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Diffeomorphic Shape Analysis

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Introduction

- Shape analysis is the study of variation of shapes in relation with other variables.
- Once a suitable "shape space" is defined, analyzing shapes involves:
  - Comparing them (using distances)
  - Finding properties of datasets in this space
  - Testing statistical hypotheses

Some entry points to the literature

- Landmarks / point sets: Kendall, Bookstein, Small, Dryden…
- Active shapes: Taylor, Cootes,…
- Registration: Demons, Diffeomorphic Demons (Thirion, Guimond, Ayache, Pennec, Vercauteren,…)
- Harmonic analysis: SPHARM (Gerig, Steiner,…)
- Medial axis and related, M-REPS (Pizer, Damon,…)
- Manifolds of curves / surfaces – Theory (Mumford, Michor, Yezzi, Mennucci, Srivastava, Mio, Klassen…)
- Statistics on manifolds of curves/surfaces (Pennec, Fletcher, Joshi, Marron…)

On "Diffeomorphometry"…

- Precursors (fluid registration): Christensen-Miller-Rabbit; Thirion…
- Large Deformation Diffeomorphic Metric Mapping – LDDMM
  – Images: Beg, Miller, Trouvé, Y.;
  – Landmarks Miller, Joshi;
  – Measures (Glaunès, Trouvé, Y.), Currents (Glaunès, Vaillant)
  – Hamiltonian methods (Glaunès, Trouvé, Vialard, Y…)
- Metamorphosis (Miller, Trouvé, Holm, Y…)

Shape Spaces

- Shape spaces are typically modeled as differential manifolds, but…
- Almost all practical methods use a shape representation in a linear space of "local coordinates"
- Linear statistical methods can then be employed to analyze the data.
- For some of these methods (e.g., PCA), it is also important that linear combinations of the representations make sense, too.

Example: Kendall Shape Space

- Consider the family of collections of N distinct points in $\mathbb{R}^d$
- This forms an open subset of $Q = (\mathbb{R}^d)^N$
- Identify collections that are can be deduced from each other by rotation, translation and scaling.
- It is a set of subsets of Q (quotient space).
- It can be structured as a differential manifold.
- The Euclidean metric on Q transforms into a Riemannian metric in the quotient space.

Example: Spaces of Curves

- The set Q of smooth functions $q:[0,1]\to\mathbb{R}^2$ is a Fréchet space.
- Quotient out translation rotations scaling and **change of parameter** to obtain a shape space.
- Sobolev norms on Q trickle down to Riemannian metrics on the shape space.
- See papers from Michor, Mumford, Shah…

Shapes Spaces and Deformable Templates

- Ulf Grenander's metric pattern theory involves transformation groups that act on shapes.
- The transformations have a cost, represented by an *effort functional*.
- Under additional assumptions, this induces a metric in the shape space.
- The construction that follows will be based on these principles.
- The group is the group of diffeomorphisms.
- The shapes are anything that can be deformed.

Tangent space representations

- There is a natural way to build linear representations when the the shape space is modeled as a Riemannian manifold, i.e.:
  - a topological space that can be mapped locally to a vector space on which differentials can be computed (with consistency relations between local maps).
  - with a metric which can be used to compute lengths, and shortest paths between two points, which are called geodesics.

Exponential Charts (I)

- Geodesics can be characterized by a second order differential equation on the manifold.
- This equation has (in general) a unique solution given its initial position and first derivative.
- Fix the initial position ("template"). Denote it $\bar{S}$.
- The space of all derivatives of curves in $\mathcal{S}$ that start from $\bar{S}$ is the tangent space to $\mathcal{S}$ at $\bar{S}$ (notation $T_{\bar{S}}\mathcal{S}$).

Exponential Charts (II)

- The exponential map associates to each vector $v \in T_{\bar{S}}\mathcal{S}$ the solution at time $t = 1$ of the geodesic equation starting at $\bar{S}$ in the direction v.
- It is a map from $T_{\bar{S}}\mathcal{S}$ to $\mathcal{S}$, with notation

$$v \in T_{\bar{S}}\mathcal{S} \mapsto \exp_{\bar{S}}(v) \in \mathcal{S}$$

- It can (generally) be restricted to a neighborhood of 0 in $T_{\bar{S}}\mathcal{S}$ over which it is one to one, providing so-called normal local coordinates or an exponential chart at $\bar{S}$.

SHAPES AND DIFFEOMORPHISMS

General Approach

- We will define shape spaces via the action of diffeomorphisms on them.
- This action will induce a differential structure on the shape space.
- It also allows to compare them: two shapes are similar if one can be obtained from the other via a small deformation.

Notation

- Diffeomorphisms of $\mathbb{R}^d$ will be denoted φ, ψ, etc.
  They are invertible differentiable transformations with a differentiable inverse.

- Vector fields over $\mathbb{R}^d$ will be denoted v, w, etc.
  They are differentiable mappings from $\mathbb{R}^d$ onto itself.

Ordinary Differential Equations

- Diffeomorphisms can be built as flows associated to ordinary differential equations (ODEs).
- Let $(t,x) \mapsto v(t,x)$ be a time-dependent vector field. Assume that v is differentiable in x with bounded first derivative over a time interval $[0,T]$.
- Then there exists a unique solution of the ODE $\dot{y} = v(t,y)$ with initial condition $y(0) = x_0$ defined over the whole interval $[0,T]$

Flows

- The flow associated with the ODE $\dot{y} = v(t, y)$ is the mapping
$$(t,x) \mapsto \varphi(t,x)$$
such that $\varphi(t,x)$ is the solution at time t of the ODE initialized with $y(0) = x$.
- In other terms:

$$\boxed{\begin{cases} \partial_t \varphi = v(t,\varphi) \\ \varphi(0,x) = x \end{cases}}$$

Flows (II)

- Assuming that $v(t,\cdot)$ is continuously differentiable with bounded derivative, uniformly in time, the associated flow is such that

$$x \mapsto \varphi(t,x)$$

  is a diffeomorphism at all times.
- If v has more (space) derivatives, they are inherited by φ .
- We will build diffeomorphisms as flows associated to vector fields that belong in a specified reproducing kernel Hilbert space.

Hilbert Spaces

- A Hilbert space H is an infinite-dimensional vector space with an inner-product, such that the associated norm that makes it a complete metric space.
- The inner product between two elements in H is denoted

$$\left\langle h, h' \right\rangle_H$$

- The set of bounded linear functionals $\mu : H \to \mathbb{R}$ is the topological dual of H, denoted H^* .
- We will use the notation $\left(\mu \mid h\right) := \mu(h)$ for $\mu \in H^*, h \in H$

Riesz Theorem

- The Riesz representation theorem states that H and H^* are isometric.
- $\mu \in H^*$ if and only if there exists $h \in H$ such that, for all $h' \in H$:
$$\left(\mu \mid h'\right) = \left\langle h, h' \right\rangle_H$$
- The correspondence $\mu \mapsto h$ will be denoted $\mathbf{K}_H$, so that $\mathbf{K}_H : H^* \to H$ and its inverse $\mathbf{A}_H : H \mapsto H^*$
- We therefore have
$$\left(\mu \mid h\right) = \left\langle \mathbf{K}_H \mu, h \right\rangle_H \text{ and } \left\langle h, h' \right\rangle_H = \left(\mathbf{A}_H h \mid h'\right)$$

RKHS

- A Hilbert space H of functions defined over $\mathbb{R}^d$, with values in $\mathbb{R}^k$ is an RKHS, if

$$H \subset L^2(\mathbb{R}^d, \mathbb{R}^k) \cap C_0^p(\mathbb{R}^d, \mathbb{R}^k)$$

  ($p \geq 0$) with continuous inclusions in both spaces. (Here $C_0^p(\mathbb{R}^d, \mathbb{R}^k)$ is the space of p times differentiable vector fields that converge to 0 (will all derivatives up to order p) at infinity, equipped with the supremum norm.
- This means that for some constant C, and for all $v \in H$

$$\max\left(\|v\|_2, \|v\|_{p,\infty}\right) \leq C\|v\|_H$$

RKHS

- If H is an RKHS, and $x \in \mathbb{R}^d, a \in \mathbb{R}^k$ the linear form
$$a\delta_x : v \mapsto a^T v(x)$$
belongs to H^*.
- General notation: if θ is a (scalar) measure and a is a vector field defined on its support, $a\theta$ is the vector measure
$$(a\theta \mid w) = \int a(x)^T w(x) d\theta(x)$$

RKHS

- The reproducing kernel of V is a matrix-valued function K_V defined on $\mathbb{R}^d \times \mathbb{R}^d$ by
$$K_H(x,y)a = \boldsymbol{K}_H(a\delta_y)(x)$$
with $a, x \in \mathbb{R}^d$
- $K_H(x,y)$ is a k by k matrix.
- We will denote K_H^i the ith column of K_H and by K_H^{ij} its i,j entry. One has, in particular

$$\left\langle K_H^i(\cdot,x), K_H^j(\cdot,y)\right\rangle_H = K_H^{ij}(x,y)$$

Usual examples (scalar kernels)

- I_k is the d by d identity matrix.
- Gaussian kernel: $K_H(x,y) \propto \exp(-\|x-y\|^2/2\sigma^2) I_k$
- Cauchy Kernel: $$K_H(x,y) \propto \frac{I_k}{1+\|x-y\|^2/\sigma^2}$$
- Power of Laplacian:

$$K_H(x,y) \propto P_m(\|x-y\|/\sigma)\exp(-\|x-y\|/\sigma) I_k$$

with $P_0 = 1,\ P_1 = 1+t$ and $\partial_t P_m - P_m = -tP_{m-1}$

The Interpolation Problem

- Let H be a Hilbert space and $\mu_1,\ldots,\mu_m \in H^*$.
- Solve the problem

$$\begin{cases} \|h\|_H \to \min \\ \text{subject to } \left(\mu_k \middle| h\right) = \lambda_k, k = 1,\ldots,m \end{cases}$$

- Solution: $h = \sum_{k=1}^m a_k \mathbf{K}_H \mu_k$ where $a_1,\ldots,a_m$ are identified using the constraints.

Application

- H is a scalar RKHS ($k = 1$).
- $x_1, \dots, x_m \in \mathbb{R}^d$
- Solve

$$\begin{cases} \|h\|_H \to \min \\ \text{subject to } h(x_k) = \lambda_k, k = 1, \dots, m \end{cases}$$

- Solution: $h(\cdot) = \sum_{k=1}^{m} K_H(\cdot, x_k) a_k$

with: $\sum_{l=1}^{m} K_H(x_k, x_l) a_l = \lambda_k, \; k = 1, \dots, m$

Attainable Diffeomorphisms

- Fix V, an RKHS of vector fields with at least one derivative ($p \geq 1$).
- We consider ODEs of the form $\dot{y} = v(t, y)$ with $v(t,\cdot) \in V$
- The flow evolution $\partial_t \varphi(t,\cdot) = v(t,\varphi(t,\cdot))$ can be interpreted as a control system in which the deformation, φ, is the state driven by the time-dependent vector field $v(t,\cdot)$
- The space of attainable diffeomorphisms is

  $$G_V = \left\{ \psi : \exists T, \exists v(t,\cdot), \left\| v(t,\cdot) \right\|_V \text{ bounded}, \psi = \varphi^v(T,\cdot) \right\}$$

  where φ^v is the flow associated to v.

Attainable Diffeomorphisms

- G_V is a subgroup of the group of diffeomorphisms of $\mathbb{R}^d$
- There is no loss of generality in taking $T = 1$ in the definition.
- One defines a distance on G_V by

$$d_V(\psi,\psi') = \min\left\{\int_0^1 \| v(t,) \|_V \, dt : \varphi^v(1,\psi) = \psi'\right\}$$

and

$$d_V(\psi,\psi')^2 = \min\left\{\int_0^1 \| v(t,) \|_V^2 \, dt : \varphi^v(1,\psi) = \psi'\right\}$$

Attainable Diffeomorphisms

- Computing $d_V(\psi,\psi') = d_V(\mathrm{id},\psi\circ(\psi')^{-1})$ is equivalent to solving the optimal control problem

$$\int_0^1 \| v(t) \|_V^2 \, dt \to \min$$

subject to $\varphi(0) = \mathrm{id},\ \partial_t \varphi = v(t,\varphi),\ \varphi(1) = \psi \circ (\psi')^{-1}$

Riemannian Interpretation

- d_V is the distance associated to the Riemannian metric

$$\left\|\delta\varphi\right\|_{\varphi} = \left\|\delta\varphi \circ \varphi^{-1}\right\|_{V}$$

since, using $\dot{\varphi} \circ \varphi^{-1} = v$,

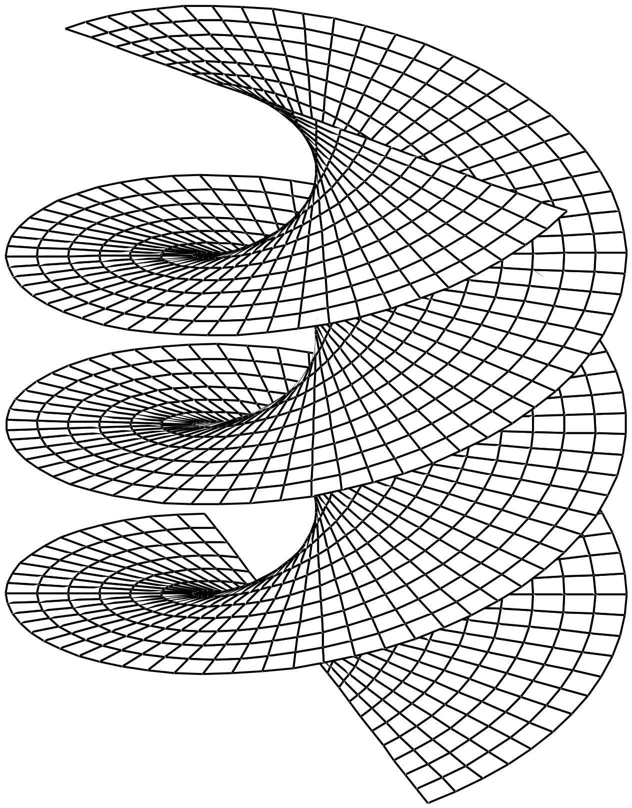
$$d_V(\psi, \psi') = \min\left\{\int_0^1 \| \dot{\varphi}(t) \|_{\varphi}\, dt : \varphi(1) = \psi', \varphi(0) = \psi\right\}$$

$$= \min\left\{\int_0^1 \| \dot{\varphi}(t) \|_{\varphi}^2\, dt : \varphi(1) = \psi', \varphi(0) = \psi\right\}^{1/2}$$

Differentiable Manifold

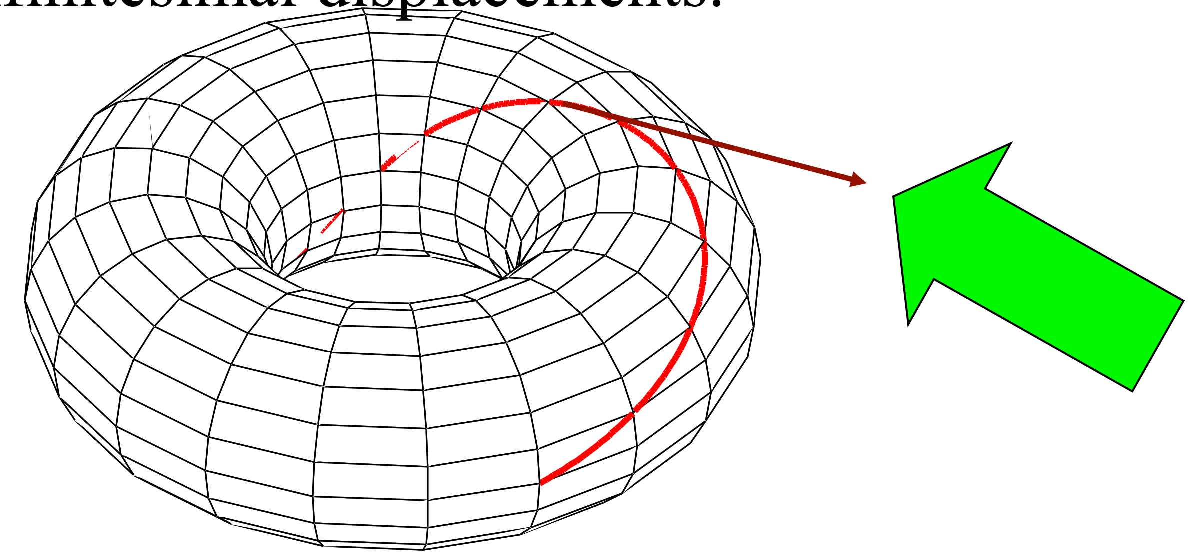
- Let M be a Hausdorff topological space. An n-dimensional local chart on M is a pair (U,Φ) where U is open in M and $\Phi : U \to V \subset \mathbb{R}^n$ is a homeomorphism.
- Two charts $(U_1,\Phi_1),(U_2,\Phi_2)$ are C^p-compatible if either $U_1 \cap U_2 = \varnothing$ or $\Phi_2 \circ \Phi_1^{-1}$ is C^p on $\Phi_1(U_1 \cap U_2) \subset \mathbb{R}^n$
- M is an n-dimensional C^p manifold if it can be covered with local charts that are all pairwise C^p compatible (which form an atlas).

Something like this



Tangent Vectors on Manifolds

Tangent Vectors on a differentiable manifold are velocities of trajectories in the manifold.
They represent infinitesimal displacements.



The collection of all tangent vectors at a given point is an *n*-dimensional vector space, called the tangent space at this point.

Riemannian Manifold

- A Riemannian manifold is a differentiable manifold with an inner product on each of its tangent spaces.

$$p \in M,\ v \text{ tangent to } M \text{ at } p \rightarrow \|v\|_p$$

Riemannian distance

- Adding the norms of infinitesimal displacements, one can compute the lengths of trajectories on a manifold.
- The Riemannian distance is the length of the shortest path between two points:

$$d(p,p') = \inf\left\{ \int_0^1 \left\| \dot{x}(t) \right\|_{x(t)} dt : x(0) = p, x(1) = p' \right\}$$

- Curves that achieve the shortest length are called (minimizing) geodesics. They extend the notion of straight lines to manifolds.

Back to Diffeomorphisms

- Manifold: group G of diffeomorphisms. It is an open space of a Banach or Fréchet space and has infinite dimension.
- Infinitesimal displacements, $\delta\varphi$, are vector fields.
- The Riemannian metric is

$$\|\delta\varphi\|_{\varphi} = \|\delta\varphi \circ \varphi^{-1}\|_{V}$$

Exponential Charts

- On a Riemannian manifold, one can define radial coordinates or exponential charts.
- Example: (Latitude, Longitude) on Earth.
  - Meridian lines stemming from the North Pole are geodesics.
  - A point on Earth is measured by specifying which meridian it belongs to (Longitude) and where it is on this meridian (latitude).

Exponential Charts

- Geodesics $t \mapsto \gamma(t)$ must satisfy a second-order differential equation.
- They are uniquely defined by their initial conditions
$$(\gamma(0), \dot\gamma(0))$$
- Definition: $\exp_p(v) = \gamma(1)$
where γ is the geodesic with initial conditions
$$\gamma(0) = p, \dot\gamma(0) = v$$
is the exponential map on the manifold.

Exponential Charts

- Fixing p, the function $v \mapsto \exp_p(v)$ is a local chart mapping a neighborhood of 0 in the tangent space to p to a neighborhood of p on the manifold.
- It is called the exponential chart.
- (On the sphere, longitude provides the direction of v and latitude provides the norm.)
- The inverse map: $p' \to v$ such that $p' = \exp_p(v)$ is defined in a neighborhood of p and provides exponential coordinates (Riemannian logarithm).

Application to Diffeomorphisms

- Take $M = G$, a group of diffeomorphisms, $p = \mathrm{id}$, the identity map.
- The Riemannian logarithm of ψ is obtained by solving the optimal control problem
$$\int_0^1 \| v(t) \|_V^2 \, dt \to \min$$
subject to $\varphi(0) = \mathrm{id}, \partial_t \varphi = v \circ \varphi, \varphi(1) = \psi$.
- The logarithm is then given by $v(0)$.

EPDiff

- The geodesic equation on diffeomorphisms is called EPDiff.
- It expresses the conservation of "momentum" along optimal trajectories.

$$\begin{cases} \partial_t \varphi = v \circ \varphi \\ \partial_t \mathbf{A}_V v + \mathrm{ad}_v^* \mathbf{A}_V v = 0 \end{cases}$$

$$\text{where } \mathrm{ad}_v : w \to Dv\, w - Dw\, w$$

- Solving this equation with initial conditions (id, v_0) provides a local chart of G around the identity.

Shape Spaces

- Assume that the shape space $\mathcal{M}$ is an open subset of a Banach space $\mathcal{Q}$.
- Assume that diffeomorphisms act on shapes, with notation:

$$(\varphi, q) \mapsto \varphi \cdot q$$

- Thus:

$$\mathrm{id} \cdot q = q$$

$$\varphi \cdot (\psi \cdot q) = (\varphi \circ \psi) \cdot q$$

Infinitesimal Action

- The infinitesimal action of vector fields: $(v,q) \mapsto v \cdot q$ is defined by

$$v \cdot q := \partial_\varepsilon (\varphi_\varepsilon \cdot q)_{\epsilon=0}, \quad \varphi_0 = \mathrm{id}, \quad (\partial_\varepsilon \varphi)_{\varepsilon=0} = v$$

- Let $\xi_q : v \mapsto v \cdot q$.
- We assume that, for all $q \in \mathcal{M}$, $\xi_q : V \to \mathcal{Q}$ is well defined and bounded.

Riemannian Metric on Shapes

- Define a metric on $\mathcal{M}$ via "Riemannian submersion", yielding

$$\left\|\delta q\right\|_q = \inf\left\{\left\|v\right\|_V : \xi_q v = \delta q\right\}$$

- The associated distance is then given by

$$d_{\mathcal{M}}(q_0,q_1) = \inf\left\{d_G(\mathrm{id},\varphi) : \varphi \cdot q_0 = q_1\right\}$$

- Or: $$\int_0^1 \| v(t) \|_V^2 \, dt \to \min$$

  subject to $$q(0) = q_0,\ \partial_t q = \xi_q v,\ q(1) = q_1.$$

Large Deformation Diffeomorphic Metric Mapping

- The generic "LDDMM" problem is

$$\frac{1}{2}\int_0^1 \| v(t,.) \|_V^2 + U(q(1)) \to \min$$

$$\text{subject to } q(0) = q^{(0)} \text{ and } \dot{q}(t) = \xi_{q(t)} v(t)$$

- This is an infinite-dimensional optimal control problem, with v as control, q as state and U an end-point cost assumed to be differentiable.
- Typically, U measures the discrepancy between $q(1)$ and the "target" shape q_1.

Geodesics equations

- Optimal paths must satisfy

$$\begin{cases} \partial_t q = \xi_q \mathbf{K}_V \xi_q^* p \\ \partial_t p + (\partial_q \xi_q v)^* p = 0 \\ v = \mathbf{K}_V \xi_q^* p \end{cases}$$

$$\text{with } \mathrm{q}(0) = \mathrm{q}_0,\ p(0) = p_0.$$

for some $p_0 \in \mathcal{M}^*$.

- The mapping $p_0 \rightarrow q(1)$ provides a coordinate system equivalent to the exponential chart.

Example: Parametrized sets

- q: continuous embedding of S (Riemannian manifold) in $\mathbb{R}^d$ with

$$\varphi \cdot q = \varphi \circ q$$

$$\xi_q v = v \circ q$$

- If p is a measure on S, $\xi_q^* a = q^* a$ and

$$(\xi_q \mathbf{K}_V \xi_q^* p)(x) = \int_S K_V(q(x), q(y)) dp(y)$$

Special case: Point Sets / Landmarks

- $q = (q_1, \ldots, q_N)$ is a finite set of distinct points in $\mathbb{R}^d$.

$$\varphi \cdot q = (\varphi(q_1), \ldots, \varphi(q_N))$$
$$\xi_q v = (v(q_1), \ldots, v(q_N))$$

- $\mathcal{Q} = \mathcal{Q}^* = (\mathbb{R}^d)^N \quad \xi_q^* p = \sum_{k=1}^{N} p_k \delta_{q_k}$

- Then

$$(\xi_q \mathbf{K}_V \xi_q^* p)_k = \sum_{l=1}^{N} K_V(q_k, q_l) p_l$$

Point Set Matching LDDMM Problem

- Plug into the generic problem:

$$\frac{1}{2}\int_0^1 \| v(t,.) \|_V^2 + U(q(1)) \to \min$$

subject to $q(0) = q^{(0)}$ and $\dot{q}(t) = \xi_{q(t)} v(t)$

the constraint that $v(t,\cdot) = \mathbf{K}_V \xi^*_{q(t)} p(t)$ for some

$$p(t) = \left\{ p_k(t) \right\}_{k=1}^N$$

- One then has

$$\left\| v(t) \right\|_V^2 = \sum_{k,l=1}^N p_k^T K_V(q_k, q_l) p_l$$

Reduction

- The problem becomes finite dimensional:

$$\frac{1}{2}\int_0^1 \sum_{k,l=1}^{N} p_k(t)^T K_V(q_k(t), q_l(t)) p_l(t)\, dt \; + U(q(1)) \to \min$$

subject to $q(0) = q^{(0)}$ and $\dot{q}_k(t) = \sum_{l=1}^{N} K_V(q_k(t), q_l(t)) p_l(t)$

- This is a classical optimal control problem with state q and control p.
- One can use the adjoint method to solve it numerically.

Adjoint Method

- Consider the general optimal control problem

$$\int_0^1 g(q(t),u(t))\,dt + U(q(1)) \to \min$$

subject to $q(0) = q^{(0)}$ and $\dot{q}(t) = f(q(t),u(t))$

- Consider q as a function of u, say q^u uniquely defined by

$$q^u(0) = q^{(0)} \text{ and } \dot{q}^u(t) = f(q^u(t),u(t))$$

- Let
$$F(u) = \int_0^1 g(q^u(t),u(t))\,dt + U(q^u(1)) \to \min$$

Adjoint Method

- The adjoint methods computes $\nabla F(u)$
- Introduce the Hamiltonian

$$H_u(p,q) = p^T f(q,u) - g(q,u)$$

- Step 1: Given u, solve for the state equation $\dot{q} = f(q,u)$ or

$$\dot{q} = \partial_p H_u$$

- Step 2: Set $p(1) = -\nabla U(q(1))$
- Step 3: Solve $\dot{p} = -\partial_q H_u$ (backward in time)
- Step 4: Let $\nabla F(u)(t) = -\partial_u H(p(t), q(t))$

Data Terms

- Several types of data terms $q \mapsto U(q)$ have been developed depending on the interpretation made for q.
- If $q = (q_1, \ldots, q_N)$ are labeled landmarks, use

$$U(q) = \sum_{k=1}^{N} \left| q_k - q_k^{(1)} \right|^2$$

- If $q = \{q_1, \ldots, q_N\}$ are unlabeled, introduce the measure

$$\mu_q = \sum_{k=1}^{N} \delta_{q_k}$$

Data Terms

- Let $U(q) = \| \mu_q - \mu_{q^{(1)}} \|^2$ with

$$\|\mu\|^2 = \iint K_H(x,y)\, d\mu(x)\, d\mu(y)$$

- This is also applicable to weighted sums of point masses.
- Example: discretize the line measure *dl* along a curve by

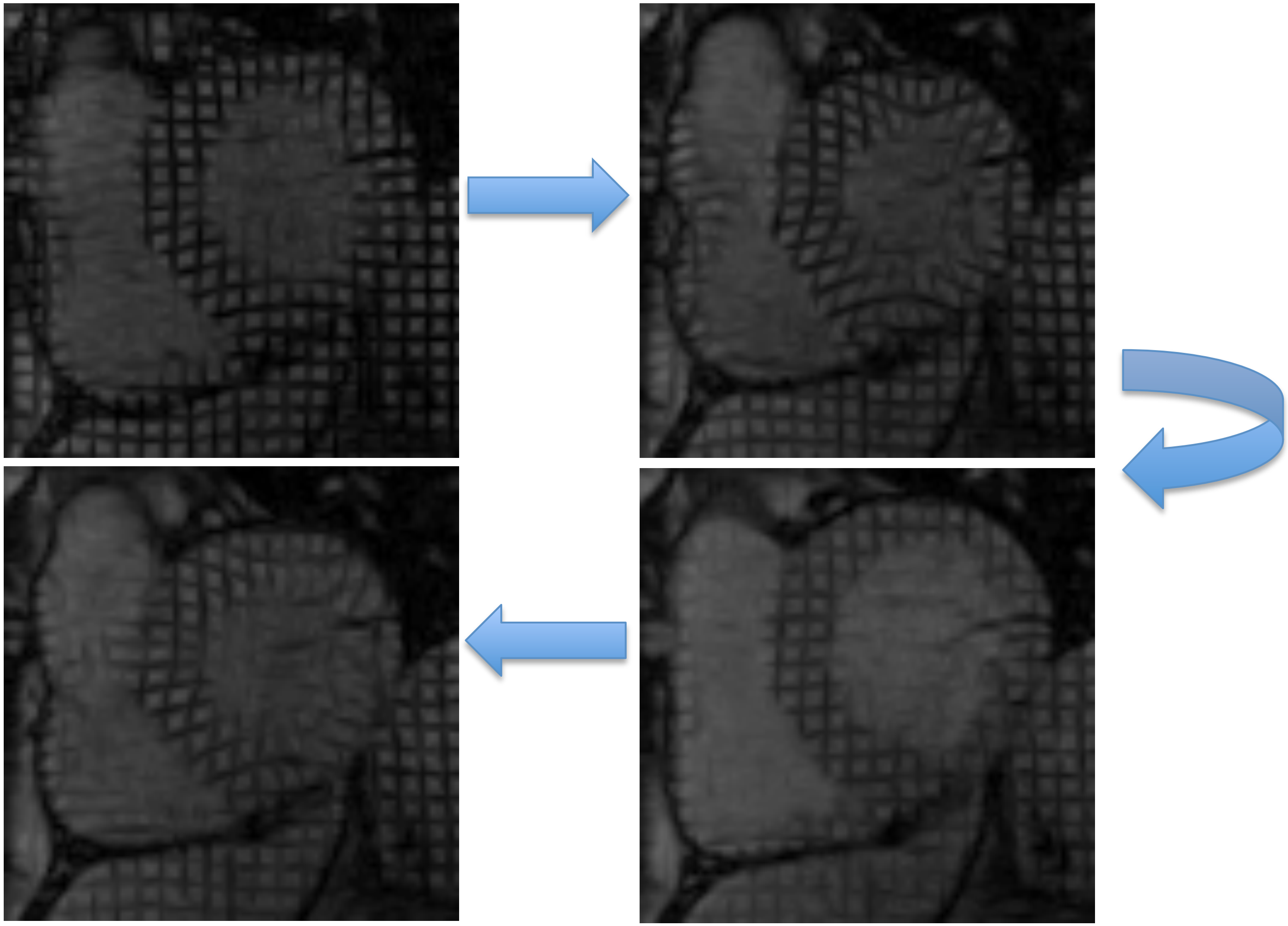
$$\mu_q = \sum_{k=1}^{N} (dl_k)\delta_{q_k}$$

  and use this representation for curve comparison.
- Same idea for triangulated surfaces.

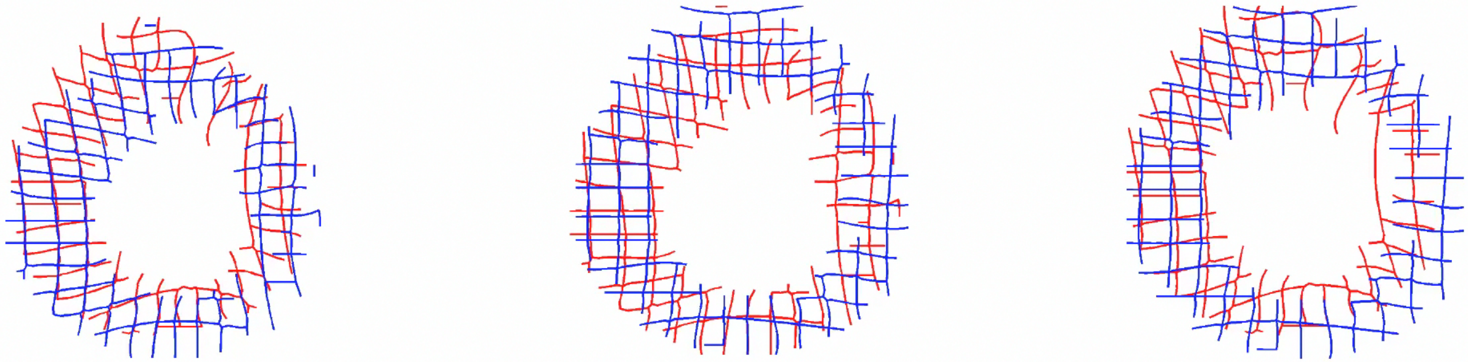
Data Terms

- For oriented curves and surfaces: use vector measures instead of scalar ones (involving normal vector).
- Equivalent to current-based surface comparison (Vaillant-Glaunès).
- Other variants have been developed (collections of curves, surfaces to sections,…)

Application: tracking tagged MRI



Matching curves from tagged MRI data



Matching Triangulated Surfaces