Topology-Invariant Similarity and Diffusion Geometry

Lecture 7
Intrinsic similarity – limitations

Suitable for near-**isometric** shape deformations

Unsuitable for deformations modifying shape **topology**
Numerical geometry of non-rigid shapes  Topology-Invariant Similarity & Diffusion Geometry

Extrinsically dissimilar
Intrinsically similar

Extrinsically similar
Intrinsically dissimilar

Desired result:
THIS IS THE SAME SHAPE!
Joint extrinsic/intrinsic similarity

\[ Z = f(X) \]

\[ d_J(X, Y) = \min_{f: X \to \mathbb{R}^3} d_E(f(X), Y) + \lambda d_I(f(X), X) \]

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Glove fitting example

Misfit = Extrinsic dissimilarity

Stretching = Intrinsic dissimilarity

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Numerical geometry of non-rigid shapes

Topology-Invariant Similarity & Diffusion Geometry

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Computation of the joint similarity

\[
\min_Z d_E(Z, Y) + \lambda d_I(X, Z)
\]

- **Optimization variable**: the deformed shape vertex coordinates \( Z \)
- Assuming \( Z \) has the **connectivity** of \( X \)
- Split into computation of \( d_E(Z, Y) \) and \( d_I(X, Z) \)
- **Gradients** w.r.t. \( Z \) are required for optimization
Computation of the extrinsic term

- Find and fix correspondence $Y^*(Z)$ between current $Z$ and $Y$
- Can be e.g. the closest points

$$y^*(z) = \arg\min_{y \in Y} \|y - z\|$$

- Compute an $L_2$ variant of a one-sided Hausdorff distance

$$d_E(Z) = \text{trace}\left\{(Z - Y^*(Z))^T (Z - Y^*(Z))\right\}$$
$$= \|Z - Y^*(Z)\|_F^2$$

and its gradient

$$\frac{d}{dZ} d_E(Z) = 2(Z - Y^*(Z))^T$$

- Similar in spirit to ICP

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Computation of the intrinsic term

- Fix trivial correspondence $z_i \leftrightarrow x_i$ between $Z$ and $X$

- Compute $L_2$ distortion of geodesic distances

\[ d_1(Z) = \sum_{i,j} (d_X(x_i, x_j) - d_Z(z_i, z_j))^2 \]

\[ = ||D(X) - D(Z)||^2_F \]

and gradient

\[ \frac{d}{dZ} d_1(Z) = 2(D(X) - D(Z))^{\top} \frac{dD(Z)}{dZ} \]

- $D(X)$ is a fixed matrix of all pair-wise geodesic distances on $X$

- Can be precomputed using Dijkstra’s algorithm or fast marching

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Computation of the intrinsic term

- $D(Z)$ is a function of the optimization variables and needs to be recomputed.
- First option: modify the Dijkstra’s algorithm or fast marching to compute the gradient $dD(Z)/dZ$ in addition to the distance $D(Z)$ itself.
- Second option: compute and fix the path of the geodesic.

\[
D(Z) = \mathcal{I}D_{\text{loc}}(Z)
\]

- $D_{\text{loc}}(Z)$ is a matrix of Euclidean distances between adjacent vertices.
- $\mathcal{I}$ is a linear operator integrating the path length along fixed path.
Computation of the joint similarity

- **Alternating minimization** algorithm

1. Compute corresponding points  \( Y^*(Z) \)
2. Compute shortest paths and assemble  \( \mathcal{I} \)
3. Update  \( Z \) to sufficiently decrease

\[
\|Z - Y^*(Z)\|^2_F + \lambda \|D(X) - D(Z)\|^2_F
\]

4. If change is small, stop; otherwise, go to Step 1
Numerical example – dataset

Data: tosca.cs.technion.ac.il = topology change
Numerical example – intrinsic similarity

no topological changes
Numerical example – intrinsic similarity

- Insensitive to strong deformations
- Sensitive to topological changes $d_I$

- Red circle = topology-preserving
- Yellow circle = topology change
Numerical example – extrinsic similarity

- Insensitive to topological changes
- Sensitive to strong deformations

- \(d_E\)

\(\bullet\) = topology-preserving
\(\circ\) = topology change
Numerical example – joint similarity

Insensitive to topological changes...

...and to strong deformations

= topology-preserving  = topology change
Numerical example – ROC curves

- **Extrinsic**: EER=10.3%
- **Intrinsic**: EER=7.7%
- **Joint**: EER=1.6%

**Intrinsic, no topological changes**: EER=1.1%
Shape morphing

Stronger intrinsic similarity (larger $\lambda$)

Stronger extrinsic similarity (smaller $\lambda$)
Other intrinsic geometries

Geodesic distance

\[ d(x, x') = \min_{\Gamma} L(\Gamma) \]

is sensitive to topology changes

Possible more robust alternatives

- “Average path length”
- “Density of paths”
- Transition probability
Diffusion on manifolds

- **Kernel** *(aka affinity function)* $k : X \times X \rightarrow \mathbb{R}$
  - Non-negative $k(x, y) \geq 0$
  - Symmetric $k(x, y) = k(y, x)$
  - **Positive semi-definite**: for any $f : X \rightarrow \mathbb{R}$
    \[
    \int_{X \times X} k(x, y) f(x) f(y) \, da \, da \geq 0
    \]

- **Discrete case**: $N \times N$ symmetric positive semi-definite matrix $K$

- **Examples**:
  - Adjacency matrix
  - Heat kernel $k(x, y) = \exp \left\{ -\frac{d_X^2(x, y)}{t^2} \right\}$

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Diffusion on manifolds

- **Normalized** kernel \( \bar{p}(x, y) = \frac{k(x, y)}{v(x)} \)

  where \( v(x) = \int_X k(x, y) d\mu(y) \)

- Because of normalization \( \int_X \bar{p}(x, y) d\mu(y) = 1 \)

- \( \bar{p}(x, y) \) is no more symmetric

- **Symmetrized** kernel \( p(x, y) = \bar{p}(x, y) \sqrt{\frac{v(x)}{v(y)}} \)

- \( p(x, y) \) = probability of step from \( x \) to \( y \) by random walk

- **Discrete case: Markovian matrix** \( P \) (each row sums to 1)

Diffusion on manifolds

- Diffusion operator: \( P f(x) = \int_X p(x, y) f(y) d\mu(y) \quad f \in L^2(X) \)

- Discrete case: matrix \( P f \quad f \in \mathbb{R}^N \)

- Spectral theorem: the kernel of operator \( P \) admits the spectral decomposition

\[
p(x, y) = \sum_{i \geq 0} \lambda_i \phi_i(x) \phi_i(y)
\]

where \( \lambda_i \) and \( \phi_i(x) \) are eigenvalues and eigenfunctions of \( P \)

- Discrete case: \( P = \sum_{i \geq 0} \lambda_i u_i u_i^T \) where \( u_i \) are eigenvectors of \( P \)

Diffusion on manifolds

- **Power** of the diffusion operator

\[ P^m f(x) = \int_X p^{(m)}(x, y) f(y) d\mu(y) \]

where the kernel is

\[ p^{(m)}(x, y) = \sum_{i \geq 0} \lambda_i^m \phi_i(x) \phi_i(y) \]

- **Discrete case**: matrix power \( P^m \)

\[ p^{(m)}(x, y) = \text{transition probability from } x \text{ to } y \text{ in } m \text{ steps} \]
Diffusion distance

- **“Connectivity rate”** from $x$ to $y$ by paths of length $m$

\[
d_m^2(x, y) = p^{(m)}(x, x) + p^{(m)}(y, y) - 2p^{(m)}(x, y)
\]

- **Small** if there are many paths connecting $x$ and $y$
- **Large** if there are few paths connecting $x$ and $y

Diffusion distance

A mathematical exercise: find the kernel of $P^{2m}$

\[
P^{2m} f(x) = P^m P^m f(x) = \int_X p^{(m)}(x, z) \left( \int_X p^{(m)}(z, y) f(y) d\mu(y) \right) d\mu(z)
= \int_X \left( \int_X p^{(m)}(x, z) p^{(m)}(z, y) d\mu(z) \right) f(y) d\mu(y)
\]

\[
p^{(2m)}(x, y) = \int_X p^{(m)}(x, z) p^{(m)}(y, z) d\mu(z)
\]

Discrete case: $(P^{2m})_{ij} = \sum_k (P^m)_{ik} (P^m)_{kj} = \sum_k (P^m)_{ik} (P^m)_{jk}$

Diffusion distance

Substitute

\[ p^{(2m)}(x, y) = \int_X p^{(m)}(x, z)p^{(m)}(y, z)d\mu(z) \]

into diffusion distance

\[
\begin{align*}
\tilde{d}_{2m}^2(x, y) &= p^{(2m)}(x, x) + p^{(2m)}(y, y) - 2p^{(2m)}(x, y) \\
&= \int_X p^{(m)}(x, z)p^{(m)}(x, z)d\mu(z) + \int_X p^{(m)}(y, z)p^{(m)}(y, z)d\mu(z) \\
&\quad - 2\int_X p^{(m)}(x, z)p^{(m)}(y, z)d\mu(z) \\
&= \int_X \left( (p^{(m)}(x, z))^2 - 2p^{(m)}(x, z)p^{(m)}(y, z) + (p^{(m)}(y, z))^2 \right) d\mu(z) \\
&= \int_X \left( p^{(m)}(x, z) - p^{(m)}(y, z) \right)^2 d\mu(z)
\end{align*}
\]

Diffusion distance

\[ d_{2m}^2(x, y) = \int_X \left( p^{(m)}(x, z) - p^{(m)}(y, z) \right)^2 d\mu(z) \]

- \( p^{(m)}(x, \cdot) = \text{bump centered at } x \)
- Becomes wider as \( m \) increases
- \( d_{2m}(x, y) = \text{distance between two bumps} \)
  - Small if there is “cross-talk” between bumps
  - Large if bumps do not overlap
Kernels
Diffusion distance

Substitute \( p^{(m)}(x, y) = \sum_{i \geq 0} \lambda_i^m \phi_i(x) \phi_i(y) \)
into diffusion distance

\[
d_m^2(x, y) = p^{(m)}(x, x) + p^{(m)}(y, y) - 2p^{(m)}(x, y)
= \sum_{i \geq 0} \lambda_i^m (\phi_i(x) \phi_i(x) + \phi_i(y) \phi_i(y) - 2\phi_i(x) \phi_i(y))
= \sum_{i \geq 0} \lambda_i^m (\phi_i(x) - \phi_i(y))^2 = \sum_{i \geq 0} \left(\sqrt{\lambda_i^m} \phi_i(x) - \sqrt{\lambda_i^m} \phi_i(y)\right)^2
= \|\Phi_m(x) - \Phi_m(y)\|_2^2
\]

where \( \Phi_m(x) = \left(\sqrt{\lambda_0} \phi_0(x), \sqrt{\lambda_1} \phi_1(x), \ldots\right) \)

Canonical forms, bis

- $d_m$ is a metric on $X$

- $d_m$ is isometrically embeddable into $\ell^2$ by means of $\Phi_m : X \to \ell^2$

$$d_m = d_{\ell^2} \circ (\Phi_m \times \Phi_m)$$

- Infinitely dimensional canonical form ("diffusion map")

$$\Phi_m(x) = \left(\sqrt{\lambda_0 \phi_0(x)}, \sqrt{\lambda_1 \phi_1(x)}, \ldots\right)$$

- Truncated $\tilde{\Phi}_m(x) = \left(\sqrt{\lambda_0 \phi_0(x)}, \sqrt{\lambda_1 \phi_1(x)}, \ldots \sqrt{\lambda_n \phi_n(x)}\right)$

gives good convergence rate

$$d_m^2(x, y) = \|\tilde{\Phi}_m(x) - \tilde{\Phi}_m(y)\|_{\mathbb{R}^n}^2(1 + O(e^{-\alpha m}))$$
Diffusion maps

Canonical form

Diffusion map

No topology change

Topology change