Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion

Estimating metrics suitable to an empirical manifold of shapes, using transport against the curse of dimensionality

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Pulsar Project

INRIA Workshop on Statistical Learning IHP

05/12/2011

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion

Мар

- Introduction
 - Motivation
 - Issues
- Searching for solutions
 - Main existing approaches and their limitations
 - Main idea
- The approach
 - Shape matching
 - Transport
 - Metric estimation (statistics on deformations)
 - Theory
- Future work

Introduction ●○○	Searching for solutions	Shape matching	Transport 00000	Metric estimation	Theory 000	Conclusion
Motivation						

Image Segmentation

- Find a contour in a given image
- The best curve for a given segmentation criterion
- Criterion based on color homogeneity, texture, edge detectors, etc.



Image



Segmentation

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Motivation						

Image Segmentation

Find the best contour for a given criterion

Variational Method

- Energy E to minimize with respect to a curve C
- Compute the derivative of the energy
- Gradient descent: $\partial_t C = -\nabla E(C)$
- ► Initialization → local minimum
- Other methods: graph cuts (suitable for few energies)

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Motivation						

Image Segmentation

Find the best contour for a given criterion

Variational Method

- Minimize criterion by gradient descent with respect to the contour
- Most criteria: no shape information



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Motivation						

Image Segmentation

Find the best contour for a given criterion

Variational Method

Minimize criterion by gradient descent with respect to the contour

Shape Statistics

- Sample set of contours from already segmented images
- Shape variability ?
- Shape prior ?

Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion
Motivation						

- Shape spaces : which metric ?
 - (to define similarity/distance between shapes)
 - Hausdorff distance
 - Symmetric difference area
 - Quotients by transformation groups (rotation, translation, scaling, affine...)



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion
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- Shape spaces : which metric ? (to define similarity/distance between shapes)
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- Shape evolution, morphing : priors on probable deformations ?
 - \implies Which local metric on deformations ?

(metric on the manifold of shapes)



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 - (metric on the manifold of shapes)
 - L² norm of instantaneous deformations
 - L² + curvature, H¹
 - \blacktriangleright rigid motion more probable \implies associated metric

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 - rigid motion more probable \implies associated metric



 L^2 inner product





rigidifying inner product

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 - L² norm of instantaneous deformations
 - L² + curvature, H¹
 - \blacktriangleright rigid motion more probable \implies associated metric

$\blacktriangleright \implies$ learn the suitable metric from examples (datasets of shapes)

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Introduction ○○●	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion
Issues						

- Sparse sets of highly varying shapes
 - e.g. human silhouettes
 - high intrinsic dimension (\geq 30)
 - $\blacktriangleright \implies$ no dense training set



Guillaume Charpiat Metrics that suit an empirical manifo<u>ld of shapes</u>

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Metrics that suit an empirical manifold of shapes

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Metrics that suit an empirical manifold of shapes

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Metrics that suit an empirical manifold of shapes

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- Sparse sets of highly varying shapes
 - e.g. human silhouettes
 - ▶ high intrinsic dimension (≥ 30)
 - no dense training set



 to compare quantities defined on different shapes : need for correspondences

- match shape with different topologies ?
- very frequent topological changes



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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion
State of the art						

Searching for solutions

Main existing approaches and their limitations

Approach 1 : *mean* + *modes* model

Approach 2 : distance-based approaches, such as kernel methods

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State of the art						

• Mean M, shapes S_i , warpings $W_{M \to S_i}$



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• Mean *M*, shapes S_i , warpings $W_{M \to S_i}$



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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• Mean M, shapes S_i , warpings $W_{M \to S_i}$



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
State of the art						

- Mean M, shapes S_i , warpings $W_{M \to S_i}$
- ▶ PCA : diagonalize correlation matrix C : $C_{ij} = \langle W_{M \to S_i} | W_{M \to S_i} \rangle$
 - \implies eigenmodes e_k with eigenvalues λ_k : best coordinate system



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
State of the art						

- ▶ Mean *M*, shapes S_i , warpings $W_{M \to S_i}$
- ▶ PCA : diagonalize correlation matrix C : $C_{ij} = \langle W_{M \to S_i} | W_{M \to S_j} \rangle$ ⇒ eigenmodes e_k with eigenvalues λ_k : best coordinate system
- ▶ any new deformation *W* of *M* :

$$W = \sum_{k} \alpha_k e_k + \text{ noise}$$



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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• Mahalanobis distance : $d(M + W, (S)) = \sum_{k} \frac{\alpha_{k}^{2}}{\lambda_{k}^{2}}$



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- Mahalanobis distance : $d(M + W, (S)) = \sum_{k} \frac{\alpha_{k}^{2}}{\lambda_{k}^{2}}$
- ► associated inner product on deformations, in the tangent space of *M*: $\langle W_1 | W_2 \rangle = \sum_k \frac{1}{\lambda_k^2} \alpha_{1,k} \alpha_{2,k}$



Guillaume Charpiat Metrics that suit an empirical manifold of shapes

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- ► associated inner product on deformations, in the tangent space of *M*: $\langle W_1 | W_2 \rangle = \sum_k \frac{1}{\lambda_k^2} \alpha_{1,k} \alpha_{2,k}$
- defines a deformation cost $||W||^2 = \langle W |W \rangle$



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▶ probability $p(W) \propto exp(-\sum_k \frac{\alpha_k^2}{2\lambda_k^2})$: Gaussian distribution



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▶ probability
$$p(W) \propto exp(-\sum_{k} \frac{\alpha_k^2}{2\lambda_k^2})$$
: Gaussian distribution

defines a Gaussian shape prior



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Empirical distribution : $\mathcal{D}_{emp} = \sum_{i} \delta_{W_{M \to S_i}}$ (possibly smoothed by a kernel)



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► Empirical distribution : $\mathcal{D}_{emp} = \sum_{i} \delta_{W_{M \to S_i}}$ (possibly smoothed by a kernel)

Any inner product < | >_P in tangent space of the mean ⇒ Gaussian distribution D_P(W) ∝ exp(-||W||²_P)



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State of the ar	t					

► Empirical distribution : $\mathcal{D}_{emp} = \sum_{i} \delta_{W_{M \to S_i}}$ (possibly smoothed by a kernel)

Any inner product $\langle | \rangle_P$ in tangent space of the mean \Rightarrow Gaussian distribution $\mathcal{D}_P(W) \propto \exp(-||W||_P^2)$

▶ Best *P* for Kullback-Leibler($\mathcal{D}_P | \mathcal{D}_{emp}$) : PCA!



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Approach 1 : mean + modes model

\hookrightarrow example from my PhD thesis



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Statistics (PCA) on deformation fields

between the mean shape and each sample



modes of deformation = deformation prior = Gaussian probabilistic model

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Example of application : image segmentation with shape prior



without shape prior



with shape prior

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Example of application : image segmentation with shape prior



without shape prior



with shape prior

requires a mean shape (does not always make sense, e.g. person walking)

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Example of application : image segmentation with shape prior



without shape prior



with shape prior

requires a mean shape (does not always make sense, e.g. person walking) Δ

requires all deformations between the mean and samples : \implies relatively similar sample shapes (otherwise, not reliable)

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- Kernel : symmetric definite positive function k(x, y)
- Expresses the similarity between x and y
- ▶ Typically, the Gaussian kernel : $k(x, y) = exp(-d(x, y)^2)$
- For each point x_i : $k_i(y) := k(x_i, y)$

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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- choice of a distance, of a kernel ?
- distance between 2 shapes : not much informative (wrt deformations)
- rebuild geometry of space of shapes from distances ?
- distances are not reliable/meaningful for far shapes
- needs for a representative neighborhood, i.e. a high dataset density (not affordable)

Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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State of the art	:					



- choice of a distance, of a kernel ?
- distance between 2 shapes : not much informative (wrt deformations)
- rebuild geometry of space of shapes from distances ?
- distances are not reliable/meaningful for far shapes
- \blacktriangleright \implies needs for a representative neighborhood, i.e. a high dataset density
- in a high-dimensional manifold, all distances are similar, and all points are on the boundary of the manifold
- $lacksim \Longrightarrow$ cannot work, need for more information than distances

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion
Main idea						

- consider deformations (not just distances)
- should not require high density of training set
- no magic (to handle/interpolate sparse sets) : add a prior

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- no magic (to handle/interpolate sparse sets) : add a prior
- prior chosen : transported deformations make sense,
 - i.e. a deformation observed on one shape can be applied to other shapes



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transport requires correspondences

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- transport requires correspondences
- but shape matching reliable only for close shapes

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- prior chosen : transported deformations make sense,
 - i.e. a deformation observed on one shape can be applied to other shapes



- transport requires correspondences
- but shape matching reliable only for close shapes
- compute correspondences between close shapes only, and combine small steps of reliable correspondences to build longer-distance correspondences

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Main idea						

Мар

- Close shape matching
- Transport
- Metric estimation (statistics on transported deformations)
- Theoretical justifications

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Close shape mat	tching					

Shape matching

Simple case : two shapes, A and B, with one connected component



$$\inf_{f:A\to B} \int_{A} \|f\|^2 + \alpha \|\nabla f\|^2 dA$$

- shape sampling
- dynamic time warping
- theory & experiments :

higher sampling rate on target





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Metrics that suit an empirical manifold of shapes

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Shape matching

Simple case : two shapes, A and B, with one connected component



$$\inf_{f:A\to B}\int_{A}\|f\|^{2}+\alpha\|\nabla f\|^{2}dA$$

- shape sampling
- dynamic time warping
- theory & experiments :
 - higher sampling rate on target

Usual case : random topologies



Usual cases = more complex (more than 10 connected components in this silhouette) but one connected component $\rightarrow \bigcup_{i}$ connected components = the same

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Close shape mat	tching					

Further possible improvements

- as such, allows appearing points (mismatches)
- > allows disappearing points : matching to \varnothing with a fixed high cost
- pb : better matchings, but energy value loses meaning

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Close shape mat	tching					

Further possible improvements

- as such, allows appearing points (mismatches)
- > allows disappearing points : matching to \varnothing with a fixed high cost
- pb : better matchings, but energy value loses meaning

Drawbacks

- specific to planar curves
- not symmetric : $m_{A \to B} = m_{B \to A}^{-1}$

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Local transport						

Local transport

Set of shapes $(S_i)_{i \in I}$ (e.g. from a video segmentation)

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Local transport						

Local transport

- Set of shapes $(S_i)_{i \in I}$ (e.g. from a video segmentation)
- ▶ Two shapes S_i and $S_j \implies$ their correspondence field $m_{i \rightarrow j}$



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Transport (translation, naive) :



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Local transport						

Local transport

- Set of shapes $(S_i)_{i \in I}$ (e.g. from a video segmentation)
- ▶ Two shapes S_i and $S_j \implies$ their correspondence field $m_{i \rightarrow j}$
- Transport (translation, naive) :

$$egin{array}{lll} orall \ h: S_j
ightarrow \mathcal{X}, & T^L_{j
ightarrow i}(h): \ S_i \
ightarrow \mathcal{X} \ & \left(T^L_{j
ightarrow i}(h)
ight)(s) \ = \ h\left(m_{i
ightarrow j}(s)
ight) \end{array}$$

Associated cost : $E(m_{i \rightarrow j}) \implies$ reliability $w_{i \rightarrow j}^L \propto \exp\left(-\alpha E(m_{i \rightarrow j})\right)$

Introduction	Searching for solutions	Shape matching	Transport ○●○○○	Metric estimation	Theory	Conclusion
Global transport						

Global transport

- ► Associated cost : $E(m_{i \to j}) \implies$ reliability $w_{i \to j}^L \propto \exp\left(-\alpha E(m_{i \to j})\right)$
- close shapes : reliable; distant shapes : not reliable
- $\blacktriangleright \implies$ search for paths of small steps in the training set (S_i)
- graph : nodes = shapes, edges = transport, weights = transport cost
- shortest path between pairs of shapes : global transport



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Global transport

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- $\blacktriangleright \implies$ search for paths of small steps in the training set (S_i)
- graph : nodes = shapes, edges = transport, weights = transport cost
- shortest path between pairs of shapes : global transport
- ► compose : $T_{i \to j}^{\mathcal{G}} = T_{i_n \to j}^{\mathcal{L}} \circ T_{i_{n-1} \to i_n}^{\mathcal{L}} \circ \dots \circ T_{i_1 \to i_2}^{\mathcal{L}} \circ T_{i \to i_1}^{\mathcal{L}}$

• reliability :
$$w_{i \rightarrow j}^{G} = \prod_{i} w_{i_k \rightarrow i_{k+1}}^{L}$$

use transport to propagate information



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Metrics that suit an empirical manifold of shapes

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Transported arm rotation (translation)

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Transported arm rotation (better)

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Transported forearm rotation

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Transported forearm rotation (better)

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Transport to another shape

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Transported forearm rotation (translation)

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Transported forearm rotation (better)

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Transported arm rotation (translation)

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Transported arm rotation (better)

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Remarks about transport

Why ?

transport : of deformations : needed to increase training set density

Which ?

- "translation" : ok for short pathes
- transport : not obvious (muscles + T-shirt artifacts)
- criterion to assess transport quality / suitability ?
- transport : should be learned (from video sequences ?)
- path could depend on deformation transported

What properties ?

- probability of a deformation transported : can differ
- inner product : no reason to be transport-invariant

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Transport in differential geometry

A connection ∇ is **Riemannian** if the parallel transport it defines preserves the metric *g*. Metric connection :

 $abla_X g(\cdot, \cdot) = 0$ for all vector fields X on \mathcal{M}

- not satisfied (probability of a deformation depends on the shape)
 - \implies **not Riemannian** : transport and metric are independent

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Transport in differential geometry

A connection ∇ is **Riemannian** if the parallel transport it defines preserves the metric *g*. Metric connection :

 $abla_X g(\cdot, \cdot) = 0$ for all vector fields X on \mathcal{M}

not satisfied (probability of a deformation depends on the shape)

⇒ not Riemannian : transport and metric are independent

Transport \implies connection

Given transport, under few hypotheses (e.g. smoothness), it is possible to recover the associated infinitesimal connection :

$$\nabla_X V = \lim_{h \to 0} \left. \frac{T_{\gamma}^{h \to 0} V_{\gamma(h)} - V_{\gamma(0)}}{h} = \left. \frac{d}{dt} T_{\gamma}^{t \to 0} V_{\gamma(t)} \right|_{t=0}.$$

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Introduction	Searching for solutions	Shape matching	Transport 0000●	Metric estimation	Theory	Conclusion
Global transport						

Transport in differential geometry

A connection ∇ is **Riemannian** if the parallel transport it defines preserves the metric *g*. Metric connection :

 $abla_X g(\cdot, \cdot) = 0$ for all vector fields X on \mathcal{M}

not satisfied (probability of a deformation depends on the shape)

 \implies not Riemannian : transport and metric are independent

Transport \implies connection

Given transport, under few hypotheses (e.g. smoothness), it is possible to recover the associated infinitesimal connection :

$$\nabla_X V = \lim_{h \to 0} \frac{T_{\gamma}^{h \to 0} V_{\gamma(h)} - V_{\gamma(0)}}{h} = \left. \frac{d}{dt} T_{\gamma}^{t \to 0} V_{\gamma(t)} \right|_{t=0}.$$

Connection \implies **transport**: Given a covariant derivative ∇ , the transport along a curve γ is obtained by integrating the condition $\nabla_{\dot{\gamma}} = 0$.

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation ●000	Theory	Conclusion	
Statistics on deformations							

- ▶ set of shapes (S_i) , local deformations $m_{i \to j}$, transport $T_{i \to k}^G$
- ► ⇒ transport deformations to a particular shape S_k : $f_{i \to j}^{i \to k} = T_{i \to k}^G(m_{i \to j})$ are, $\forall i, j$, deformations defined on the same shape S_k with reliability weights $w_{ij}^k = w_{i \to k}^G w_{i \to j}^L$



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- statistics, for k fixed : PCA
- PCA with weights, and with H¹-norm
- \blacktriangleright \implies eigenmodes e_n (= principal deformations) with eigenvalues λ_n
- \implies defines an inner product P_k = metric in the tangent space of the shape S_k
- \triangleright P_k varies smoothly as a function of k

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Example of results								

Example of results : dancing sequence (9s, 24Hz), shape 1



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Example of results							

Example of results : shape 2



Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion	
Example of results							

Example of results : shape 3



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Theoretical justifications							

The best metric ?

Searching for principal modes of deformations which vary smoothly (as a function of the shape S_k) ?

 vain quest : hairy ball theorem on best smooth direction field (or then it has to vanish sometimes)

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Best metric for a given distribution (on one shape) ?

PCA gives the best metric for a criterion based on Kullback-Leibler divergence between distributions

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Best metric for a given distribution (on one shape) ?

PCA gives the best metric for a criterion based on Kullback-Leibler divergence between distributions

Best metric for a given empirical manifold (all shapes together) ?

- needs a smoothness criterion (\implies transport)
- $\blacktriangleright \implies$ best metric for a criterion involving transport & K-L divergence.
- best metric for another criterion involving transport & L²-norm of distributions.

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Best metric						

- ▶ set of shapes (S_i), local deformations $\mathbf{f}_{i \rightarrow j}$, transport $T_{i \rightarrow k}^{G}$
- Empirical distributions : $\mathcal{D}_{emp_i} = \sum_j w_{i \rightarrow j}^L \delta_{f_{i \rightarrow j}}$



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- Empirical distributions : $\mathcal{D}_{emp_i} = \sum_j w_{i \to j}^L \delta_{\mathbf{f}_{i \to j}}$
- ► Transported distribution : via $T_{i \to k}(\delta_{\mathbf{f}}) = \delta_{T_{i \to k}(\mathbf{f})}$.

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory ○●○	Conclusion
Best metric						

- ▶ set of shapes (S_i), local deformations $\mathbf{f}_{i \rightarrow j}$, transport $\mathcal{T}_{i \rightarrow k}^{\mathsf{G}}$
- Empirical distributions : $\mathcal{D}_{emp_i} = \sum_j w_{i \to j}^L \delta_{\mathbf{f}_{i \to j}}$
- ► Transported distribution : via $T_{i \to k}(\delta_{\mathbf{f}}) = \delta_{T_{i \to k}(\mathbf{f})}$.
- $\blacktriangleright \quad \text{Criterion} : \text{ best } (P_k) \text{ for } \sum_{i,k} \quad w_{ik}^{\mathcal{G}} \quad \textit{KL} (\mathcal{D}_{P_k} \mid T_{i \to k} (\mathcal{D}_{emp_i}))$

$$= \text{ best } (P_k) \text{ for } \sum_{k} KL(\mathcal{D}_{P_k} | \mathcal{D}_{emp_k}^{\mathsf{T}})$$
where $\mathcal{D}_{emp_k}^{\mathsf{T}} = \sum_{i,j}^{k} w_{i \to j}^k \, \delta_{\mathfrak{f}_{i \to j}^k}$

- ► Transported deformations to any shape S_k : $f_{i \to j}^k = T_{i \to k}^G(f_{i \to j})$ with reliability weights $w_{i \to j}^k = w_{i \to k}^G w_{i \to j}^L$
- the one obtained by weighted PCA on transported deformations

Introduction	Searching for solutions	Shape matching	Transport 00000	Metric estimation	Theory ○○●	Conclusion
Best metric						

- empirical distributions : D_{empi}
- ▶ kernel-smoothed empirical distributions : $\mathcal{D}_{emp_i}^{\mathcal{K}} = g_i^0 d\mu$
- \triangleright g_i^0 : density functions in the tangent space of the shape S_i

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- \triangleright g_i^0 : density functions in the tangent space of the shape S_i
- search for g_i : close to g_i and smooth from shape to shape

$$E(g) = \sum_{i} \|g_{i} - g_{i}^{0}\|_{L^{2}(T_{i})}^{2} + \sum_{ij} w_{ij} \|T_{i \to j}(g_{i}) - g_{j}\|_{L^{2}(T_{j})}^{2}$$

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▶ $A = Id + \varepsilon \Delta$ where $\Delta =$ graph Laplacian (with transports)

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$$E(g) = \sum_{i} \|g_{i} - g_{i}^{0}\|_{L^{2}(T_{i})}^{2} + \sum_{ij} w_{ij} \|T_{i \to j}(g_{i}) - g_{j}\|_{L^{2}(T_{j})}^{2}$$

$$\begin{array}{l} \bullet \quad \text{minimization} \quad \Longrightarrow \quad Ag = g^0 \text{ with }: \\ \left\{ \begin{array}{l} A_{ii} = 1 + \sum_j w_{ij} \ T_{i \to j}^* \ T_{i \to j} + w_{ji} \\ A_{ij} = -w_{ij} \ T_{i \to j}^* - w_{ji} \ T_{j \to i} & \text{for } i \neq j \end{array} \right. \end{array}$$

- $A = Id + \varepsilon \Delta$ where $\Delta =$ graph Laplacian (with transports)
- $\blacktriangleright \ g = A^{-1}g^0 = (Id + \varepsilon \Delta)^{-1}g^0 \simeq (Id \varepsilon \Delta)g^0 \simeq \mathcal{N}_{\varepsilon} * g^0.$
- g = (Id − εΔ) g⁰ coincides with the D^T_{emp} and the inner products (P_i) which suit g = (g_i) the best (for K-L) are the ones we computed

Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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Conclusion

- transport is useful to reduce required training set size
- transport is useful to propagate information between shapes
- globally optimal metrics (and low complexity)

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[NORDIA 2009 : Learning Shape Metrics based on Deformations and Transport]

Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory	Conclusion
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Future works

- learning functions defined on shape spaces / with values in shape spaces
- statistics on image patches through correspondences/transport

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PCA and Kullba	nck-Leibler					

Link between PCA and Kullback-Leibler divergence

Aim : to find a metric suitable for a given distribution of deformations (f_i) on one particular shape

Guillaume Charpiat Metrics that suit an empirical manifold of shapes

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PCA and Kullba	ck-Leibler					

Link between PCA and Kullback-Leibler divergence

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Empirical distribution of deformations : $\mathcal{D}_{emp} = \sum_{i} w_i \, \delta_{\mathbf{f}_i}$
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PCA and Kullba	ck-Leibler					

Aim : to find a metric suitable for a given distribution of deformations (f_i) on one particular shape

- Empirical distribution of deformations : $\mathcal{D}_{emp} = \sum_{i} w_i \, \delta_{\mathbf{f}_i}$
- Any inner product (= metric) *P* is associated to a probability distribution: $\mathcal{D}_P(\mathbf{f}) \propto \exp(-\|\mathbf{f}\|_P^2)$

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PCA and Kullba	ck-Leibler					

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Given an inner product P_0 (= H^1) of reference, with its orthonormal basis (e_n) , supposing that P is continuous wrt. P_0 :

$$\forall \mathbf{f} \in \mathcal{T}, \quad \|\mathbf{f}\|_{P}^{2} = \sum_{n} \alpha_{n} \langle \mathbf{f} | \mathbf{e}_{n} \rangle_{P_{0}}^{2}$$

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n

$$\forall \mathbf{f} \in T, \quad \|\mathbf{f}\|_{P}^{2} = \sum_{n} \alpha_{n} \langle \mathbf{f} | \mathbf{e}_{n} \rangle_{P_{0}}^{2}$$
$$\implies \mathcal{D}_{P} \text{ is Gaussian} : \mathcal{D}_{P}(\mathbf{f}) := \prod \left(\frac{\alpha_{n}}{\pi}\right)^{\frac{1}{2}} \exp(-\alpha_{n} \langle \mathbf{f} | \mathbf{e}_{n} \rangle_{P_{0}}^{2})$$

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PCA and Kullba	ick-Leibler					

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• Given an inner product P_0 (= H^1) of reference, with its orthonormal basis (e_n), supposing that P is continuous wrt. P_0 : $\forall \mathbf{f} \in T$, $\|\mathbf{f}\|_P^2 = \sum \alpha_n \langle \mathbf{f} | \mathbf{e}_n \rangle_{P_0}^2$

$$\blacktriangleright \implies \mathcal{D}_{P} \text{ is Gaussian} : \mathcal{D}_{P}(\mathbf{f}) := \prod_{n} \left(\frac{\alpha_{n}}{\pi} \right)^{\frac{1}{2}} \exp(-\alpha_{n} \langle \mathbf{f} | \mathbf{e}_{n} \rangle_{P_{0}}^{2})$$

 \blacktriangleright \implies search over inner products = search over Gaussian distributions

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PCA and Kullba	ick-Leibler					

► Gaussian distribution that fits \mathcal{D}_{emp} the best ?

Guillaume Charpiat Metrics that suit an empirical manifold of shapes Pulsar project - INRIA

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PCA and Kullba	ick-Leibler					

- Gaussian distribution that fits \mathcal{D}_{emp} the best ?
- ▶ search for best Gaussian (= for best P) that minimize $KL(D_P|D_{emp})$

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PCA and Kullba	ick-Leibler					

- Gaussian distribution that fits \mathcal{D}_{emp} the best ?
- search for best Gaussian (= for best P) that minimize $KL(\mathcal{D}_P|\mathcal{D}_{emp})$
- best inner product P is the one given by weighted PCA with norm P_0 !

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PCA and Kullba	ick-Leibler					

- ► Gaussian distribution that fits \mathcal{D}_{emp} the best ?
- search for best Gaussian (= for best P) that minimize $KL(\mathcal{D}_P|\mathcal{D}_{emp})$
- **b** best inner product P is the one given by weighted PCA with norm P_0 !
- similar result for kernel-smoothed distributions : $\mathcal{D}_{emp}^{\mathcal{K}}(\mathbf{f}) = \sum_{j} w_{j} \mathcal{K}(\mathbf{f}_{j} - \mathbf{f}).$

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Introduction	Searching for solutions	Shape matching	Transport 00000	Metric estimation	Theory	Conclusion ○○○○●
weighted, H^1 -P	CA					

- PCA = find the best axes (to project data on this subspace)
- Minimize projection error :

$$\inf_{\left\langle \mathbf{e}_{n} \middle| \mathbf{e}_{n'} \right\rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{i,j} w_{i \to j}^{k} \left\| \mathbf{f}_{i \to j}^{k} - \sum_{n} \left\langle \mathbf{f}_{i \to j}^{k} \middle| \mathbf{e}_{n} \right\rangle_{H_{\alpha}^{1}} \mathbf{e}_{n} \right\|_{H_{\alpha}^{1}}^{2}$$

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$$\blacktriangleright \sup_{\left\langle \mathbf{e}_{n} \middle| \mathbf{e}_{n'} \right\rangle_{\mathcal{H}_{\alpha}^{1}} = \delta_{n=n'}} \sum_{n} \sum_{i,j} w_{i \to j}^{k} \left\langle \mathbf{f}_{i \to j}^{k} \middle| \mathbf{e}_{n} \right\rangle_{\mathcal{H}_{\alpha}^{1}}^{2}$$

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$$\begin{aligned} & \sup_{\langle \mathbf{e}_n | \mathbf{e}_{n'} \rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{n} \sum_{i,j} w_{i \to j}^{k} \left\langle \mathbf{f}_{i \to j}^{k} | \mathbf{e}_n \right\rangle_{H_{\alpha}^{1}}^{2} \\ & \sum_{\langle \mathbf{e}_n | \mathbf{e}_{n'} \rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{n} \mathbf{e}_n HFH \mathbf{e}_n \\ & \text{where } F = \sum_{i,j} w_{i \to j}^{k} \mathbf{f}_{i \to j}^{k} \otimes \mathbf{f}_{i \to j}^{k} = \text{weighted covariance matrix,} \\ & \text{and } H = Id - \alpha\Delta = \text{symmetric definite operator s.t.} \\ & \langle a | b \rangle_{H_{\alpha}^{1}} = \langle H a | b \rangle_{L^2} \end{aligned}$$

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion 0000●
weighted, H ¹ -PCA						

- PCA = find the best axes (to project data on this subspace)
- Minimize projection error :

$$\inf_{\left\langle \mathbf{e}_{n} | \mathbf{e}_{n'} \right\rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{i,j} w_{i \to j}^{k} \left\| \mathbf{f}_{i \to j}^{k} - \sum_{n} \left\langle \mathbf{f}_{i \to j}^{k} | \mathbf{e}_{n} \right\rangle_{H_{\alpha}^{1}} \mathbf{e}_{n} \right\|_{H_{\alpha}^{1}}^{2}$$

$$\begin{split} \sup_{\left\langle \mathbf{e}_{n} \middle| \mathbf{e}_{n'} \right\rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{n} \sum_{i,j} w_{i \to j}^{k} \left\langle \mathbf{f}_{i \to j}^{k} \middle| \mathbf{e}_{n} \right\rangle_{H_{\alpha}^{1}}^{2} \\ & \sum_{\left\langle \mathbf{e}_{n} \middle| \mathbf{e}_{n'} \right\rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{n} \mathbf{e}_{n} HFH \mathbf{e}_{n} \\ & \text{where } F = \sum_{i,j} w_{i \to j}^{k} \mathbf{f}_{i \to j}^{k} \otimes \mathbf{f}_{i \to j}^{k} = \text{weighted covariance matrix,} \\ & \text{and } H = Id - \alpha \Delta = \text{symmetric definite operator s.t.} \\ & \left\langle a \middle| b \right\rangle_{H_{\alpha}^{1}} = \left\langle H a \middle| b \right\rangle_{L^{2}} \end{split}$$

Change of variables:
$$\mathbf{d}_n = H^{1/2} \mathbf{e}_n$$
:
$$\sup_{\langle \mathbf{d}_n | \mathbf{d}_{n'} \rangle_{i,2} = \delta_{n=n'}} \sum_n \mathbf{d}_n H^{1/2} F H^{1/2}$$

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Introduction	Searching for solutions	Shape matching	Transport	Metric estimation	Theory 000	Conclusion ○○○○●		
weighted, H ¹ -PCA								

- PCA = find the best axes (to project data on this subspace)
- Minimize projection error :

$$\inf_{\left\langle \mathbf{e}_{n} \middle| \mathbf{e}_{n'} \right\rangle_{H_{\alpha}^{1}} = \delta_{n=n'}} \sum_{i,j} w_{i \to j}^{k} \left\| \mathbf{f}_{i \to j}^{k} - \sum_{n} \left\langle \mathbf{f}_{i \to j}^{k} \middle| \mathbf{e}_{n} \right\rangle_{H_{\alpha}^{1}} \mathbf{e}_{n} \right\|_{H_{\alpha}^{1}}^{2}$$

classical PCA problem, with correlation matrix : $M_{(i,j),(i',j')} = \left\langle \sqrt{w_{i \to j}^{k}} \mathbf{f}_{i \to j}^{k} \left| \sqrt{w_{i' \to j'}^{k}} \mathbf{f}_{i' \to j'}^{k} \right\rangle_{H_{\Omega}^{1}} \right.$

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- eigenvectors :

$$\mathbf{e}_n = \sum_{ij} \gamma_n^{(i,j)} \sqrt{w_{i \to j}^k} \mathbf{f}_{i \to j}^k$$

Guillaume Charpiat