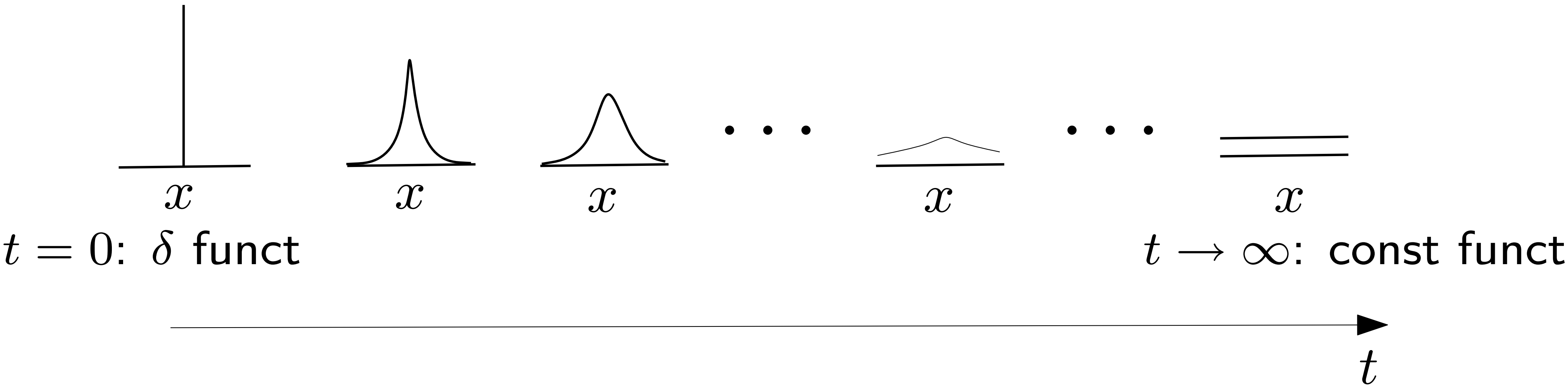

  - local features in small t's; global summaries in big t's

- however, $\{k_t(x,\cdot)\}_t$'s complexity is extremely high
  - difficult to compare $\{k_t(x,\cdot)\}_t$ with $\{k_t(x',\cdot)\}_t$

Heat Kernel Signature

- HKS is the restriction of $\{k_t(x,\cdot)\}_t$ to the temporal domain
  - $\mathsf{HKS}_x : \mathbb{R}^+ \to \mathbb{R}^+$ by $\mathsf{HKS}_x(t) = k_t(x,x)$

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  - isometric invariant
  - informative?

Heat Kernel Signature

- $\{\mathsf{HKS}_x\}_{x \in M}$ is informative

Informative Theorem. If the eigenvalues of M and N are not repeated, a homeomorphism $T : M \to N$ is isometric iff $k_t^M(x,x) = k_t^N(T(x),T(x))$ for any $x \in M$ and any $t > 0$.

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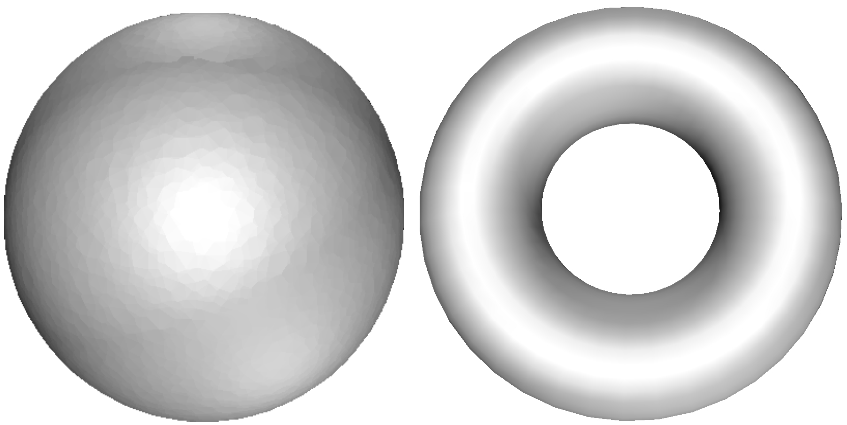
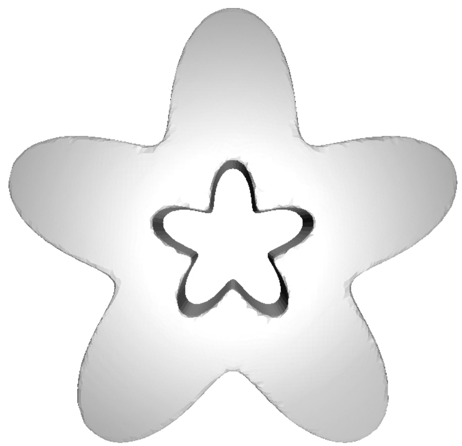
  - the theorem fails if there are repeated eigenvalues



fails!

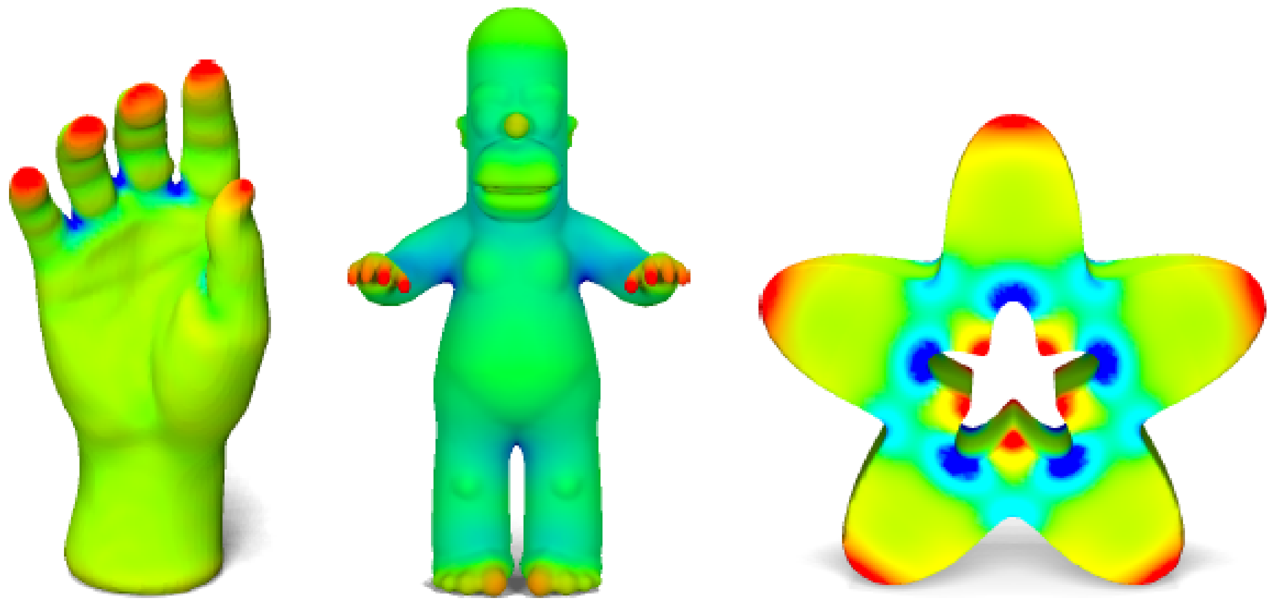


fails?

Relation to Curvature

- the polynomial expansion of HKS at small t:

$$\mathsf{HKS}_x(t) = k_t(x,x) = (4\pi t)^{-d/2}(1 + \tfrac{1}{6}s(x)t + O(t^2))$$



plot of $k_t(x,x)$ for a fixed t

Relation to Diffusion Distance

- diffusion distance [Laf04]

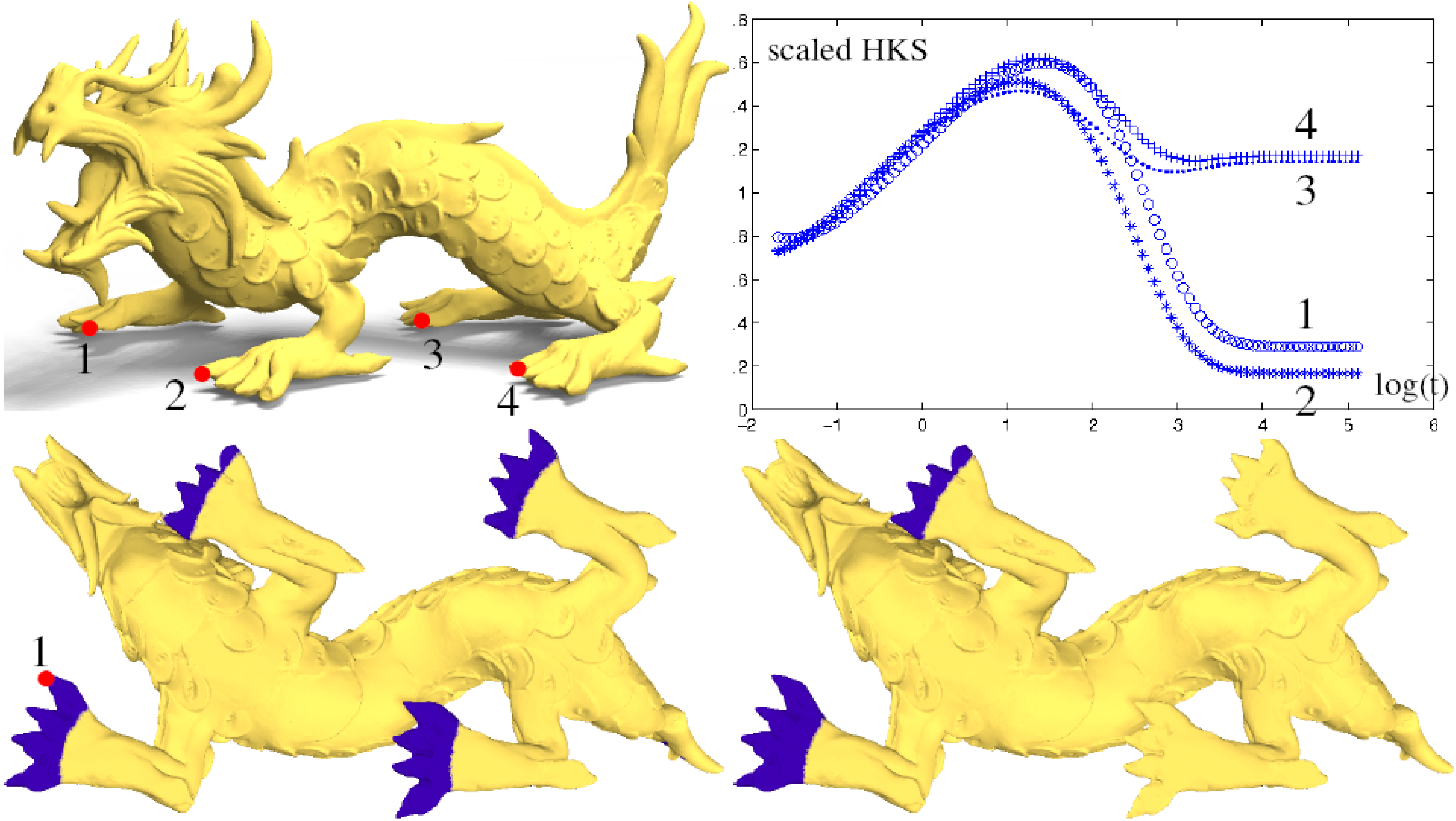
$$d_t^2(x,y) = k_t(x,x) + k_t(y,y) - 2k_t(x,y)$$

  - eccentricity in terms of diffusion distance

$$\begin{aligned} ecc_t(x) &= \frac{1}{A_M}\int_M d_t^2(x,y)dy \\ &= k_t(x,x) + H_M(t) - \frac{2}{A_M}, \end{aligned}$$

    - $ecc_t(x)$ and $k_t(x,x)$ have the same level sets, in particular, extrema points
    - shape segmentation [dGGV08]

Multi-Scale Matching



scaled HKS: $\frac{k_t(x,x)}{\int_M k_t(x,x)dx}$

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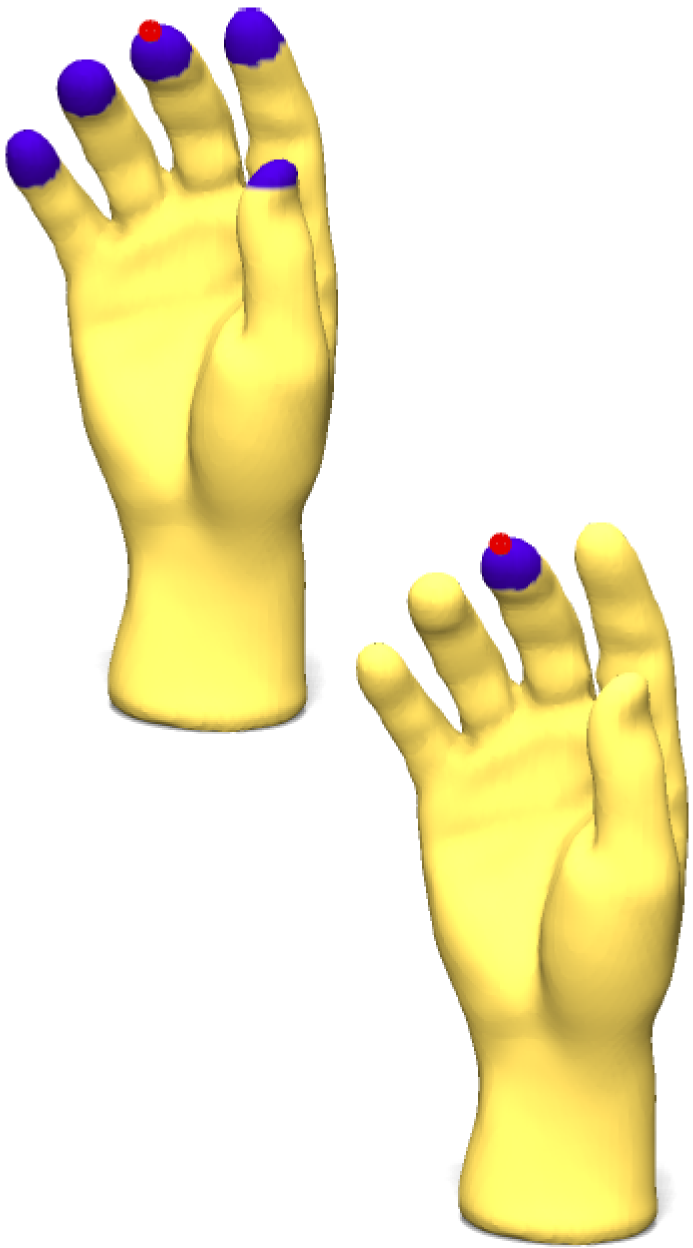

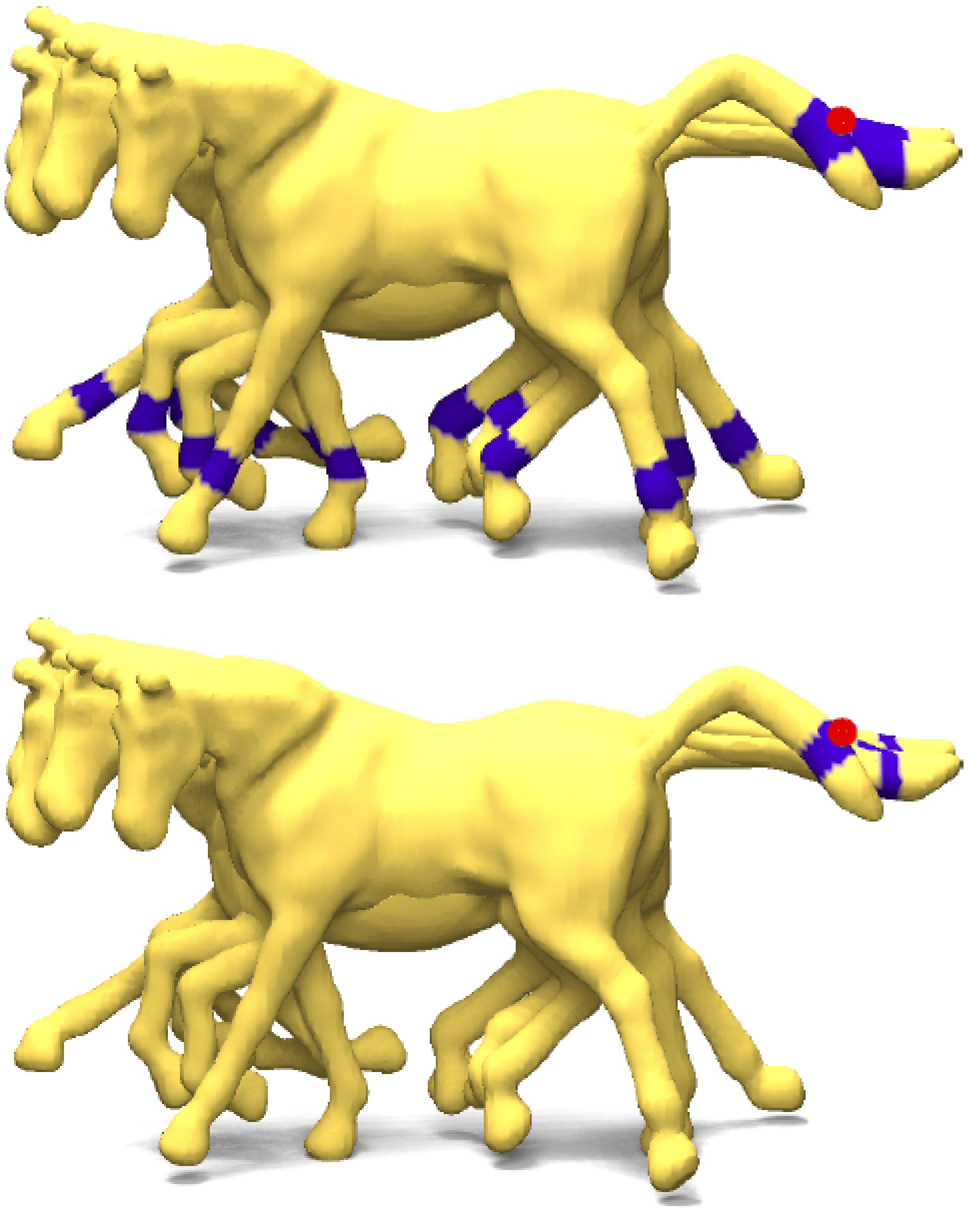

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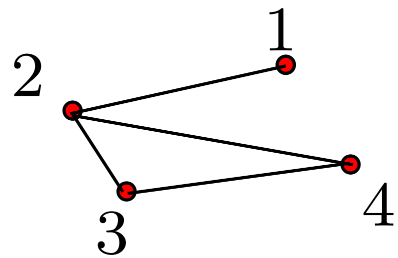
Graph Laplace Operator

- given an undirected graph G=(V, E),
  - Adjacency matrix A:

$$A(u,v) = \left\{ \begin{array}{ll} 1 & \text{if } u \sim v \\ 0 & \text{o.w.} \end{array} \right\}$$

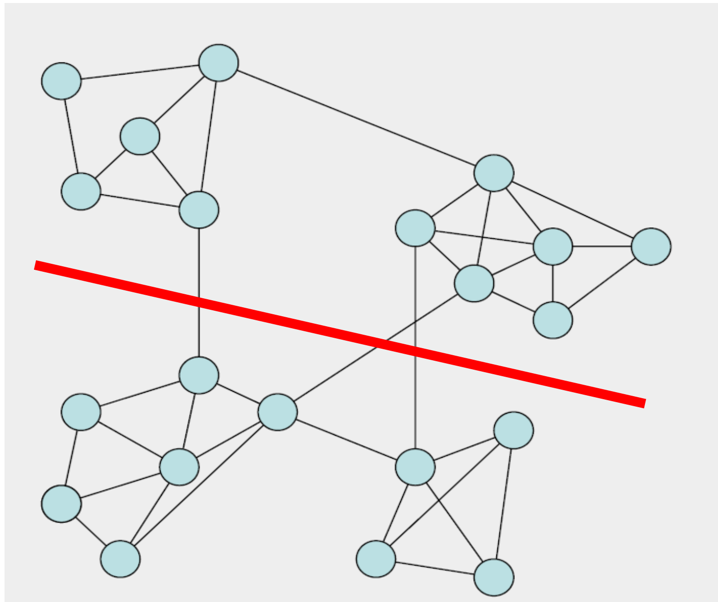


  - Diagonal degree matrix $D = diag(d_{v_1}, \cdots, d_{v_n})$
  - Graph Laplace Operator $L = D^{-1}(D - A)$
  - Tranistion probability matrix $W = D^{-1}A = I - L$,
  - $Wv = \lambda v$ implies $Lv = (1-\lambda)v$
  - 1 is the largest eigenvalue for W; 0 is the smallest eigenvalue for L.

Graph Partition Problem

- goal: find a cut with the smallest Cheeger ratio (conductance)
  - For $S \subset V$, volume of S: $vol(S) = \sum_{v \in S} d_v$
  - $\partial S = \{(u, v) \in E : u \in S \& v \in S\}$
  - Cheeger ratio of S, $h(S) = \frac{|\partial S|}{\min\{vol(S), vol(G) - vol(S)\}}$

- applications
  - clustering
  - segmentation
  - task partitioning for parallel processing
  - a preprocessing step to divide-and-conquer algorithms



Graph Partition Problem

- Rayleigh quotient $R(f) = \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_u f^2(u) d_u}$ for $f \neq 0$
  - find a boolean function f minimizing $R(f)$ $\quad \Leftarrow$ NP-complete
  - RELAXATION: find a real valued function f minimizing $R(f)$
  - $R(f) = \frac{< f, (D-A) f >}{< f, D f >}$
  - $\lambda_1 = \inf_f R(f) \;\Rightarrow\; \lambda_1$ and f are the first nonzero eigenvalue and eigenvector of L.

How good is this relaxation? Cheeger inequality

Cheeger Inequality

$$2h_G \geq \lambda_1 \geq \frac{h_f^2}{2} \geq \frac{h_G^2}{2}.$$

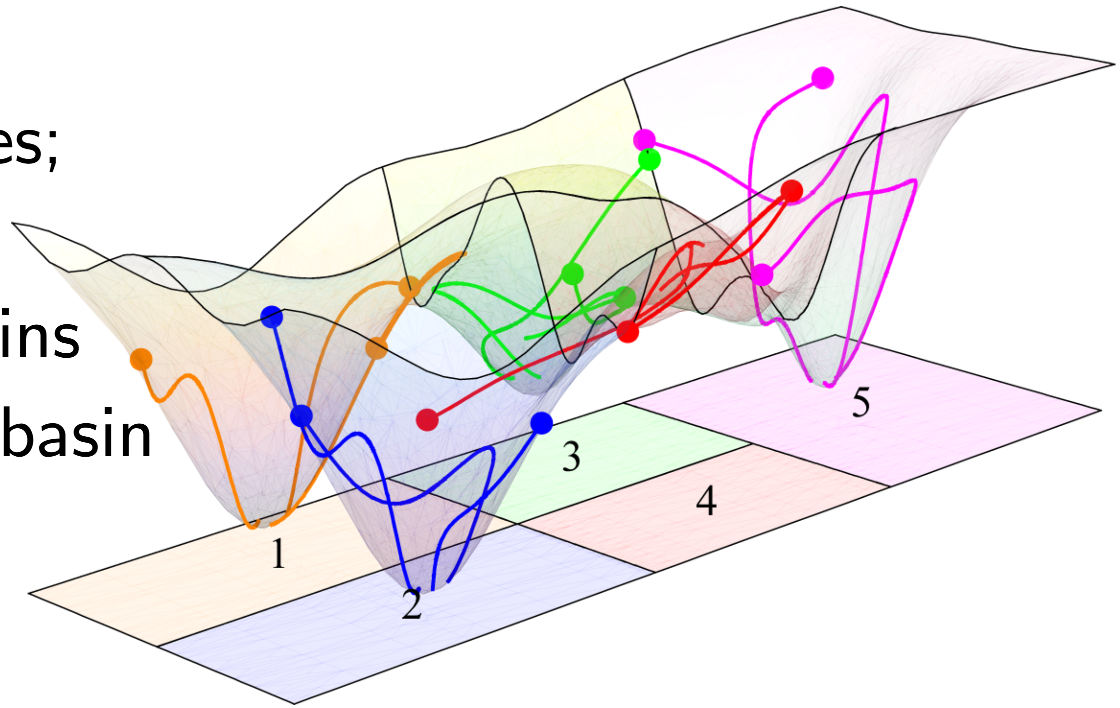
- f is the eigenvector of L corresponding to λ_1
- h_G is the smallest conductance (Cheeger ratio) of graph G
- h_f: the minimum Cheeger ratio determinded by a sweep of f
  - order the vertices: $f(v_1) \geq f(v_2) \geq \cdots \geq f(v_n)$.
  - $S_i = \{v_1, \cdots, v_i\}$
  - $h_f = \min_i h_{S_i}$
- find a partition whose conductance is within $2\sqrt{h_G}$

Local Graph Partition on Heat Kernel

- Heat kernel $H_t = e^{-tL} = I - tL + \cdots + (-1)^k \frac{t^k}{k!} L^k + \cdots$
  - induce a random walk on the graph
  - a version of local Cheeger inequality for local graph partition
  - see the following references for details:
    - "A local graph partitioning algorithm using heat kernel pagerank," WAW 2009, LNCS 5427, (2009), 62-75
    - "The heat kernel as the pagerank of a graph," PNAS, 105 (50), (2007), 19735–19740.

Cluster Biomolecular Folding Data

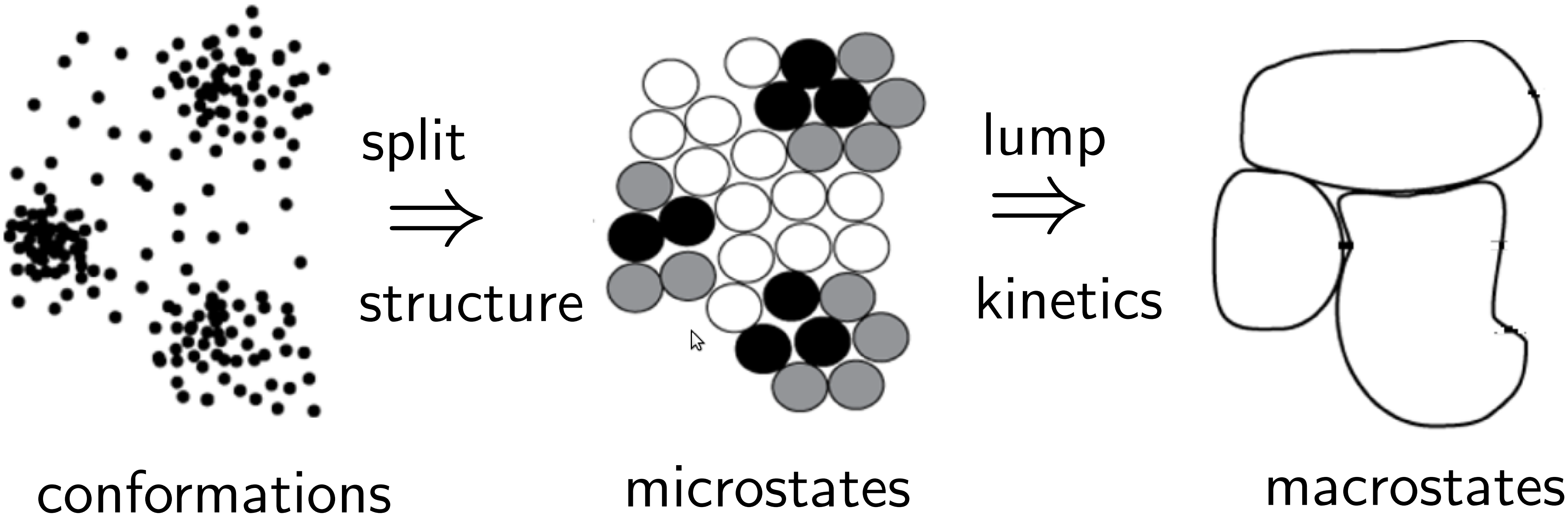
- molecular dynamics simulation
  - sample the energy landscape according to Boltzmann distribution
  - generate a set of trajectories;
  - sampled conformations concentrated at energy basins
  - lots of transitions within a basin but few across basins



- goal: cluster together the conformations within a basin

Cluster Biomolecular Folding Data

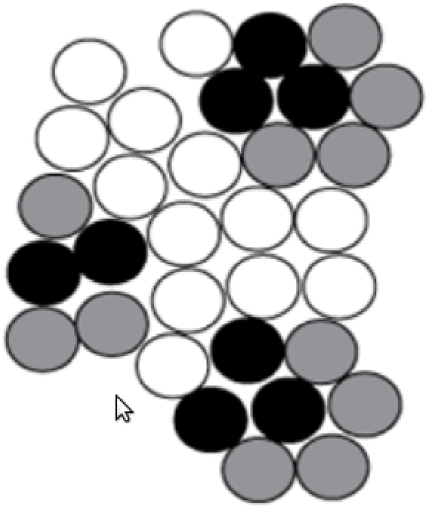
- a two stage approach



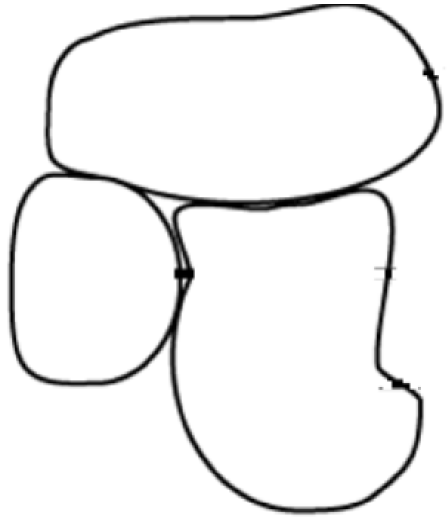
Cluster Biomolecular Folding Data

- a two stage approach

split
$\Rightarrow$
structure



lump
$\Rightarrow$
kinetics



conformations

microstates

macrostates

$\Uparrow$

RMSD,
k-center clustering

$\Uparrow$

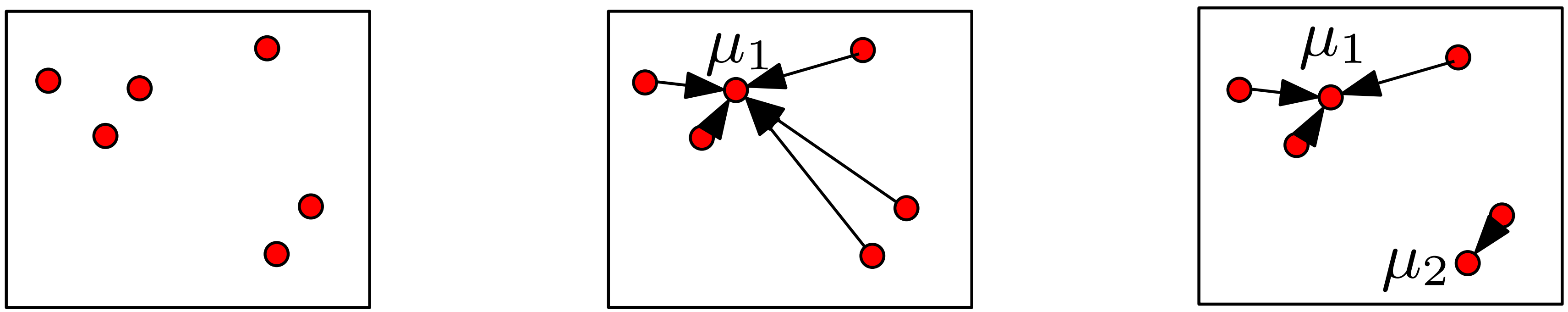
transition matrix,
spectral clustering

k-center clustering

- input: conformations in a metric space (RMSD) and a number k
- goal: obtain a partition of the points into clusters $C_1, \cdots, C_k$ with centers $\mu_1, \cdots, \mu_k$.
  - condition: minimize the maximum cluster radius:

$$\max_{i} \max_{x \in C_i} d(x, \mu_i)$$

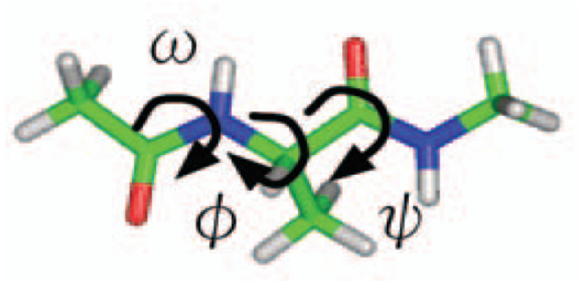
- NP-hard problem
- 2-approximation algorithm (greedy k-center algorithm)



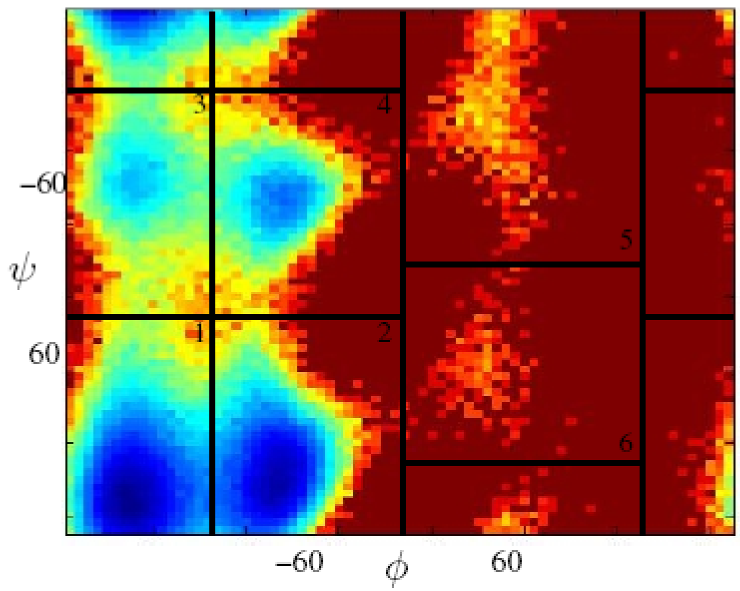
k-center clustering

- simple
- fast
  - Generate thousands of clusters from millions of conformations within several hours on a single machine
  - 20-60 times faster than K-means with triangle inequality
- Clusters have approximately equal radii, thus their size is a good indicator of the density.
  - note that accurate density estimation at high dimensional space is extremely difficult

Alanine dipeptide

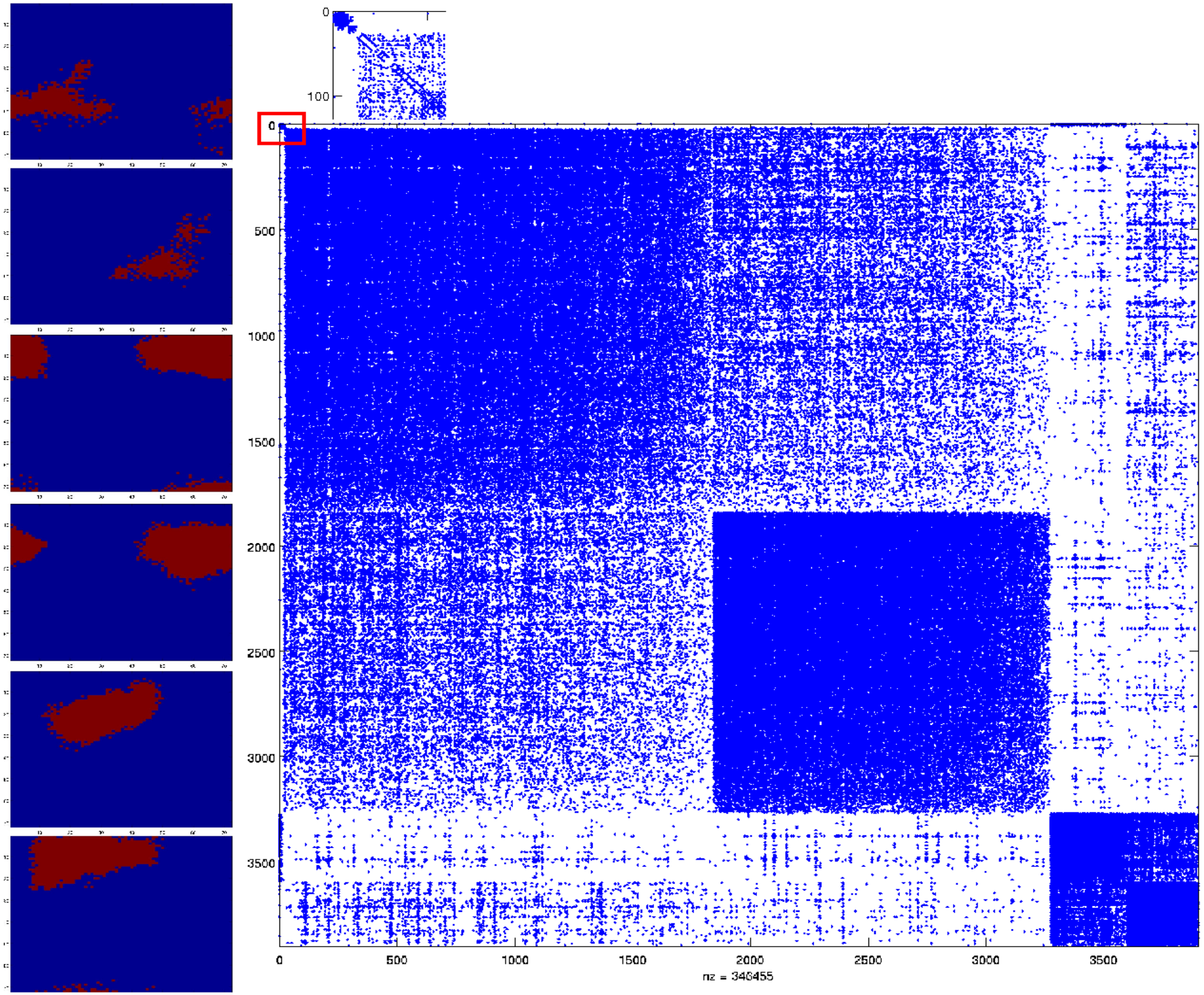


[Chodera et al. 2007]
975 trajectories
200 conformations per trajectory



density on $\phi - \psi$ plane

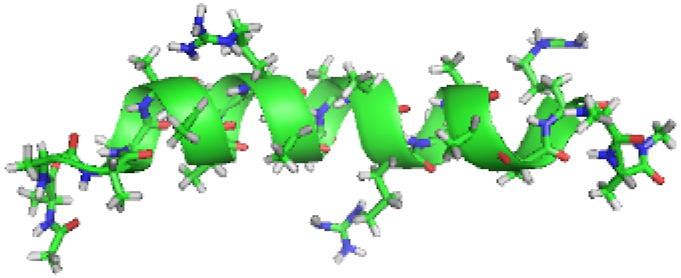
Alanine dipeptide



energy basins and re-indexed transition matrix

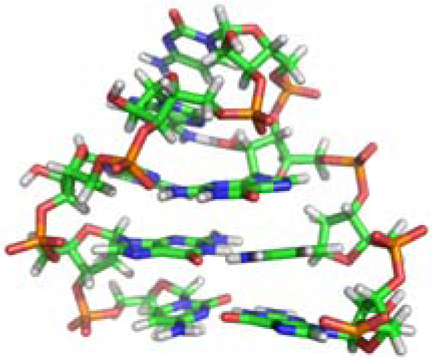
On Complicated Systems

- Fs-peptide



[Sun et al. submitted]

- RNA Hairpin



[Huang et al. PSB 2010]

Outline

- manifold Laplacian (Laplace-Beltrami operator)
  - detection of intrinsic symmetry
    - transforming theorem
  - heat kernel signature
    - informative theorem
- graph Laplacian
  - graph partition
    - Cheeger inequality
  - application on clustering biomolecule conformations
- relation between manifold Laplacian and graph Laplacian

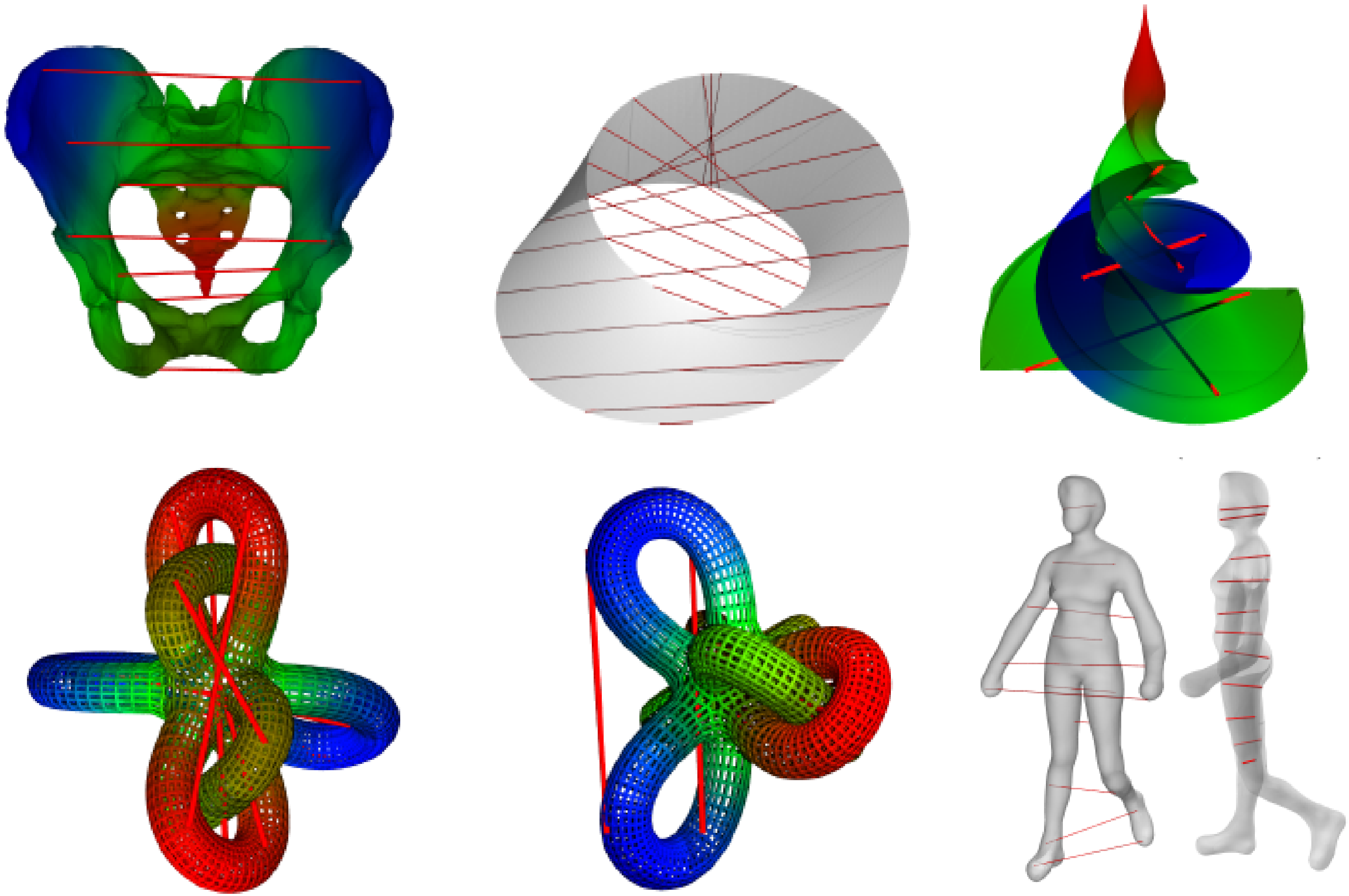
Graph Laplacian and Manifold Laplacian

- assume data points $x_1, \cdots, x_n$ are sampled from a uniform distribution on a manifold M [Belkin and Niyogi 05]
  - consider the complete graph G with nodes $\{x_i\}_{i=1}^n$
  - $A_{ij} = e^{-\frac{\|x_i - x_j\|^2}{4t}}$
  - $L = I - A$ in probability converges to Δ_M up to a constant

Thank you for your attention

Questions?

Results



Computation

- Laplace-Beltrami Operator:
  - based on its eigenfunctions and eigenvalues

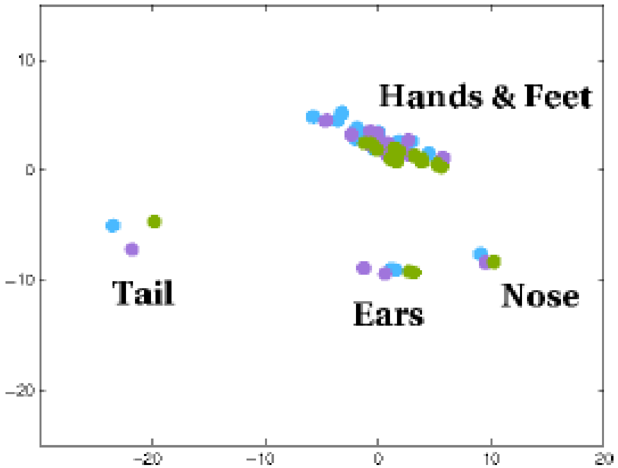
    $k_t(x, y) = \sum_i e^{-\lambda_i t} \phi_i(x)\phi_i(y)$

    $\Rightarrow \quad \mathsf{HKS}_x(t) = k_t(x, x) = \sum_i e^{-\lambda_i t} \phi_i^2(x)$

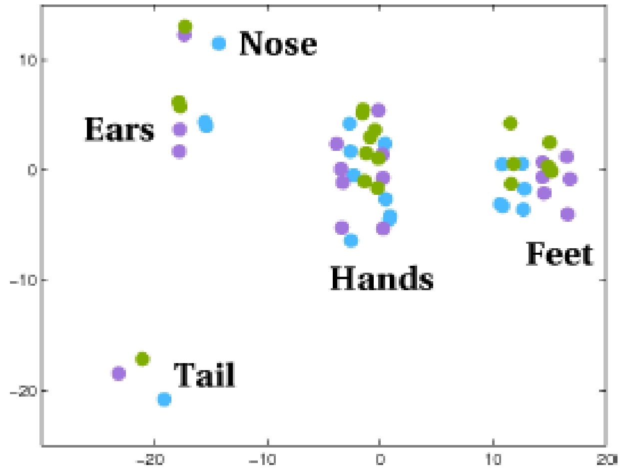
- discrete case:
  - build the discrete Laplace operator $L = A^{-1}W$ [BSW08]
  - solve $W\phi = \lambda A\phi$
  - compute $\mathsf{HKS}_x(t) = \sum_i e^{-\lambda_i t} \phi_i^2(x)$

Multi-Scale Matching

(a) maxima of $k_t(x, x)$ for a fixed t.



(b) $t = [0.1,\ 4]$



(c) $t = [0.1,\ 80]$

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  - second level bulletin
    - third level bulletin