Polynomial Regression on Riemannian Manifolds

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../Figs/UlogoDrumFeather

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Nonparametric Regression

Number of parameters tied to amount of data present

Has been extended to shape spaces, diffeomorphisms (Davis2007)
Parametric Regression

Small number of parameters can be estimated more efficiently

Geodesic shape regression (Niethammer-Huang-Vialard2011, Fletcher2011) has recently received attention.
Polynomial Regression

Polynomials enable more flexible parametric regression
Riemannian Polynomials

At least three ways to define polynomial in $\mathbb{R}^d$

- **Algebraic:** $\gamma(t) = c_0 + \frac{1}{1!} c_1 t + \frac{1}{2!} c_2 t^2 + \cdots + \frac{1}{k!} c_k t^k$
Riemannian Polynomials

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- **Variational:** $\gamma = \operatorname{argmin}_\varphi \int_0^T | \left( \frac{d}{dt} \right)^{k+1} \varphi(t) |^2 dt \quad \text{s.t. BC/ICs}$
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- Variational: $\gamma = \text{argmin} \varphi \int_0^T \left| \frac{d^{k+1}}{dt^{k+1}} \varphi(t) \right|^2 dt$ s.t. BC/ICs

- Differential: $\left( \frac{d}{dt} \right)^{k+1} \gamma(t) = 0$ s.t. initial conditions $\left( \frac{d}{dt} \right)^i \gamma(0) = c_i$
Riemannian Polynomials

At least three ways to define polynomial in $\mathbb{R}^d$

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  \[
  \gamma(t) = c_0 + \frac{1}{1!} c_1 t + \frac{1}{2!} c_2 t^2 + \cdots + \frac{1}{k!} c_k t^k
  \]

- **Variational:**
  \[
  \gamma = \arg\min_\varphi \int_0^T \left| \left( \frac{d}{dt} \right)^{k+1} \varphi(t) \right|^2 \, dt \quad \text{s.t. BC/ICs}
  \]

- **Differential:**
  \[
  \left( \frac{d}{dt} \right)^{k+1} \gamma(t) = 0 \quad \text{s.t. initial conditions} \quad \left( \frac{d}{dt} \right)^i \gamma(0) = c_i
  \]

**Covariant derivative:** replace $\frac{d}{dt}$ with $\frac{D}{dt} = \nabla \dot{\gamma}$
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**Covariant derivative:** replace $\frac{d}{dt}$ with $\frac{D}{dt} = \nabla \dot{\gamma}$

**Geodesics** ($k = 1$) have both interpretations

- $\gamma = \arg\min_\varphi \int_0^T |\dot{\varphi}(t)|^2 dt$

- $\nabla \dot{\gamma} \dot{\gamma} = 0$ s.t. initial conditions $\gamma(0), \dot{\gamma}(0)$

- Well-studied (Fletcher, Younes, Trouve, Vialard, Niethammer...
Riemannian Polynomials

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**Covariant derivative:** replace $\frac{d}{dt}$ with $\frac{D}{dt} = \nabla \dot{\gamma}$

**Cubic spline** satisfies (Noakes1989, Leite, Machado,...)

- $\gamma = \arg\min_\varphi \int_0^T |\nabla \dot{\varphi(t)}|^2 dt$

- **Euler-Lagrange equation:** $(\nabla \dot{\gamma})^3 \ddot{\gamma} = R(\dot{\gamma}, \nabla \dot{\gamma} \dot{\gamma}) \dot{\gamma}$

- **Shape splines** (Trouve&Vialard)

- **Quantum splines** (Brody-Holm-Meier)
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**Covariant derivative:** replace $\frac{d}{dt}$ with $\frac{D}{dt} = \nabla \dot{\gamma}$

**$k$-order polynomial** satisfies

- $$(\nabla \dot{\gamma})^k \dot{\gamma} = 0$$ subject to initial conditions $\gamma(0), (\nabla \dot{\gamma})^i \dot{\gamma}(0), i = 0, \ldots, k - 1$$
Riemannian Polynomials

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$k$-order polynomial satisfies

- $(\nabla \dot{\gamma})^k \dot{\gamma} = 0$
  subject to initial conditions $\gamma(0), (\nabla \dot{\gamma})^i \dot{\gamma}(0), i = 0, \ldots, k - 1$

- Introduced via *rolling maps* by Jupp&Kent1987
- Mentioned in Leite&Krakowski2008
Rolling maps

Unroll curve $\alpha$ on manifold to curve $\alpha_{dev}$ on $\mathbb{R}^d$ without twisting or slipping. Then

$$(\nabla_{\dot{\alpha}})^k \dot{\alpha} = 0 \iff \left( \frac{d}{dt} \right)^k \dot{\alpha}_{dev} = 0$$

* Leite & Krakowski. Covariant Differentiation Under Rolling Maps. 2008.
Polynomial Regression

To compute, $\left(\nabla \dot{\gamma}\right)^k \dot{\gamma} = 0$ becomes linearized system

\[
\begin{align*}
\dot{\gamma} &= v_1 \\
\nabla \dot{\gamma} v_1 &= v_2 \\
\vdots \\
\nabla \dot{\gamma} v_{k-1} &= v_k & i = 1, \ldots, k - 1 \\
\nabla \dot{\gamma} v_k &= 0.
\end{align*}
\]

Want to find initial conditions $\gamma(0), v_i(0)$ for this ODE to minimize

\[
E(\gamma) = \sum_{i=1}^{N} d(\gamma(t_i), y_i)^2
\]
Riemannian Polynomials

Forward Polynomial Evolution

repeat
  \( w \leftarrow v_1 \)
  for \( i = 1, \ldots, k - 1 \) do
    \( v_i \leftarrow \text{ParallelTransport}_\gamma(\Delta t w, v_i + \Delta t v_{i+1}) \)
  end for
  \( v_k \leftarrow \text{ParallelTransport}_\gamma(\Delta t w, v_k) \)
  \( \gamma \leftarrow \text{Exp}_\gamma(\Delta t w) \)
  \( t \leftarrow t + \Delta t \)
until \( t = T \)

Parametrized by ICs:
- \( \gamma(0) \): position
- \( v_1(0) \): velocity
- \( v_2(0) \): acceleration
- \( v_3(0) \): jerk

Polynomial Regression on Riemannian Manifolds
Intrinsic adjoint optimization method (details in arXiv paper): initialize $\lambda_i = 0$ at $t = 1$ then integrate backward to $t = 0$:

\[
\nabla_{\dot{\gamma}} \lambda_0 = - \sum_{i=1}^{N} \delta(t - t_i) \log_{\gamma(t_i)} y_i + \sum_{j=1}^{k} R(\lambda_j, v_j) v_1
\]

\[
\nabla_{\dot{\gamma}} \lambda_1 = -\lambda_0
\]

\[
\vdots
\]

\[
\nabla_{\dot{\gamma}} \lambda_k = -\lambda_{k-1}
\]

Parameter gradients are

\[
\delta_{\gamma(0)} E = -\lambda_0(0)
\]

\[
\delta_{v_1(0)} E = -\lambda_1(0)
\]

\[
\vdots
\]

\[
\delta_{v_k(0)} E = -\lambda_k(0)
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Intrinsic adjoint optimization method (details in arXiv paper): initialize $\lambda_i = 0$ at $t = 1$ then integrate backward to $t = 0$:

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$$\nabla \dot{\gamma} \lambda_1 = - \lambda_0$$

$$\vdots$$

$$\nabla \dot{\gamma} \lambda_k = - \lambda_{k-1}$$

Parameter gradients are

$$\delta_{\gamma(0)} E = - \lambda_0(0)$$

$$\delta_{v_1(0)} E = - \lambda_1(0)$$

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$$\delta_{v_1(0)} E = - \lambda_1(0)$$

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Polynomial Regression

Algorithm

repeat

Integrate $\gamma$, $\{v_i\}$ forward to $t = 1$

Initialize $\lambda_i(1) = 0, i = 0, \ldots, k$

Integrate $\{\lambda_i\}$ via adjoint equations back to $t = 0$

Gradient descent step:

$\gamma(0)^{n+1} = \text{Exp}_{\gamma(0)^n}(\epsilon \lambda_0(0))$

$v_i(0)^{n+1} = \text{ParTrans}_{\gamma(0)^n}(\epsilon \lambda_0(0), v_i(0)^n + \epsilon \lambda_i(0))$

until convergence
Special Case: Geodesic ($k = 1$)

Adjoint system is

\[ \nabla_{\dot{\gamma}} \lambda_0 = - \sum_{i=1}^{N} \delta(t - t_i) \log_{\gamma(t_i)} y_i + R(\lambda_1, v_1) v_1 \]

\[ \nabla_{\dot{\gamma}} \lambda_1 = -\lambda_0 \]

Between data points this is

\[ (\nabla_{\dot{\gamma}})^2 \lambda_1 = -R(\lambda_1, \dot{\gamma}) \dot{\gamma} \]

This is the Jacobi equation, $\lambda_1$ is an (adjoint) Jacobi field.
Coefficient of Determination ($R^2$)

Define the following

$$R^2 = 1 - \frac{SSE_\gamma}{SSE_\mu}$$

where $SSE_\mu$ is the sum squared error at the Frechet mean $\mu$:

$$SSE_\mu = \sum_i d(\mu, y_i)^2$$

and $SSE_\gamma$ is sum squared residuals of the curve $\gamma$:

$$SSE_\gamma = \sum_i d(\gamma(t_i), y_i)^2$$

$R^2 \in [0, 1]$ measures how much variance is explained away by the curve $\gamma$
Kendall Shape Space

Space of $N$ landmarks in $d$ dimensions, $\mathbb{R}^{N \times d}$, modulo translation, scale, rotation. Geometry is well-known.
Bookstein Rat Calvarium Growth

- 8 landmark points
- 18 subjects
- 8 ages

| $k$ | $R^2$ |
|-----|-------|
| 1   | 0.79  |
| 2   | 0.85  |
| 3   | 0.87  |
Corpus Collosum Aging (www.oasis-brains.org)

Fletcher 2011

- $N = 32$ patients
- Age range 18–90
- 64 landmarks using ShapeWorks sci.utah.edu

| $k$ | $R^2$ |
|-----|-------|
| 1   | 0.12  |
| 2   | 0.13  |
| 3   | 0.21  |

Polynomial Regression on Riemannian Manifolds
Initial conditions are collinear, implying time reparametrization
LDDMM Landmark Space

Space $\mathcal{L}$ of $N$ points in $\mathbb{R}^d$. Geodesic equations:

$$\frac{d}{dt} x_i = \sum_{j=1}^{N} \gamma(|x_i - x_j|^2) \alpha_j$$

$$\frac{d}{dt} \alpha_i = -2 \sum_{j=1}^{N} (x_i - x_j) \gamma'(|x_i - x_j|^2) \alpha_j^T \alpha_j$$

Use Gaussian kernel (or Cauchy, Laplace, etc.)

$$\gamma(r) = e^{-r/(2\sigma^2)}$$

$x \in \mathcal{L}$ and $\alpha \in T_x^*\mathcal{L}$ is a covector (momentum)
LDDMM Landmark Space

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Use Gaussian kernel (or Cauchy, Laplace, etc.)

$$\gamma(r) = e^{-r/(2\sigma^2)}$$

$x \in \mathcal{L}$ and $\alpha \in T_x^* \mathcal{L}$ is a covector (momentum)
Have simple formula for cometric $g^{ij}$ (the kernel)
Parallel transport in terms of covectors, cometric:

$$\frac{d}{dt} \beta_{\ell} = \frac{1}{2} g_{i\ell} g_{jn}^{\text{in}} g^{jm} (\alpha_m \beta_n - \alpha_n \beta_m) - \frac{1}{2} g_{,\ell}^{mn} \alpha_m \beta_n$$

Curvature more complicated (Mario’s Formula, Micheli 2010):

$$2 R^{ursv} = -g^{ur,sv} - g^{rv,us} + g^{rs,uv} + g^{uv,rs} + 2 \Gamma^r_{\rho v} \Gamma^u_{\sigma s} g^{\rho \sigma} - 2 \Gamma^r_{\rho s} \Gamma^{uv}_{\sigma} g^{\rho \sigma} + g^{r \lambda, u} g_{\lambda \mu} g^{\mu v, s} - g^{r \lambda, u} g_{\lambda \mu} g^{\mu s, v} + g^{u \lambda, r} g_{\lambda \mu} g^{\mu s, v} - g^{u \lambda, r} g_{\lambda \mu} g^{\mu v, s} + g^{r \lambda, s} g_{\lambda \mu} g^{\mu v, u} + g^{u \lambda, v} g_{\lambda \mu} g^{\mu s, r} - g^{r \lambda, v} g_{\lambda \mu} g^{\mu s, u} - g^{u \lambda, s} g_{\lambda \mu} g^{\mu v, r}.$$
Landmark parallel transport in momenta (Younes2008):

\[
\frac{d}{dt} \beta_i = K^{-1} \left( \sum_{j=1}^{N} (x_i - x_j)^T \left( (K \beta)_i - (K \beta)_j \right) \gamma'(|x_i - x_j|^2) \alpha_j \right)
\]

\[
- \sum_{j=1}^{N} (x_i - x_j)^T \left( (K \alpha)_i - (K \alpha)_j \right) \gamma'(|x_i - x_j|^2) \beta_j \right)
\]

\[
- \sum_{j=1}^{N} (x_i - x_j) \gamma'(|x_i - x_j|^2) \left( \alpha_j^T \beta_i + \alpha_i^T \beta_j \right)
\]

This is enough to integrate polynomials.
For curvature, need Christoffel symbols and their derivatives:

\[
(\Gamma(u, v))_i = -\sum_{j=1}^{N} (x_i - x_j)^T (v_i - v_j) \gamma'(|x_i - x_j|^2)(K^{-1}u)_j \\
- \sum_{j=1}^{N} (x_i - x_j)^T (u_i - u_j) \gamma'(|x_i - x_j|^2)(K^{-1}v)_j \\
+ \sum_{j=1}^{N} \gamma(|x_i - x_j|^2) \sum_{k=1}^{N} (x_j - x_k) \gamma'(|x_j - x_k|^2)((K^{-1}u)_k^T (K^{-1}v)_j + (K^{-1})}
\]

Take derivative with respect to \( x \), and combine using

\[
R^\ell_{ijk} = \Gamma^\ell_{ki,j} - \Gamma^\ell_{ji,k} + \Gamma^\ell_{jm} \Gamma^m_{ki} - \Gamma^\ell_{km} \Gamma^m_{ji}
\]
\[
(\langle D\Gamma (u, v) \rangle w)_i = \sum_{j=1}^{N} (w_i - w_j)^T (u_i - u_j) \gamma'(\|x_i - x_j\|^2) (K^{-1} v)_j \\
+ 2 \sum_{j=1}^{N} (x_i - x_j)^T (u_i - u_j) (x_i - x_j)^T (w_i - w_j) \gamma''(\|x_i - x_j\|^2) (K^{-1} v)_j \\
+ \sum_{j=1}^{N} (x_i - x_j)^T (u_i - u_j) \gamma'(\|x_i - x_j\|^2) (\frac{d}{d\epsilon} K^{-1}) v)_j \\
+ \sum_{j=1}^{N} (w_i - w_j)^T (v_i - v_j) \gamma'(\|x_i - x_j\|^2) (K^{-1} u)_j \\
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+ \sum_{j=1}^{N} (x_i - x_j)^T (v_i - v_j) \gamma'(\|x_i - x_j\|^2) (\frac{d}{d\epsilon} K^{-1}) u)_j \\
- 2 \sum_{j=1}^{N} (x_i - x_j)^T (w_i - w_j) \gamma'(\|x_i - x_j\|^2) \sum_{k=1}^{N} (x_j - x_k) \gamma'(\|x_j - x_k\|^2) ((K^{-1} u)_k^T (K^{-1} v)_j + (K^{-1} u)_j^T (K^{-1} v)_k) \\
- \sum_{j=1}^{N} \gamma(\|x_i - x_j\|^2) \sum_{k=1}^{N} (w_j - w_k) \gamma'(\|x_j - x_k\|^2) ((K^{-1} u)_k^T (K^{-1} v)_j + (K^{-1} u)_j^T (K^{-1} v)_k) \\
- 2 \sum_{j=1}^{N} \gamma(\|x_i - x_j\|^2) \sum_{k=1}^{N} (x_j - x_k)(x_j - x_k)^T (w_j - w_k) \gamma''(\|x_j - x_k\|^2) ((K^{-1} u)_k^T (K^{-1} v)_j + (K^{-1} u)_j^T (K^{-1} v)_k) \\
- \sum_{j=1}^{N} \gamma(\|x_i - x_j\|^2) \sum_{k=1}^{N} (x_j - x_k) \gamma'(\|x_j - x_k\|^2) \\
\times ((\frac{d}{d\epsilon} K^{-1} u)_k^T (K^{-1} v)_j + (K^{-1} u)_k^T (\frac{d}{d\epsilon} K^{-1} v)_j + (\frac{d}{d\epsilon} K^{-1} u)_j^T (K^{-1} v)_k + (K^{-1} u)_j^T (\frac{d}{d\epsilon} K^{-1} v)_k) \\
\left( \frac{d}{d\epsilon} K^{-1} v \right)_i = -(K^{-1} \frac{d}{d\epsilon} KK^{-1} v)_i \\
= -2(K^{-1} \sum_{j=1}^{N} (x_k - x_j)^T (w_k - w_j) \gamma'(\|x_k - x_j\|^2) (K^{-1} v)_j)
Same Bookstein rat data. Procrustes alignment, no scaling.

\[ R^2 = 0.92 \text{ geodesic, } 0.94 \text{ quadratic} \]
Question: how to choose polynomial order $k$?

$R^2$ always increases with increased $k$, but overfitting is bad
Testing Against the Frechet Mean

To test whether a model enables significant decrease in SSE:

- Generate a large number of permutations of indices $1, \ldots, N$
- Shuffle data by permuting times $t_i$
- Fit curve to permuted data and store list of $R^2$ values
- Percentage of $R^2$ greater than that of unpermuted fit is $p$-value

Fletcher (2011) used this to test for significant geodesic regression
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**Problem:** How to test against a lower order curve instead of the mean?
Testing against a curve

- $H_0$: data is generated by order $k$ polynomial $\gamma_k$ – samples $y_i$ are independent and exchangeable
Testing against a curve

- $H_0$: data is generated by order $k$ polynomial $\gamma_k$ – samples $y_i$ are independent and exchangeable via group action
- In homogeneous space, use transitive group action to exchange points
- Assumes noise distribution is isotropic: distribution invariant under action of isotropy group $H_{\gamma(t_i)}$
Permutation through group action

Given data (yellow stars) on the sphere
Permutation through group action

Fit base curve (green) under null hypothesis
Permutation through group action

Idealized points (black) along curve
Permutation through group action

Pair of points determines axis/angle of rotation
Permutation through group action

Apply rotations to original data points
Permutation through group action

Resulting data (orange) are shuffled under exchangeability assumption of the null hypothesis
Thank You!