Diffusion geometry in deformable shape analysis

Alex Bronstein, Michael Bronstein, Umberto Castellani

May 14, 2012

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Array of pixels

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Array of pixels



Splines, Mesh, Point cloud, etc

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Affine, projective

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Affine, projective



deformations

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Diffusion geometry in shape analysis



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Diffusion geometry in shape analysis



- Endow shapes with a structre
- Similarity, correspondence, retrieval, etc. = similarity and correspondence between structures

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- Endow shapes with a structre
- Similarity, correspondence, retrieval, etc. = similarity and correspondence between structures
- Invariance under bending, scale, affine transformations, etc.

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Local structure Point descriptors

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Glocal structure Stable regions **Local structure** Point descriptors

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Glocal structure Stable regions **Local structure** Point descriptors

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- Diffusion processes on surfaces
- Spectral point of view
- Global structure: diffusion geometry
- Local structure: diffusion kernel descriptors
- Semi-local structure: maximally stable components
- Extensions

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• Heat equation

$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

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governs heat propagation on manifold \boldsymbol{X}

• Heat equation

$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

governs heat propagation on manifold X

- Solution u(x, t): heat distribution at point x at time t
- Initial condition $u_0(x)$: heat distribution at time t = 0
- Boundary condition if manifold has a boundary

For two smooth functions $f,g:X
ightarrow\mathbb{R}$ and standard inner product on X

$$\langle f,g
angle = \int_X f(x)g(x)\,da$$

the Laplacian satisfies the following properties:

• Constant eigenfunction: $\Delta_X f = 0$ if f = const

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- Maximum principle: functions satisfying Δ_Xf = 0 (harmonic) have no minima/maxima in the interior of X

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• Surface X is *discretized* at *n* points {*x*₁,...,*x_n*} and points are connected to form a *triangular mesh*

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- Discrete version of the Laplacian

$$(L_X f)_i = \frac{1}{a_i} \sum_j w_{ij} (f_i - f_j)$$

 w_{ij} – edge weights, a_i vertex normalization coefficients.

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In matrix notation

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$$L_X f = A^{-1} L f$$

ere $A = \text{diag}\{a_i\}$ and $(L)_{ij} = \text{diag}\left\{\sum_{k \neq i} w_{ik}\right\} - w_{ij}$





Discrete Laplacian

$$w_{ij} = \left\{ egin{array}{ccc} 1 & : & x_j \in \mathcal{N}_1(x_i) \ 0 & : & ext{else} \end{array}
ight.$$

 $a_i = 1$ (umbrella operator); or $a_i = |\mathcal{N}_1(x_i)|$, valence (Tutte)

Discretized Laplacian

$$w_{ij} = \begin{cases} \cot \alpha_{ij} + \cot \beta_{ij} & : x_j \in \mathcal{N}_1(x_i) \\ 0 & : \text{ else} \end{cases}$$

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$$a_i =$$
sum of areas of triangles
sharing vertex x_i

• Constant eigenfunction: $\Delta_X f = 0$ if f = const

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• Constant eigenfunction: Satisfied by construction of L_X

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• Locality:
$$w_{ij} = 0$$
 if $x_j \neq \mathcal{N}_1(x_i)$

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- Constant eigenfunction: Satisfied by construction of L_X
- Symmetry: $L_X = L_X^T$ Reason: To have real eigenvalues and orthogonal eigenvectors
- Locality: w_{ij} = 0 if x_j ≠ N₁(x_i)
 w_{ij} stand for random walk transition probabilities along the graph edges.
- Linear precision: if X as a plane and f = ax + by + c, then $\Delta_X f = 0$

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Desired properties of discrete Laplacians

- Constant eigenfunction: Satisfied by construction of L_X
- Symmetry: $L_X = L_X^T$ Reason: To have real eigenvalues and orthogonal eigenvectors

• Linear precision: equivalently, if X is a plane, then

$$(L_X x)_i = \sum_j w_{ij}(x_i - x_j) = 0$$

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Reason: Flat plate must have zero bending energy.

• Positive semi-definiteness: $\langle \Delta_X f, f \rangle \geq 0$

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• Positive semi-definiteness: $f^{\mathrm{T}}L_X f \ge 0$, i.e., $L_X \succeq 0$

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- Positive semi-definiteness: $f^{T}L_{X}f \geq 0$, i.e., $L_{X} \succeq 0$
- Positive weights: $w_{ij} \ge 0$ and each vertex i has at least one $w_{ij} > 0$

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Reasons: Sufficient condition to satisfy discrete *maximum principle*

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Positive weights + Symmetry \Rightarrow PSD

- Positive semi-definiteness: $f^{T}L_{X}f \geq 0$, i.e., $L_{X} \succeq 0$
- Positive weights: w_{ij} ≥ 0 and each vertex i has at least one w_{ij} > 0
 Reasons: Sufficient condition to satisfy discrete maximum principle
 Positive weights + Symmetry ⇒ PSD
- Convergence: solution of discrete PDE with L_X converges to solution of continuous PDE with Δ_X as $n \to \infty$

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- Positive semi-definiteness: $f^{\mathrm{T}}L_X f \geq 0$, i.e., $L_X \succeq 0$
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Reasons: Sufficient condition to satisfy discrete maximum principle Positive weights + Symmetry \Rightarrow PSD

 Convergence: solution of discrete PDE with L_X converges to solution of continuous PDE with Δ_X as n → ∞
 Indispensable for discretization of PDE solutions

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• Discrete Laplacians are not convergent

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- cot weight discretized Laplacians is *convergent* but has *negative weights*

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- Many attempts have been made to construct discrete Laplacians satisfying above desired properties

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- Discrete Laplacians are not convergent
- cot weight discretized Laplacians is *convergent* but has *negative weights*
- Many attempts have been made to construct discrete Laplacians satisfying above desired properties
- "No free lunch theorem" (Wardetzky et al., 2007) There is no discrete Laplacian satisfying the above properties simultaneously!

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Eigendecomposition of Laplacian

• On *compact* domains Laplacian admits *countable orthogonal eigendecomposition*

$$\Delta_X \phi_i = \lambda_i \phi_i$$

 λ_i – eigenvalues; $\phi_i(x)$ – corresponding eigenfunctions

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• Discrete generalized eigendecomposition for $L_X = A^{-1}L$

$$A\Phi = \Lambda L\Phi$$

 $\Lambda = \operatorname{diag}\{\lambda_1, \dots, \lambda_k\} - \text{diagonal matrix of first } k \text{ eigenvalues} \\ \Phi - n \times k \text{ matrix of corresponding eigenvectors}$

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• Spectral decomposition theorem

$$(\Delta_X f)(x) = \sum_{i\geq 0} \lambda_i \phi_i(x) \cdot \langle \phi_i, f \rangle$$

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Discrete equivalent:
$$L_X f = \sum_{i \geq 0} \lambda_i \phi_i \phi_i^{\mathrm{T}} f$$

• Discretize $\{\lambda_i, \phi_i\}$ directly!

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- Weak form eigendecomposition

$$\langle \Delta_{\boldsymbol{X}} \phi, \alpha \rangle = \lambda \langle \phi, \alpha \rangle$$

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Fix a sufficiently regular basis {α₁,..., α_m} spanning a subspace of L²(X)

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- $\phi(x) \approx u_1 \alpha_1(x) + \cdots + u_m \alpha_m(x)$

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- Write a system of equations for $k=1,\ldots,m$

$$\sum_{i=1}^{m} u_i \langle \underbrace{\Delta_X \alpha_i, \alpha_j}_{a_{ij}} \rangle = \lambda \sum_{i=1}^{m} u_i \underbrace{\langle \alpha_i, \alpha_j \rangle}_{b_{ij}}$$

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- Weak form eigendecomposition

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• In matrix notation: $Au = \lambda Bu$

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• Solutions to stationary Helmholtz equation

 $\Delta_X f = \lambda f$

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• Solutions to stationary Helmholtz equation

$$\Delta_X f = \lambda f$$

• Laplacian *eigenfunctions* = plate vibration modes



(Reuter *et al.*, 2006) use Laplacian spectrum $\{\lambda_i\}$ as an isometry-invariant shape descriptor – *shape DNA*

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Shape DNA





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Shape similarity using Shape DNA

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"Can we hear the shape of the drum?"

• Isometric shapes are isospectral

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"Can we hear the shape of the drum?"

- Isometric shapes are isospectral
- Are isospectral shapes isometric?

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"Can we hear the shape of the drum?"

- Isometric shapes are isospectral
- Are isospectral shapes isometric?
- Can one hear the shape of the drum? (Mark Kac)



The following shape properties can be recovered ("heard") from the spectrum of the Laplacian:

Area

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The following shape properties can be recovered ("heard") from the spectrum of the Laplacian:

- Area
- Euler characteristic (genus)

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- Total Gaussian curvature

The following shape properties can be recovered ("heard") from the spectrum of the Laplacian:

- Area
- Euler characteristic (genus)
- Total Gaussian curvature
- Can we hear the metric?

One cannot hear the shape of the drum!



Counter example of isospectral non-isometric shapes (Gordon *et al.*, 1991)

Relation to harmonic analysis



1D signals

$$-\frac{d^2}{dx^2}e^{inx}=n^2e^{inx}$$

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Relation to harmonic analysis





1D signals

$$-\frac{d^2}{dx^2}e^{inx} = n^2 e^{inx}$$

3D shapes

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$$\Delta_X \phi_i(x) = \lambda_i \phi_i(x)$$

• Synthesis:
$$f(x) = \sum_{i \ge 0} F(\lambda_i)\phi_i(x)$$

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• Synthesis:
$$f(x) = \sum_{i \ge 0} F(\lambda_i)\phi_i(x)$$

• Analysis: $F(\lambda_i) = \int_X f(x)\phi_i(x)da = \langle f, \phi_i \rangle$

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$$\lambda = frequency$$

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• Synthesis:
$$f(x) = \sum_{i \ge 0} F(\lambda_i)\phi_i(x)$$

• Analysis: $F(\lambda_i) = \int_X f(x)\phi_i(x)da = \langle f, \phi_i \rangle$

•
$$\lambda = frequency$$

•
$$\{F(\lambda_i)\} = Fourier \ coefficients$$

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$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

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• Solution given by heat operator

$$u(x,t) = (\mathbf{H}^{t}u_{0})(x) = \int_{X} h_{t}(x,y)u_{0}(y)da(y)$$

• Heat equation

$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

• Solution given by heat operator

$$u(x,t) = (\mathbf{H}^t u_0)(x) = \int_X h_t(x,y) u_0(y) da(y)$$

 Heat kernel h_t(x, y) : solution at point x at time t with point heat source at y

Heat equation

$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

• Solution given by heat operator

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• Impulse response of heat equation

Heat equation

$$\left(\Delta_X + \frac{\partial}{\partial t}\right) u = 0$$

• Solution given by heat operator

$$u(x,t) = (\mathbf{H}^t u_0)(x) = \int_X h_t(x,y) u_0(y) da(y)$$

- Heat kernel h_t(x, y) : solution at point x at time t with point heat source at y
- Impulse response of heat equation
- Intrinsic quantity invariant to inelastic (isometric) bending

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Heat equation

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• Heat operator can be interpreted as a non shift-invariant version of convolution

Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis

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Probabilistic interpretation

• Brownian motion x(t) starts at point x



Probabilistic interpretation

• Brownian motion x(t) starts at point x



•
$$\Pr(x(t) \in C) = \int_C h_t(x, y) da(y)$$

Probabilistic interpretation

• Brownian motion x(t) starts at point x



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$$\Pr(x(t) \in C) = \int_C h_t(x, y) da(y)$$

• $h_t(x, y) = transition probability$ density from x to y by random walk of length t

• Let $\Delta_X \phi_i = \lambda_i \phi_i$ be the Laplacian eigendecomposition

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- Let $\Delta_X \phi_i = \lambda_i \phi_i$ be the Laplacian eigendecomposition
- By spectral decomposition theorem

$$h_t(x,y) = \sum_{i\geq 0} e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

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•
$$e^{-\lambda t} = frequency \ response$$
 of heat operator \mathbf{H}^t
 $(\mathbf{H}^t = e^{-\Delta_X t})$

• General diffusion operator

$$(\mathbf{K}u)(x) = \int_X k(x, y)u(y)da(y)$$

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• General diffusion operator

$$(\mathbf{K}u)(x) = \int_X k(x, y)u(y)da(y)$$

• Diffusion kernel

$$k(x,y) = \sum_{i\geq 0} K(\lambda_i)\phi_i(x)\phi_i(y)$$

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• $K(\lambda)$ = frequency response (lowpass filter)

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- \mathbf{K}^t is also a diffusion operator with response $K^t(\lambda)$

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- $K(\lambda) =$ frequency response (lowpass filter)
- \mathbf{K}^t is also a diffusion operator with response $K^t(\lambda)$
- A scale space of operators $\{\mathbf{K}^t\}_{t\geq 0}$

• Non-negativity: $k(x, y) \ge 0$

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- Non-negativity: $k(x, y) \ge 0$
- Symmetry: k(x, y) = k(y, x)

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$$\int \int k(x,y)f(x)f(y)da(x)da(y) \geq 0$$

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• Square integrability:

$$\int \int k^2(x,y) da(x) da(y) < \infty$$

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Conservation:

$$\int k(x,y)da(x)=1$$

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Properties of diffusion operators

- Non-negativity: $k(x, y) \ge 0$
- Symmetry: k(x, y) = k(y, x)
- Positive semidefiniteness: $K(\lambda_i) \ge 0$
- Square integrability: by Parseval's theorem

$$\sum_{i\geq 0} {\mathcal K}^2(\lambda_i) < \infty$$

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Properties of diffusion operators

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- Square integrability: by Parseval's theorem

$$\sum_{i\geq 0} {\mathcal K}^2(\lambda_i) < \infty$$

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• Conservation: by Perron-Frobenius theorem $\lambda_i \leq 1$

Diffusion geometry

• Family of *diffusion metrics*

$$d^{2}(x,y) = ||k(x,\cdot) - k(y,\cdot)||_{L^{2}(X)}^{2}$$

= $\int_{X} (k(x,z) - k(y,z))^{2} da(z)$

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Diffusion geometry

• Family of *diffusion metrics*

$$d^{2}(x,y) = ||k(x,\cdot) - k(y,\cdot)||_{L^{2}(X)}^{2}$$

=
$$\int_{X} (k(x,z) - k(y,z))^{2} da(z)$$

• Alternatively,

$$d^{2}(x,y) = \|K(\lambda_{i})\phi_{i}(x) - K(\lambda_{i})\phi_{i}(y)\|_{\ell^{2}}$$
$$= \sum_{i\geq 0} K^{2}(\lambda_{i})(\phi_{i}(x) - \phi_{i}(y))^{2}$$

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• Equivalent due to Parseval's theorem

Diffusion geometry

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- Equivalent due to Parseval's theorem
- $\{\mathbf{K}^t\}_{t\geq 0}$ define a scale space of metrics $\{d_t\}_{t\geq 0}$

• Heat diffusion metric

•
$$K(\lambda) = e^{-\lambda t}$$

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- Heat diffusion metric
- $K(\lambda) = e^{-\lambda t}$
- $d_t^2(x,y) =$

$$\sum_{i\geq 0} e^{-2\lambda_i t} (\phi_i(x) - \phi_i(y))^2$$

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Commute time metric
K(λ) = 1/√λ

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- Heat diffusion metric
- $K(\lambda) = e^{-\lambda t}$
- $d_t^2(x, y) =$

$$\sum_{i\geq 0} e^{-2\lambda_i t} (\phi_i(x) - \phi_i(y))^2$$

• Commute time metric

•
$$K(\lambda) = \frac{1}{\sqrt{\lambda}}$$

• $d^2(x, y) =$

$$\sum_{i\geq 1} \frac{1}{\lambda_i} (\phi_i(x) - \phi_i(y))^2$$

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• "Connectability" of x and y by random walks of length t

- Heat diffusion metric
- $K(\lambda) = e^{-\lambda t}$
- $d_t^2(x, y) =$

$$\sum_{i\geq 0} e^{-2\lambda_i t} (\phi_i(x) - \phi_i(y))^2$$

• Commute time metric

•
$$K(\lambda) = \frac{1}{\sqrt{\lambda}}$$

•
$$d^2(x, y) =$$

$$\frac{1}{2}\int_0^\infty d_t^2(x,y)dt$$

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- Heat diffusion metric
- $K(\lambda) = e^{-\lambda t}$
- $d_t^2(x, y) =$

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• "Connectability" by random walks of any length

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- Heat diffusion metric
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• "Connectability" by random walks of any length

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Scale invariant!

$$\Phi(x) = \{K(\lambda_i)\phi_i(x)\}_{i\geq 0}$$

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 $\Phi(x) = \{K(\lambda_i)\phi_i(x)\}_{i\geq 0}$

• $\Phi(x)$ are embedding coordinates of x in ℓ^2 (" \mathbb{R}^{∞} ")

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$$\Phi(x) = \{K(\lambda_i)\phi_i(x)\}_{i\geq 0}$$

- $\Phi(x)$ are embedding coordinates of x in ℓ^2 (" \mathbb{R}^{∞} ")
- By Parseval's theorem

$$\begin{split} \|\Phi(x) - \Phi(y)\|_{\ell^2}^2 &= \sum_{i>0} K^2(\lambda_i) (\phi_i(x) - \phi_i(y))^2 \\ &= d^2(x, y) \end{split}$$

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• Diffusion distance is represented by *Euclidean distance* in embedding space



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• Embed one shape into the other



- Embed one shape into the other
- Find minimum distortion correspondence

$$\min_{\varphi:X\to Y} \|d_X - d_Y \circ (\varphi \times \varphi)\|$$

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- Embed one shape into the other
- Find minimum distortion correspondence (e.g., L2 norm)

$$\min_{\varphi:X\to Y} \int \int (d_X(x,x') - d_Y(\varphi(x),\varphi(x')))^2 da(x) da(x')$$

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- Embed one shape into the other
- Find minimum distortion correspondence (e.g., L2 norm)

$$\min_{\varphi:X\to Y} \int \int (d_X(x,x') - d_Y(\varphi(x),\varphi(x')))^2 da(x) da(x')$$

• Solved using generalized multidimensional scaling



• Represent shape as distribution of diffusion distances



- Represent shape as distribution of diffusion distances
- Compare shapes using *divergence* of distributions



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Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis

Particular case I: Rustamov's GPS embedding



Particular case II: Mahmoudi & Sapiro



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• Diffusion distances generated by other norms, e.g. $\|\cdot\|_{L^1(X)}$



- Diffusion distances generated by other norms, e.g. $\|\cdot\|_{L^1(X)}$
- Construct (or learn) optimal task-specific diffusion kernels







Global structure Metric space Glocal structure Stable regions **Local structure** Point descriptors

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Diffusion kernel descriptors



• Associate each point x with a vector $(k_{t_1}(x, x), \dots, k_{t_n}(x, x))$

(Sun *et al.*, SGP'09)

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Diffusion kernel descriptors



- Associate each point x with a vector $(k_{t_1}(x, x), \dots, k_{t_n}(x, x))$
- Multi-scale *point-wise descriptor*

(Sun et al., SGP'09)

Diffusion kernel descriptors



- Associate each point x with a vector $(k_{t_1}(x, x), \dots, k_{t_n}(x, x))$
- Multi-scale *point-wise descriptor*
- Heat kernel signature (HKS): $x \mapsto (h_{t_1}(x, x), \dots, h_{t_n}(x, x))$

(Sun et al., SGP'09)

Heat kernel signature



$$h_t(x,x) = \frac{1}{4\pi t} \left(1 + \frac{1}{3} \kappa(x) t + \mathcal{O}(t^2) \right)$$

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 $\kappa(x) =$ Gaussian curvature at point x (Sun *et al.*, SGP'09)

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- Original shape
- Eigenvalues λ_i
- Eigenfunctions $\phi_i(x)$
- Heat kernel $h_t(x, x)$



- Scaled by $\frac{1}{\alpha}$
- Eigenvalues $\alpha^2 \lambda_i$
- Eigenfunctions $\alpha \phi_i(x)$
- Heat kernel $\alpha^2 h_{\alpha^2 t}(x, x)$

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• Not scale invariant!





$\begin{array}{l} \text{Scale} \rightarrow \\ \text{shift} + \text{factor} \end{array}$

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Scale invariance



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Scale invariance



(B&Kokkinos, CVPR'09)

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(B&Kokkinos, CVPR'09)

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• Let C(p) be a curve on manifold X

- Let C(p) be a curve on manifold X
- Demand $det(x_1, x_2, C_{pp}) = 1$ and obtain *equi-affine invariant* arclength

$$dp^{2} = \det(x_{1}, x_{2}, x_{11}du_{1}^{2} + 2x_{12}du_{1}du_{2} + x_{22}du_{2}^{2}) = \tilde{g}_{11}du_{1}^{2} + 2\tilde{g}_{12}du_{1}du_{2} + \tilde{g}_{22}du_{2}^{2}$$

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where $\tilde{g}_{ij} = \det(x_1, x_2, x_{ij})$

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where $\tilde{g}_{ij} = \det(x_1, x_2, x_{ij})$

• Construct invariant pre-metric tensor

$$\hat{g}_{ij} = \tilde{g}_{ij} |\det \tilde{g}|^{-1/4}$$

where $|\det \tilde{g}|^{-1/4}$ guarantees reparametrization invariance

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Positive definite only on *convex* surfaces

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- Positive definite only on *convex* surfaces
- Construct g from \hat{g} enforcing positivity of eigenvalues

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- Demand $det(x_1, x_2, C_{pp}) = 1$ and obtain *equi-affine invariant* arclength

$$dp^{2} = \det(x_{1}, x_{2}, x_{11}du_{1}^{2} + 2x_{12}du_{1}du_{2} + x_{22}du_{2}^{2}) = \tilde{g}_{11}du_{1}^{2} + 2\tilde{g}_{12}du_{1}du_{2} + \tilde{g}_{22}du_{2}^{2}$$

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• Construct invariant pre-metric tensor

$$\hat{g}_{ij} = \tilde{g}_{ij} |\det \tilde{g}|^{-1/4}$$

where $|\det \tilde{g}|^{-1/4}$ guarantees reparametrization invariance

- Positive definite only on *convex* surfaces
- Construct g from \hat{g} enforcing positivity of eigenvalues
- g is a valid metric on manifolds with non-vanishing curvature

- Define equi-affine Laplacian Δ_g
- Equi-affine Laplacian + scale-invariance = affine-invariance



Fusing geometric and photometric information



Fusing geometric and photometric information



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Fusing geometric and photometric information



Color = embedding



metric h_{ij}

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Color = embedding



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• Given point-wise descriptor $\mathbf{h}(x)$

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- Given point-wise descriptor **h**(*x*)
- Quantize each **h** in a fixed vocabulary $V = {\mathbf{v}_1, \dots, \mathbf{v}_n}$

Image: A image: A



- Given point-wise descriptor **h**(*x*)
- Quantize each **h** in a fixed vocabulary $V = {\mathbf{v}_1, \dots, \mathbf{v}_n}$
- Bag-of-words shape descriptor

$$\mathsf{H} = \int_X \mathsf{v}(x) d\mathsf{a}(x)$$



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• Spatially-sensitive bags of pairs of words

$$\mathbf{H} = \int_{X imes X} \mathbf{v}(x) \mathbf{v}(y) h_t(x, y) da(x) da(y)$$

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 $\bullet\,$ Given a bag-of-features descriptor ${\boldsymbol{\mathsf{H}}}'$ of a part $Y'\subset\,Y$

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- Given a bag-of-features descriptor \mathbf{H}' of a part $Y' \subset Y$
- Find part $X' \subset X$ with equal area such that the descriptor

$$\mathbf{H} = \int_{X'} \mathbf{v} d\mathbf{a}$$

best matches \mathbf{H}'

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- $\bullet\,$ Given a bag-of-features descriptor H' of a part $Y'\subset\,Y$
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best matches \mathbf{H}'

• Regularize part boundary length a lá Mumford-Shah

$$\min_{X'} \left\| \int_{X'} \mathbf{v} da - \mathbf{H}' \right\|^2 + \mu L(\partial X') \quad \text{s.t.} \quad A(X') = A(Y')$$

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• Ambrosio-Tortorelli approximation

$$\min_{u,\rho} \left\| \int_X \mathbf{v} u d\mathbf{a} - \mathbf{H}' \right\|^2 + \mu_1 \int_X \rho^2 \|\nabla u\|^2 d\mathbf{a} + \mu_2 \epsilon \int_X \|\nabla \rho\|^2 d\mathbf{a}$$

$$+ \frac{\mu_2}{4\epsilon} \int_X (1-\rho)^2 da \text{ s.t. } \int_X u da = A(Y')$$

Alex Bronstein, Michael Bronstein, Umberto Castellani



Global + local structures



Global structure Metric space **Local structure** Point descriptors

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Correspondence encore



• Find minimum distortion correspondence

$$\min_{\varphi:X \to Y} \|d_X - d_Y \circ (\varphi \times \varphi)\|$$

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Correspondence encore



• Find minimum distortion correspondence

$$\min_{\varphi: X \to Y} \| d_X - d_Y \circ (\varphi \times \varphi) \| + \mu \| \mathbf{h}_X - \mathbf{h}_Y \circ \varphi \|$$

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- d_X, d_Y global structures $\mathbf{h}_X, \mathbf{h}_Y$ – local structures
- Combine local and global structure distortion

Heat kernel signature encore



Poor spatial feature localization!

Aubry et al., CVPR'11; B, PAMI'11

Alex Bronstein, Michael Bronstein, Umberto Castellani

Heat kernel signature encore



• Collection of *low pass filters*

$$\mathbf{p}(x) = \sum_{k \ge 0} \begin{pmatrix} p_1(\lambda_k) \\ \vdots \\ p_n(\lambda_k) \end{pmatrix} \phi_k^2(x)$$
$$p_i(\lambda) = \exp(-\lambda t_i)$$

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Wave kernel signature

• Different physical model: a quantum particle with initial energy distribution $f(\nu)$.



Alex Bronstein, Michael Bronstein, Umberto Castellani

Diffusion geometry in shape analysis

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Wave kernel signature

- Different physical model: a quantum particle with initial energy distribution $f(\nu)$.
- Described by the Schrödinger equation

$$\left(i\Delta+\frac{\partial}{\partial t}\right)\psi(x,t) = 0$$

Aubry et al., CVPR'11

Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion ge

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- $|\psi(x,t)|^2$ = probability to find particle at point x at time t.
- Solution in spectral domain

$$\psi(x,t) = \sum_{k\geq 0} e^{i\nu_k t} f(\nu_k) \phi_k(x)$$

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Aubry et al., CVPR'11

• Family of log-normal initial energy distributions

$$f_e(
u) \propto \exp\left(-rac{(\log e - \log
u)^2}{2\sigma^2}
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Aubry et al., CVPR'11

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$$p_e(x) = \lim_{T \to \infty} \frac{1}{T} \int_0^T |\psi(x, t)|^2 dt = \sum_{k \ge 1} f_e^2(\nu_k) \phi_k^2(x)$$

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Aubry et al., CVPR'11

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• Each point is associated the wave kernel signature

$$\mathbf{p}(x): x \mapsto (p_{e_1}(x), \dots, p_{e_n}(x))$$

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Aubry et al., CVPR'11



• Collection of band pass filters

$$\mathbf{p}(x) = \sum_{k \ge 0} \begin{pmatrix} p_1(\nu_k) \\ \vdots \\ p_n(\nu_k) \end{pmatrix} \phi_k^2(x)$$
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Aubry et al., CVPR'11

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- Better spatial feature localization
- Lower discriminativity

Aubry et al., CVPR'11; B, PAMI'11

Alex Bronstein, Michael Bronstein, Umberto Castellani



• WKS has higher *sensitivity* than HKS (better at low FPR)

B, PAMI'11



• WKS has higher *sensitivity* than HKS (better at low FPR)

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• Yet has lower specificity (worse at low FNR)



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- Yet has lower specificity (worse at low FNR)
- WKS is better for *correspondence* problems



- WKS has higher *sensitivity* than HKS (better at low FPR)
- Yet has lower specificity (worse at low FNR)
- WKS is better for *correspondence* problems
- HKS is better for shape retrieval problems

B, PAMI'11

• Localization: changes a lot under a small displacement on the surface.



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- Localization: changes a lot under a small displacement on the surface.
- **Sensitivity**: a small set of best matches should contain a correct match with high probability.

B. PAMI'11

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Image: A image: A

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Image: A image: A

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- Localization: changes a lot under a small displacement on the surface.
- **Sensitivity**: a small set of best matches should contain a correct match with high probability.
- **Discriminativity**: distinguish between shapes belonging to different classes.
- **Invariance**: invariant (insensitive) to a class of transformations.
- Efficiency: maximum information per number of dimensions.

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• Build optimal spectral descriptor of the form

$$\mathbf{p}(x) = \sum_{k\geq 0} \begin{pmatrix} f_1(\nu_k) \\ \vdots \\ f_n(\nu_k) \end{pmatrix} \phi_k^2(x)$$

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- Similar in spirit to Wiener filter.
 - attenuate frequencies with large noise content (deformation)

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- pass frequencies with large signal content (discriminative geometric features)
- Hard to model axiomatically
- ...yet easy to *learn* from examples!

• To do learning, we need a *finite* set of parameters

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Parametrization

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- Problem: each shape has distinct eigen-frequencies $\{\nu_i\}$.



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- Independent parametrization: select basis functions

$$\{b_1(\nu),\ldots,b_m(\nu)\}$$

spanning a sufficiently wide interval of frequencies $[0, \nu_{\rm max}]$

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• Represent responses as

$$\begin{pmatrix} f_1(\nu) \\ \vdots \\ f_n(\nu) \end{pmatrix} = \mathbf{A} \begin{pmatrix} b_1(\nu) \\ \vdots \\ b_m(\nu) \end{pmatrix}$$

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with the matrix of parameters A

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• Select sufficiently large s for which $\nu_s \geq \nu_{\max}$

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- Select sufficiently large s for which $\nu_s \geq \nu_{\max}$
- Represent the point descriptor

$$\mathbf{p}(x) = \sum_{k \ge 0} \begin{pmatrix} f_1(\nu_k) \\ \vdots \\ f_n(\nu_k) \end{pmatrix} \phi_k^2(x)$$
$$\approx \mathbf{A} \begin{pmatrix} b_1(\nu_1) & \cdots & b_1(\nu_s) \\ \vdots & \ddots & \vdots \\ b_m(\nu_1) & \cdots & b_m(\nu_s) \end{pmatrix} \begin{pmatrix} \phi_1^2(x) \\ \vdots \\ \phi_s^2(x) \end{pmatrix} = \mathbf{Ag}(x)$$

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• Geometry vector **g** consistently represents all geometric information at point *x*.



x a point, x₊ a knowingly similar point (*positive*), x₋ a knowingly dissimilar point (*negative*).



Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis

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- x a point, x₊ a knowingly similar point (*positive*), x₋ a knowingly dissimilar point (*negative*).
- $\bullet~g,g_+,g_-$ corresponding geometry vectors.

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- $\mathbf{p}, \mathbf{p}_+, \mathbf{p}_-$ corresponding descriptors.

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- $\mathbf{p}, \mathbf{p}_+, \mathbf{p}_-$ corresponding descriptors.
- Simultaneously maximize $d(\mathbf{p}, \mathbf{p}_{-})$ and minimize $d(\mathbf{p}, \mathbf{p}_{+})$.

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- Using Euclidean distance on descriptor space

$$\begin{aligned} d_{\pm}^2 &= \|\mathbf{p} - \mathbf{p}_{\pm}\|^2 = \|\mathbf{A}(\mathbf{g} - \mathbf{g}_{\pm})\|^2 \\ &= (\mathbf{g} - \mathbf{g}_{\pm})^{\mathrm{T}} \mathbf{A}^{\mathrm{T}} \mathbf{A} (\mathbf{g} - \mathbf{g}_{\pm}). \end{aligned}$$

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• Mahalanobis distance on geometry vectors space.

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- Mahalanobis distance on geometry vectors space.
- Mahalanobis *metric learning* problem.
• Taking expectation over positive/negative pairs

$$\begin{split} \mathbb{E}\{d_{\pm}^2\} &= \mathbb{E}\left\{\|\mathbf{p} - \mathbf{p}_{\pm}\|^2\right\} = \mathbb{E}\left\{(\mathbf{g} - \mathbf{g}_{\pm})^{\mathrm{T}} \mathbf{A}^{\mathrm{T}} \mathbf{A} (\mathbf{g} - \mathbf{g}_{\pm})\right\} \\ &= \mathrm{tr}\left\{\mathbf{A} \mathbb{E}((\mathbf{g} - \mathbf{g}_{\pm}) (\mathbf{g} - \mathbf{g}_{\pm})^{\mathrm{T}}) \mathbf{A}^{\mathrm{T}}\right\} \\ &= \mathrm{tr}\left\{\mathbf{A} \mathbf{C}_{\pm} \mathbf{A}^{\mathrm{T}}\right\} \end{split}$$

Strecha, Fua, BB, PAMI'11; B, PAMI'11

Alex Bronstein, Michael Bronstein, Umberto Castellani

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• Taking expectation over positive/negative pairs

$$\mathbb{E}\{d_{\pm}^{2}\} = \mathbb{E}\{\|\mathbf{p} - \mathbf{p}_{\pm}\|^{2}\} = \mathbb{E}\{(\mathbf{g} - \mathbf{g}_{\pm})^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}(\mathbf{g} - \mathbf{g}_{\pm})\}$$

$$= \operatorname{tr}\{\mathbf{A}\mathbb{E}((\mathbf{g} - \mathbf{g}_{\pm})(\mathbf{g} - \mathbf{g}_{\pm})^{\mathrm{T}})\mathbf{A}^{\mathrm{T}}\}$$

$$= \operatorname{tr}\{\mathbf{A}\mathbf{C}_{\pm}\mathbf{A}^{\mathrm{T}}\}$$

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• C_{\pm} is the *covariance matrix* of positives/negatives $\mathbf{g} - \mathbf{g}_{\pm}$.

Strecha, Fua, BB, PAMI'11; B, PAMI'11

• Taking expectation over positive/negative pairs

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- \textbf{C}_{\pm} is the *covariance matrix* of positives/negatives $\textbf{g}-\textbf{g}_{\pm}.$
- Minimize weighted difference

min
$$(1-\alpha)\mathbb{E}(d_+^2) - \alpha\mathbb{E}(d_-^2)$$

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Strecha, Fua, BB, PAMI'11; B, PAMI'11

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- C_{\pm} is the *covariance matrix* of positives/negatives $\mathbf{g} \mathbf{g}_{\pm}$.
- Minimize weighted difference

min tr {A(
$$(1 - \alpha)$$
C₊ - α C₋)A^T}

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Strecha, Fua, BB, PAMI'11; B, PAMI'11

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- C_{\pm} is the *covariance matrix* of positives/negatives $g g_{\pm}$.
- Minimize weighted difference

min tr $\{\mathbf{A}\mathbf{D}_{\alpha}\mathbf{A}^{\mathrm{T}}\}$

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Strecha, Fua, BB, PAMI'11; B, PAMI'11

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- C_{\pm} is the *covariance matrix* of positives/negatives $\mathbf{g} \mathbf{g}_{\pm}$.
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min tr
$$\{\mathbf{A}\mathbf{D}_{\alpha}\mathbf{A}^{\mathrm{T}}\}$$

• α controls tradeoff between *sensitivity* ($\alpha \rightarrow 1$) and *specificity* ($\alpha \rightarrow 0$).

Strecha, Fua, BB, PAMI'11; B, PAMI'11 Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis



• Scale of A is arbitrary!

B, PAMI'11

Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis

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- Scale of **A** is arbitrary!
- Recall *efficiency*: dimensions of **p** should be *statistically independent*



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- Scale of **A** is arbitrary!
- Recall *efficiency*: dimensions of **p** should be *statistically independent uncorrelated*



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- Scale of **A** is arbitrary!
- Recall *efficiency*: dimensions of **p** should be *statistically independent uncorrelated*

$$\mathbf{I} = \mathbb{E}(\mathbf{p}\mathbf{p}^{\mathrm{T}}) = \mathbf{A}\mathbb{E}(\mathbf{g}\mathbf{g}^{\mathrm{T}})\mathbf{A}^{\mathrm{T}} = \mathbf{A}\mathbf{C}\mathbf{A}^{\mathrm{T}}$$

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B, PAMI'11

- Scale of **A** is arbitrary!
- Recall *efficiency*: dimensions of **p** should be *statistically independent uncorrelated*

$$\mathbf{I} = \mathbb{E}(\mathbf{p}\mathbf{p}^{\mathrm{T}}) = \mathbf{A}\mathbb{E}(\mathbf{g}\mathbf{g}^{\mathrm{T}})\mathbf{A}^{\mathrm{T}} = \mathbf{A}\mathbf{C}\mathbf{A}^{\mathrm{T}}$$

• Minimization problem

$$\label{eq:min_star} \underset{\textbf{A}}{\text{min}} \ \mathrm{tr} \left\{ \textbf{A} \textbf{D}_{\alpha} \textbf{A}^{\mathrm{T}} \right\} \quad \mathrm{s.t.} \quad \textbf{A} \textbf{C} \textbf{A}^{\mathrm{T}} = \textbf{I}$$

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- Recall *efficiency*: dimensions of **p** should be statistically independent uncorrelated

$$\mathbf{I} = \mathbb{E}(\mathbf{p}\mathbf{p}^{\mathrm{T}}) = \mathbf{A}\mathbb{E}(\mathbf{g}\mathbf{g}^{\mathrm{T}})\mathbf{A}^{\mathrm{T}} = \mathbf{A}\mathbf{C}\mathbf{A}^{\mathrm{T}}$$

Minimization problem

$$\min_{\mathbf{A}} \ \mathrm{tr} \left\{ \mathbf{A} \mathbf{D}_{\alpha} \mathbf{A}^{\mathrm{T}} \right\} \quad \mathrm{s.t.} \quad \mathbf{A} \mathbf{C} \mathbf{A}^{\mathrm{T}} = \mathbf{I}$$

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• Solution: $\mathbf{A} = \mathbf{U}_n^{\mathrm{T}} \mathbf{C}^{-1/2}$ where \mathbf{U}_n are the *n* smallest eigenvectors of $\mathbf{C}^{-1/2} \mathbf{D}_{\alpha} \mathbf{C}^{-1/2}$.

B, PAMI'11



• Optimal filters (invariance learned from positive and negative examples)

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• Better specificity and sensitivity than HKS and WKS

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B, PAMI'11



- Better spatial feature localization than WKS
- Better discriminativity than HKS

B, PAMI'11



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• Better performance in correspondence problems

B, PAMI'11

• Spectral descriptors lack *orientation* information



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Kokkinos, Litman, BB, CVPR'12

Alex Bronstein, Michael Bronstein, Umberto Castellani

Diffusion geometry in shape analysis

- Spectral descriptors lack *orientation* information
- Given a vector field p on surface, compute its distribution over a local polar system of coordinate



Kokkinos, Litman, BB, CVPR'12

- Spectral descriptors lack *orientation* information
- Given a vector field p on surface, compute its distribution over a local polar system of coordinate
- Intrinsic shape context (ISC)
 a meta-descriptor



Kokkinos, Litman, BB, CVPR'12



Tangent plane map Inward shooting Outward shooting

• Problem I: no global coordinate system

Kokkinos, Litman, BB, CVPR'12



Tangent plane map Inward shooting Outward shooting

- Problem I: no global coordinate system
- Local chart has to be created

Kokkinos, Litman, BB, CVPR'12



Tangent plane map Inward shooting Outward shooting

- Problem I: no global coordinate system
- Local chart has to be created
- Problem II: arbitrary angular coordinate

Kokkinos,Litman,BB, CVPR'12



Tangent plane map

Inward shooting

Outward shooting

- Problem I: no global coordinate system
- Local chart has to be created
- Problem II: arbitrary angular coordinate
- Undone using Fourier transform modulus

Kokkinos, Litman, BB, CVPR'12



Scale Invariant HKS

Intrinsic Shape Context

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Kokkinos, Litman, BB, CVPR'12

Alex Bronstein, Michael Bronstein, Umberto Castellani

Diffusion geometry in shape analysis



Alex Bronstein, Michael Bronstein, Umberto Castellani

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Global structure Metric space Glocal structure Stable regions **Local structure** Point descriptors

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• Measure proximity d(x, y) in some local neighborhood $y \in \mathcal{N}(x)$

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- Measure proximity d(x, y) in some local neighborhood $y \in \mathcal{N}(x)$
- t = 0: start with single points forming disjoint clusters
- For increasing t merge clusters C_1 and C_2 if

$$d(C_1, C_2) = \min_{\substack{x \in C_1 \\ y \in C_2}} d(x, y) \le t$$

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- Measure proximity d(x, y) in some local neighborhood y ∈ N(x)
- t = 0: start with single points forming disjoint clusters
- For increasing t merge clusters C_1 and C_2 if

$$d(C_1, C_2) = \min_{\substack{x \in C_1 \\ y \in C_2}} d(x, y) \le t$$

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• Single-linkage agglomerative clustering

- Measure proximity d(x, y) in some local neighborhood y ∈ N(x)
- t = 0: start with single points forming disjoint clusters
- For increasing t merge clusters C_1 and C_2 if

$$d(C_1, C_2) = \min_{\substack{x \in C_1 \\ y \in C_2}} d(x, y) \le t$$

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- Single-linkage agglomerative clustering
- Hierarchy described as component tree

Component trees



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• Stability of a component

$$\sigma(C_t) = \frac{A(C_t)}{\frac{dA(C_t)}{dt}}$$

- Measures relative change of area as function of change of threshold
- (Better stability functions are available)



• Stability of a component

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$$\sigma(C_t) = \frac{A(C_t)}{\frac{dA(C_t)}{dt}}$$

- Measures relative change of area as function of change of threshold
- (Better stability functions are available)
- Maximally stable components: local maximizers of σ



Maximally stable components



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Is our model good?



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Volume isometry



Preserves geodesic distances inside the volume

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Boundary isometry





Preserves geodesic distances on the boundary surface

Volume isometry



Preserves geodesic distances inside the volume

3.0



• *Boundary isometry* does not always represent a realistic deformation

(image: Sumner)

Alex Bronstein, Michael Bronstein, Umberto Castellani Diffusion geometry in shape analysis



- *Boundary isometry* does not always represent a realistic deformation
- May change volume of the solid

(image: Sumner)



- Boundary isometry does not always represent a realistic deformation
- May change volume of the solid
- Solution: *volumetric* diffusion geometry

(image: Sumner)

Boundary diffusion

$$\left(\Delta_{\partial X}+\frac{\partial}{\partial t}\right)u(x,t) = 0$$

where $u: \partial X \times [0,\infty) \to \mathbb{R}$ $\Delta_{\partial X}$ - Laplace-Beltrami operator

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Boundary diffusion

$$\left(\Delta_{\partial X}+rac{\partial}{\partial t}
ight)u(x,t) = 0$$

Volumetric diffusion

$$egin{aligned} & \left(\Delta+rac{\partial}{\partial t}
ight)U(x,t)=0,\,x\in\mathrm{int}(X)\ & \left<
abla U(x,t),n(x)
ight>=0,\,x\in\partial X \end{aligned}$$

where

 $u: \partial X \times [0,\infty) \to \mathbb{R}$ $\Delta_{\partial X}$ - Laplace-Beltrami operator where

 $U: X \times [0,\infty) o \mathbb{R}$ Δ - Euclidean Laplace operator n - normal to ∂X

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$$k_t(x,y) = \sum_{i\geq 0} e^{-\lambda_i t} \phi_i(x) \phi_i(y)$$

where $\Delta_{\partial X} \phi_i(x) = \lambda_i \phi_i(x)$

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Volumetric heat kernels

$$\mathcal{K}_t(x,y) = \sum_{i\geq 0} e^{-\Lambda_i t} \Phi_i(x) \Phi_i(y)$$

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where
$$\Delta \Phi_i(x) = \Lambda_i \Phi_i(x)$$

 $\langle \nabla \Phi_i(x), n(x) \rangle = 0, x \in \partial X$

 $k_t(x,y) = \sum_{i\geq 0} e^{-\lambda_i t} \phi_i(x) \phi_i(y)$

where
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Volumetric heat kernels

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Geometric interpretation $k_t(x,x) \approx \frac{1}{4\pi t} \left(1 + \frac{1}{6}\kappa(x)\right)$

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$$\Delta \Phi_i(x) = \Lambda_i \Phi_i(x)$$

 $\langle \nabla \Phi_i(x), n(x) \rangle = 0, \ x \in \partial X$

Geometric interpretation $K_t(x,x) \approx \frac{1}{(4\pi t)^{3/2}} \left(1 + \frac{1}{6}s(x)\right)$

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Volumetric maximally stable components



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• Diffusion processes on manifolds

- Diffusion processes on manifolds
- Spectrum of the Laplacian

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- Diffusion processes on manifolds
- Spectrum of the Laplacian
- Global structure: diffusion geometry

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- Diffusion processes on manifolds
- Spectrum of the Laplacian
- Global structure: diffusion geometry
- Local structure: diffusion kernel signatures

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- Diffusion processes on manifolds
- Spectrum of the Laplacian
- Global structure: diffusion geometry
- Local structure: diffusion kernel signatures
- Semi-local structure: maximally stable components

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- Diffusion processes on manifolds
- Spectrum of the Laplacian
- Global structure: diffusion geometry
- Local structure: diffusion kernel signatures
- Semi-local structure: maximally stable components
- Extensions

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Numerical Geometry of Non-Rigid Shapes

On paper: Springer, 2008 (~ 35\$) *Online:* tosca.cs.technion.ac.il/book

- Problems & Solutions
- Tutorials, Slides & Videos
- Code & Data
- Links



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