Direct Diffeomorphic Reparameterization for Correspondence Optimization in Statistical Shape Modeling

— Ph.D. Thesis Defense

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 - Analytical formulas and quadrature approximations
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Why Statistical Shape Model (SSM)?

SSM of a shape population

Better understanding

mean & typical range of shape variations

Compact representation

mean + linear combination of variations

Classification

Medical diagnosis etc.

Shape construction

Patient-specific modeling etc.

Figures courtesy of American Academy of Orthopaedic Surgeons (AAOS)



Cam impingement



Knee implant



What is Statistical Shape Model?



- SSM = mean + modes
- Mode: shape variation pattern



How to get SSM?



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Statistical analysis steps







Shape variation pattern \sim shape correspondence



Unreasonable variation

Reasonable variation

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Manipulate correspondence by reparametrization



- Shape 6 as an example
- $\bullet\,$ Correspondence manipulation \sim landmarks redistribution
- Landmarks redistribution achieved by reparametrization



Correspondence manipulation on curve by R(u)



- Correspondence manipulation ~ Landmark redistribution
- Shape parametrized by S(u), reparametrized by R(u)
- Landmark S(u) moves to S[R(u)]



Reparametrization by concatenation: curve case



- Conventional reparametrization: sequential concatenations
- Local reparametrization: Cauchy kernel
- Cumbersome and inefficient



Proposed direct reparametrization: curve case



• $R(u) = \sum_{i=0}^{n} B_{i,p}(u)b_i, \quad 0 \le u \le 1; \ i = 0, ..., n$

• Diffeomorphic constraint: $b_i - b_{i+1} \leq 0$, i = 0, 1, ..., n - 1.



A reparametrization example



Landmarks before reparam.

Reparmeterization function

Landmarks after reparam.

- More complex geometry: hand contour
- Arbitrary landmarks redistribution achievable



Correspondence manipulation on surface by $\mathbf{R}(u, v)$



- Correspondence manipulation ~ Landmark redistribution
- Shape parametrized by S(u, v)
- Precisely controlled by reparametrization function $\mathbf{R}(u, v)$

Reparametrization by concatenation: surface case



- Conventional reparametrization: sequential concatenations
- Local reparametrization: Clamped Plate Spline warp
- Cumbersome and inefficient



Proposed direct reparametrization: surface case



Diffeomorphic constraint: Jacobian positivity

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Correspondence optimization formulation

- Description Length (DL): the message length for transmitting statistical model: x̄, {v_m} and {λ_m}
- Simplified version as objective function

$$\begin{split} f \doteq DL &= \sum_{m=1}^{n_S-1} L_m \\ \text{where } L_m &= \begin{cases} 1 + \log(\lambda_m/\lambda_{\text{cut}}) & \lambda_m \geq \lambda_{\text{cut}} \\ \lambda_m/\lambda_{\text{cut}} & \text{otherwise} \end{cases} \end{split}$$

Optimization formulation

$$\min_{\mathbf{b}} f(\mathbf{b}) = \sum_{\lambda_i \ge \lambda_{\text{cut}}} \left[1 + \log \frac{\lambda_k(\mathbf{b})}{\lambda_{\text{cut}}} \right] + \sum_{\lambda_k < \lambda_{\text{cut}}} \frac{\lambda_k(\mathbf{b})}{\lambda_{\text{cut}}}$$
(1a)

s.t.
$$\left[\mathbf{C}^{T}(\mathbf{b})\mathbf{C}(\mathbf{b})\right]\mathbf{v}_{k}(\mathbf{b}) = \lambda_{i}(\mathbf{b})\mathbf{v}_{k}(\mathbf{b})$$
 (1b)

$$\mathbf{v}_k^T(\mathbf{b})\mathbf{v}_k(\mathbf{b}) = 1, \quad k = 1, \dots, n_S$$
(1c)

$$g(\mathbf{b}) < 0 \tag{1d}$$

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Direct method

- Eigen decomposition form: $\mathbf{C}^T \mathbf{C} \mathbf{v}_m = \lambda_m \mathbf{v}_m$ (1); $\mathbf{v}_m^T \mathbf{v}_m = 1$ (2)
- Consider sensitivity for f(α, λ, V)

$$\frac{\mathrm{d}f(\boldsymbol{\alpha})}{\mathrm{d}b_r} = \frac{\partial f}{\partial b_r} + \sum_{m=1}^{n_S} \frac{\partial f}{\partial \lambda_m} \frac{\partial \lambda_m}{\partial b_r} + \sum_{m=1}^{n_S} \left(\frac{\partial f}{\partial \mathbf{v}_m}\right)^T \frac{\partial \mathbf{v}_m}{\partial b_r} = \sum_{m=1}^{n_S} \frac{\partial f(\boldsymbol{\lambda})}{\partial \lambda_m} \frac{\partial \lambda_m}{\partial b_r}$$

• Differentiating (1) and (2) w.r.t b_r for each q gives

$$\left(\lambda_m \mathbf{I}_{n_S} - \mathbf{C}^T \mathbf{C}\right) \frac{\partial \mathbf{v}_m}{\partial b_r} + \mathbf{v}_m \frac{\partial \lambda_m}{\partial b_r} = \frac{\partial (\mathbf{C}^T \mathbf{C})}{\partial b_r} \mathbf{v}_m \qquad \mathbf{v}_m^T \frac{\partial \mathbf{v}_m}{\partial b_r} = 0$$

• Direct sensitivity: solve for $\frac{\partial \lambda_m}{\partial b_r}$, $\frac{\partial \mathbf{v}_m}{\partial b_r}$ directly and plug into (3)

$$\begin{bmatrix} 0 & \mathbf{v}_m^T \\ \mathbf{v}_m & \lambda_m \mathbf{I}_{n_S} - \mathbf{C}^T \mathbf{C} \end{bmatrix} \begin{bmatrix} \frac{\partial \lambda_m}{\partial b_r} \\ \frac{\partial \mathbf{v}_m}{\partial b_r} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{\partial (\mathbf{C}^T \mathbf{C})}{\partial b_r} \mathbf{v}_m \end{bmatrix}$$

Adjoint method

 $\bullet \,$ Introduce Lagrangian with (1) and (2) as constraints

$$\mathcal{L} = f(\boldsymbol{\lambda}) + \sum_{m=1}^{n_S} \boldsymbol{\mu}_m^T \left(\mathbf{C}^T \mathbf{C} \, \mathbf{v}_m - \lambda_m \mathbf{v}_m \right) + \sum_{m=1}^{n_S} \eta_m (\mathbf{v}_m^T \mathbf{v}_m - 1)$$
(4)

Adjoint variables μ_m and η_m are just Lagrange multipliers

• Differentiation of (4) w.r.t b_r gives

$$\frac{\mathrm{d}f}{\mathrm{d}b_r} = \sum_{m=1}^{n_S} \boldsymbol{\mu}_m^T \frac{\partial (\mathbf{C}^T \mathbf{C})}{\partial b_r} \mathbf{v}_m + \sum_{m=1}^{n_S} \left(\frac{\partial f}{\partial \lambda_m} - \boldsymbol{\mu}_m^T \mathbf{v}_m \right) \frac{\partial \lambda_m}{\partial b_r} + \sum_{m=1}^{n_S} \left[\boldsymbol{\mu}_m^T (\mathbf{C}^T \mathbf{C} - \lambda_m \mathbf{I}_{n_S}) + 2\eta_m \mathbf{v}_m^T \right] \frac{\partial \mathbf{v}_m}{\partial b_r}$$
(5)

• Adjoint sensitivity: solve (6) for μ_m and η_m and plug into (5)

$$\begin{bmatrix} \mathbf{v}_m^T & \mathbf{0} \\ \mathbf{C}^T \mathbf{C} - \lambda_m \mathbf{I}_{n_S} & 2\mathbf{v}_m \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu}_m \\ \eta_m \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial \lambda_m} \\ \mathbf{0} \end{bmatrix}$$
(6)

Adjoint equation* (6) avoids the need to compute $\frac{\partial \lambda_m}{\partial b_r}$, $\frac{\partial \mathbf{v}_m}{\partial b_r}$

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Experiment 1 (curve): hand

40 hand contours

□ Control Point + Knot Point

B-spline representation

• Data courtesy of Technical University of Denmark

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Correspondence before vs. after optimziation

Statistical mode before vs. after optimization

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Time cost comparison: concatenation vs. direct reparam.

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Experiment 2 (surface): plane-bump

Correspondence before vs. after optimziation

Time cost comparison: concatenation vs. direct reparam.

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Time complexity of analytical gradient

• Adjoint sensitivity scales better w.r.t n_b and n_S

Aorta anatomy

- 1) Ascending aorta; 2) Aortic arch;
- 3) Left coronary artery; 5) Right coronary artery;
- 4) Left coronary sinus; 6) Right coronary sinus;
 - 7) Non-coronary sinus

Input raw triangle meshes

- From CT images
- 6 patients
- Shape 3 with severe aneurysm
- Courtesy of Georgia Tech

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Generatrix construction

Consistent cylindrical topology

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Training set B-splines fitting

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Statistical modes analysis

- Mode 1: Ascending aorta dilation, $\lambda_1 = 2.06 (64.5\%)$
- Mode 2: Coronary sinus dilation, $\lambda_2 = 0.44$ (13.8%)
- Mode 3: Annulus dilation, $\lambda_3 = 0.38$ (11.8%)

Raw proximal femur data

- 29 proximal femur meshes
- 17 patients
- 13 healthy, 16 unhealthy
- Courtesy of RUSH hospital

Two training sets: healthy and unhealthy

Correspondence improvement

Reference shape feature line 1

A non-ref shape corresponding line 1 before (red) and after (blue) optimization

- Feature line: intertrochanteric line
- Improvement noticeable at the greater trochanter eminence
- Similar improvement observed in unhealthy group

Statistical modes analysis: healthy group

- Mode 1: femur head ball enlarging and the trochanter shrinking (4.3mm)
- Mode 2: additional thickening pattern of intertrochanteric valley (1.2 mm)
- Mode 3: bone material depositing at femur neck near trochanter (0.7mm)

Statistical modes analysis: unhealthy group

- Mode 1: femur head ball enlarging and the trochanter shrinking (3.9mm)
- Mode 2: femur head ball enlarging (1.7 mm)
- Mode 3: bone material depositing at femur neck near head (1mm)

Statistical modes analysis: unhealthy group

- Bone material (0.7mm) of unhealthy mean on unhealthy mean
- Probable cause of cam impingement among unhealthy group

Discrete covariance matrix

- Suppose training set of n_S shapes $\{S_i\}$ $(i = 1, 2, ..., n_S)$
 - ► Landmark: $\mathbf{x}_{i}^{(j)} = \left[x_{i}^{(j)}, y_{i}^{(j)}, z_{i}^{(j)}\right] \in \mathcal{S}_{i} \quad (j \in 1, 2, ..., n_{P})$
 - Shape vector: $\mathbf{X}_i \doteq \left[\mathbf{x}_i^{(1)}, \mathbf{x}_i^{(2)}, ..., \mathbf{x}_i^{(n_P)}\right]^T$
- Mean shape: $\bar{\mathbf{X}} \doteq \frac{1}{n_S} \sum_{i=1}^{n_S} \mathbf{X}_i$.
- Shape data matrix: $\mathcal{X} = [\mathbf{X}_1 \bar{\mathbf{X}}, \ \mathbf{X}_2 \bar{\mathbf{X}}, \ ..., \ \mathbf{X}_{n_S} \bar{\mathbf{X}}]$
- Discrete covariance matrix

$$\widetilde{\mathbf{D}} \doteq \frac{1}{n_S - 1} \sum_{i=1}^{n_S} \left(\mathbf{X}_i - \bar{\mathbf{X}} \right)^T \left(\mathbf{X}_i - \bar{\mathbf{X}} \right) = \frac{1}{n_S - 1} \mathcal{X}^T \mathcal{X}$$

Or entry-wise definition: $\widetilde{D}_{i_1i_2} \doteq \frac{1}{n_S - 1} \left(\mathbf{X}_{i_1} - \bar{\mathbf{X}} \right)^T \left(\mathbf{X}_{i_2} - \bar{\mathbf{X}} \right)$

• PCA for SSM variation $\{\lambda_m\}$ and modes $\{\mathbf{v}_m\}$

$$\widetilde{\mathbf{D}}\,\mathbf{v}_m = \lambda_m \mathbf{v}_m$$

Continuous covariance matrix

• Mean shape:
$$\bar{\mathbf{S}}(\mathbf{u}) \doteq \frac{1}{n_S} \sum_{i=1}^{n_S} \mathbf{S}_i(\mathbf{u}).$$

• Continuous formulation I

$$C_{i_1i_2}^{I} \doteq \frac{1}{n_S - 1} \int_{\mathcal{U}} \left[\mathbf{S}_{i_1}(\mathbf{u}) - \bar{\mathbf{S}}(\mathbf{u}) \right]^T \left[\mathbf{S}_{i_2}(\mathbf{u}) - \bar{\mathbf{S}}(\mathbf{u}) \right] \, \mathrm{d}\mathbf{u}$$

• Continuous formulation II

$$C_{i_{1}i_{2}}^{II} \doteq \frac{\int_{\mathcal{U}} \left[\mathbf{S}_{i_{1}}(\mathbf{u}) - \bar{\mathbf{S}}(\mathbf{u}) \right]^{T} \left[\mathbf{S}_{i_{2}}(\mathbf{u}) - \bar{\mathbf{S}}(\mathbf{u}) \right] |\mathbf{J}(\mathbf{u})| \, \mathrm{d}\mathbf{u}}{(n_{S} - 1) \int_{\mathcal{U}} |\mathbf{J}(\mathbf{u})| \, \mathrm{d}\mathbf{u}},$$

$$\bullet \quad \mathsf{Curve:} \ |\mathbf{J}(u)| = \left| \frac{\mathrm{d}\bar{\mathbf{S}}(\mathbf{u})}{\mathrm{d}u} \right|$$

$$\bullet \quad \mathsf{Surface:} \ |\mathbf{J}(u, v)| = \left| \frac{\partial \bar{\mathbf{S}}(u, v)}{\partial u} \times \frac{\partial \bar{\mathbf{S}}(u, v)}{\partial v} \right|$$

Continuous formulation *I* with analytical integral

• Bézier curves:
$$\mathbf{S}_{i}(u) = \sum_{j=0}^{p} B_{j}^{p}(u) \mathbf{P}_{j}^{(i)}, \ u \in [0, 1]$$

 $C_{i_{1}i_{2}}^{I} = \frac{1}{n_{S} - 1} \int_{0}^{1} \sum_{j=0}^{2p} B_{j}^{2p}(u) Q_{j}^{(i_{1},i_{2})} du$
 $= \sum_{j=0}^{2p} \sum_{l=\max(0,j-p)}^{\min(j,p)} \frac{\binom{p}{l}\binom{p}{j-l}\widehat{\mathbf{P}}_{l}^{(i_{1})T}\widehat{\mathbf{P}}_{j-l}^{(i_{2})}}{\binom{2p}{j}(n_{S} - 1)(2p + 1)}.$
• Bézier surfaces: $\mathbf{S}_{i}(\mathbf{u}) = \sum_{j=0}^{p} \sum_{k=0}^{q} B_{j}^{p}(u) B_{k}^{q}(v) \mathbf{P}_{j,k}^{(i)}, \ u \times v \in [0,1]^{2}$
 $C_{i_{1}i_{2}}^{I} = \sum_{j=0}^{2p} \sum_{k=0}^{2q} \sum_{l=\max(0,j-p)}^{\min(j,p)} \sum_{m=\max(0,k-q)}^{\min(k,q)} \frac{\binom{p}{l}\binom{p}{j-l}\binom{q}{m}\binom{k}{n-m}\widehat{\mathbf{P}}_{l,m}^{(i_{1})T}\widehat{\mathbf{P}}_{j-l,k-m}^{(i_{2})}}{\binom{2p}{2}\binom{2p}{k}(n_{S} - 1)(2p + 1)(2q + 1)}$

• B-spline curves/surfaces: summation over knot spans

Continuous formulation II with analytical integrand

Bézier curves

$$C_{i_{1}i_{2}}^{II} \frac{\int_{0}^{1} \sum_{j=0}^{2p} \sum_{k=0}^{p-1} B_{j}^{2p}(u) B_{k}^{p-1}(u) Q_{j}^{(i_{1},i_{2})} \widetilde{P}_{k} \, \mathrm{d}u}{(n_{S}-1) \int_{0}^{1} \sum_{k=0}^{p-1} B_{k}^{p-1}(u) \widetilde{P}_{k} \, \mathrm{d}u}$$

where $\widetilde{P}_k = p(\overline{P}_{k+1} - \overline{P}_k)$. and

$$Q_{j}^{(i_{1},i_{2})} = \sum_{l=\max(0,j-p)}^{\min(j,p)} \frac{\binom{p}{l}\binom{p}{j-l}}{\binom{2p}{j}} \,\widehat{\mathbf{P}}_{l}^{(i_{1})T} \widehat{\mathbf{P}}_{j-l}^{(i_{2})}$$

- Similar for Bézier surface and B-spline curves/surfaces
- Formulation I and II can be approximated by quadrature

Incorporation of reparametrization

•
$$C_{i_1i_2}^I \doteq \frac{1}{n_S - 1} \int_{\mathcal{U}} \widehat{\mathbf{S}}_{i_1}[\mathbf{R}_{i_1}(\mathbf{u})]^T \widehat{\mathbf{S}}_{i_2}[\mathbf{R}_{i_2}(\mathbf{u})] \, \mathrm{d}\mathbf{u}$$

Shapes $\{\mathbf{S}_i(u)\}$		Reparam. $\{R_i(u)\}$	Gauss Pt. No.
Туре	Degree	Degree	n_G^*
Bézier curve	p	—	p + 1
Bézier surface	$p \times q$	—	(p+1)(q+1)
B-spline curve	p	—	p + 1
B-spline surface	$p \times q$	—	(p+1)(q+1)
Bézier curve	p	d	pd+1
Bézier surface	$p \times q$	d imes e	(pd+1)(qe+1)
B-spline curve	p	d	pd+1
B-spline surface	$p \times q$	d imes e	

•
$$C_{i_1 i_2}^{II} \doteq \frac{\int_{\mathcal{U}} \widehat{\mathbf{S}}_{i_1}[\mathbf{R}_{i_1}(\mathbf{u})]^T \widehat{\mathbf{S}}_{i_2}[\mathbf{R}_{i_2}(\mathbf{u})] |\mathbf{J}(\mathbf{R}(\mathbf{u}))| \, \mathrm{d}\mathbf{u}}{(n_S - 1) \int_{\mathcal{U}} |\mathbf{J}(\mathbf{R}(\mathbf{u}))| \, \mathrm{d}\mathbf{u}}$$

Discrete covariance matrix of qurater circles

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Continuous covariance matrix of qurater circles

- Discrete formulation subject to sampling density/pattern
- Continuous formulations independent of sampling density/pattern

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Line-bump shapes and two reparametrizations

Covariance matrix convergence under reparametriation

• Formulation II is independent of parametrization

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Influence on correspondence optimization: C^{I} vs. C^{II}

- Compare optimized landmarks by using C^I and C^{II}
- Formulation II yields more reasonable landmark distribution

Summary and outlook

Thesis contributions

- Direct diffeomorphic reparametrization achieved through B-splines
- Pull differentiability of objective function w.r.t optimization variables
- Adjoint method for analytical gradient computation
- Analytical form and efficient numerical quadrature for covariance matrix
- Viable application to real medical data with valuable clinical insights

Future work

- Extension from single patch to complex topologies
- Experiments with larger data pool

