Learning Shape Trends: Parameter Estimation in Diffusions on Shape Manifolds

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Motivation

- 100 years of mathematical study of shapes and their evolution
- Few statistical methods for learning stochastic processes of shapes

Learning Stochastic Models

Goal:

- to learn stochastic models of deforming shapes from training data

Challenges:

- shapes are high-dimensional objects in a nonlinear space
- traditional time series methods fail to capture the geometry

Approach:

- define diffusion processes on the space of discretized curves
- estimate missing parameters based on likelihood-ratio techniques

Stochastic Shape Processes Through History

- "The diffusion of Shape"(Kendall'77) introduces Brownian motion on the space of landmarks [6]
- extensions to an Ornstein - Uhlenbeck process (Ball'08) [2]
- modeling biological growth by diffeomorphisms (Grenander'06) [5]
- stochastic diffeomorphic flows for shapes (Vialard'12) [10]
- noise estimation in diffusions (Sommer'15, Arnaudon'16)[1],[9]

THE STATISTICS OF SHAPE

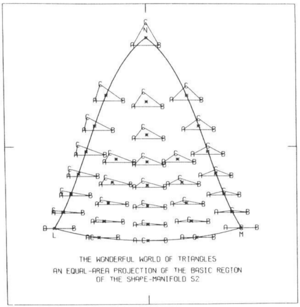

Figure 5.1 The spherical blackboard, showing 32 triangles located according to their shapes

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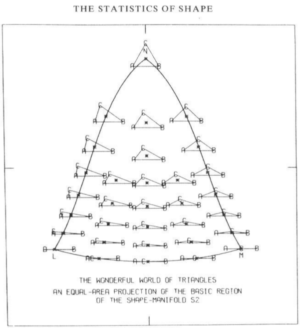

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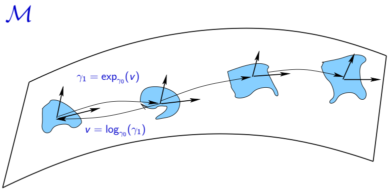
We focus on learning trends in diffusion processes on the Riemannian manifold of deformable landmarks.

The Shape Manifold



- The *shape manifold* $\mathcal{M}$ consists of simple closed plane curves γ
  - here $\gamma = \{x_1, ..., x_m \in \mathbb{R}^2, x_i \neq x_j \text{ when } i \neq j\}$

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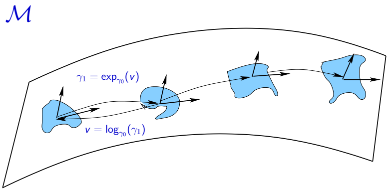

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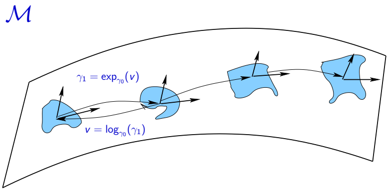

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  - $K(x_i, x_j) = \exp(\|x_i - x_j\|^2/2\sigma^2)$

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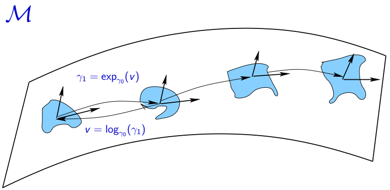

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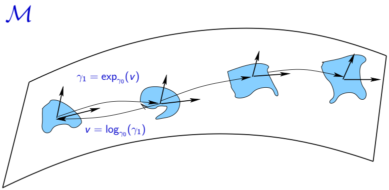

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- *Logarithm map:* $\mathbf{v} = \log_{\gamma_0}(\gamma_1)$
  - we assume it exists locally

Diffusion Models

Noise Models:

Random perturbations $\rightarrow$ random walk $\rightarrow$ Brownian motion

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Diffusion Models:

unknown parameters

$$d\gamma_t = \underbrace{A(\gamma_t, \theta)dt}_{drift} + \underbrace{B(\gamma_t)dW_t}_{noise}$$

Stratonovich Equations on Manifolds

Let $\{A, B_1, ..., B_n\}$ be vector fields on $\mathcal{M}$.

Stratonovich Equations on $\mathcal{M}$

The solution is a process X_t on $\mathcal{M}$, which satisfies for any smooth compactly supported f

$$f(X_T) - f(X_0) = \int_0^T Af(X_t)dt + \int_0^T \sum_{k=1}^{n} B_k f(X_t) \circ dw_k(t)$$

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Note: Stratonovich equations transform as tangent vectors!

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Instead we can define them through the exponential map.

Itô Equations in Belopolskaya-Daletsky form [3]:

$$dX_t = \exp_{X_t}(A(X_t, \theta)dt + \sum_{k=1}^{n} B_k \cdot dw_k(t)),$$

Generating Diffusions

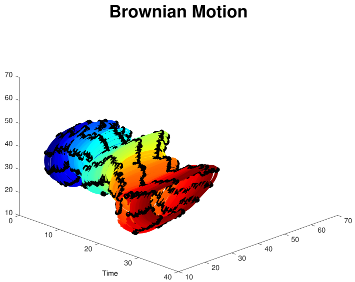
Consider a set of orthonormal vector fields: $E_1, ..., E_n$.

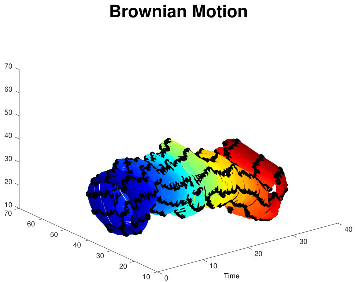
Generating Brownian motion on $\mathcal{M}$

$$\gamma_{t+dt} = \exp_{\gamma_t}\left(\sqrt{dt}\sum_{k=1}^{n} E_k(\gamma_t)\varepsilon_k\right),$$

where $\{\varepsilon_k\}_{k=1}^n \sim \mathcal{N}(\mathbf{0}, \mathbf{I_n})$.

Driftless Diffusion





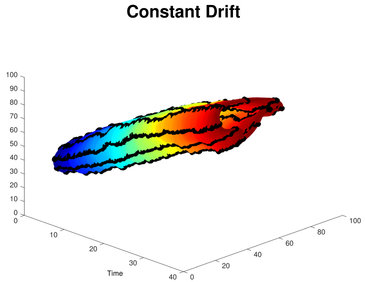
Constant drift

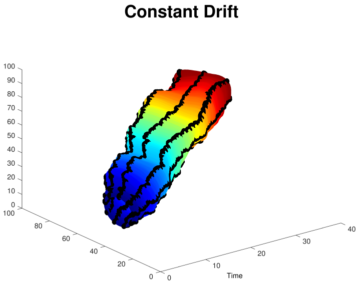
Constant with respect to the **K** basis

$$d\gamma_t = \sum_{k=1}^{n} \theta_k K(x_k, \gamma_t) dt + dW_t$$

Note: the drift will not be constant wrt to other bases.

Constant Drift Diffusion





Mean-reverting Drift

Ornstein-Uhlenbeck process on $\mathbb{R}^n$

$$dX_t = -\theta \nabla_{X_t} \left[(X_t - \mu)^2 \right] + dW_t$$

Let μ be a template shape.

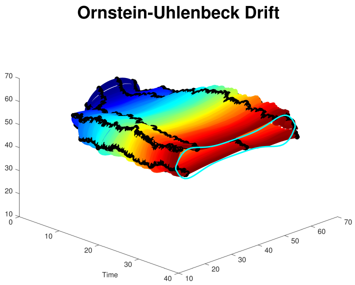
Mean-reverting process on $\mathcal{M}$

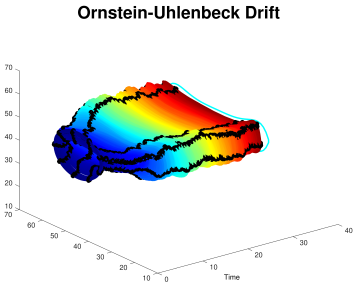
$$d\gamma_t = -\theta \nabla_{\gamma_t} dist(\gamma_t, \mu) + dW_t$$

Instead of Riemannian distance we use:

$$dist(X_t, \mu) = \text{area of mismatch of the two shapes}$$

Mean-reverting drift diffusion





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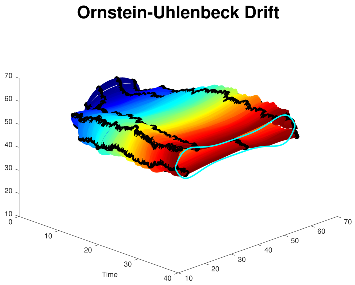
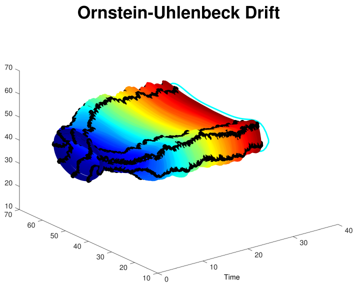




This model can be generalized for multiple templates $\mu_1, ..., \mu_p$:

$$d\chi_t = \exp_{\chi_t}\left(-\sum_{i=1}^{p}\theta_i \nabla^{\mathcal{M}} dist(\chi_t, \mu_i) + dW_t\right). \qquad (1)$$

Length-Area Drift

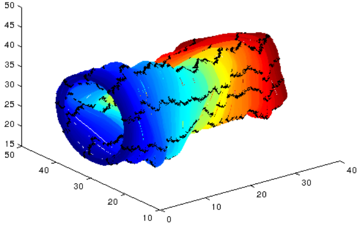
Suppose we don't have μ but only estimates for its length L_μ and area A_μ.

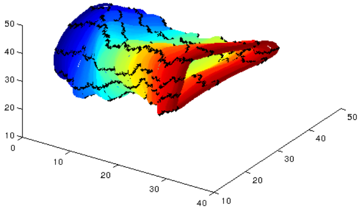
Shape process

$$dX_t = -\frac{1}{2}\theta_1 \nabla_{\gamma_t}|L_{\gamma_t} - L_\mu|^2 - \frac{1}{2}\theta_2 \nabla_{\gamma_t}|A_{\gamma_t} - A_\mu|^2 + dW_t$$

The above gradients can be explicitly computed.

Length-Area drift diffusion





Parameter Estimation in Diffusion Models

We are given a sequence of observations: $\gamma_{t_0}, ..., \gamma_{t_n}$.

We would like to maximize the joint likelihood:

$$p_\theta(\gamma_{t_1}, ..., \gamma_{t_n}) = p_\theta(\gamma_{t_n}|\gamma_{t_{n-1}})p_\theta(\gamma_{t_{n-1}}|\gamma_{t_{n-2}})...p_\theta(\gamma_{t_1}|\gamma_{t_0})p(\gamma_{t_0})$$

We do not have a closed form for the transition probability $p_\theta(\gamma_{t_i}|\gamma_{t_{i-1}})$.

Likelihood-ratio Parameter Estimation [7, 8]

Idea:

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   - driftless process
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   - Girsanov formula
3. estimate θ by maximizing the likelihood ratio
   - when the drift is linear wrt to θ the estimate has a closed form

Parameter Estimation in Diffusions on $\mathbb{R}^n$

Let X_t be a diffusion process on $\mathbb{R}^n$:

$$\begin{aligned} P_X: \quad dX_t &= A(X_t, \theta)dt + dW_t \\ P_Y: \quad dY_t &= dW_t \end{aligned}$$

Girsanov Formula:

$$\frac{dP_X}{dP_Y}(X_t) = \exp\left(\int_0^T A(X_t, \theta)^T \cdot dX_t - \frac{1}{2} \int_0^T A(X_t, \theta)^T A(X_t, \theta) dt \right).$$

Parameter estimate of θ can be obtained by maximizing $\frac{dP_X}{dP_Y}(X_t)$ wrt θ.

Girsanov Formula on Manifolds (Elworthy'82 [4])

$$\frac{dP_X}{dP_Y}(X_t) = \exp\left(\int_0^T \langle A(X_t,\theta), \cdot dX_t\rangle_{X_t} - \frac{1}{2}\int_0^T \langle A(X_t,\theta), A(X_t,\theta)\rangle_{X_t} dt\right),$$

where $\cdot dX_t$ should be interpreted as $\log_{X_t}(X_{t+dt})$

Likelihood-ratio Estimators

- Constant Drift

$$\hat{\theta} = \frac{1}{Ndt} \sum_{i=1}^{N-1} K_{\gamma_i}^{-1/2} \log(\gamma_i, \gamma_{i+1})$$

- Mean-Reverting Drift

$$\hat{\theta} = \frac{\sum_{i=1}^{N-1} \langle \nabla dist(\gamma_i, \mu), \log(\gamma_i, \gamma_{i+1}) \rangle}{\sum_{i=1}^{N} \|\nabla dist(\gamma_i, \mu)\|^2 dt}$$

- Shape-Gradient Drift

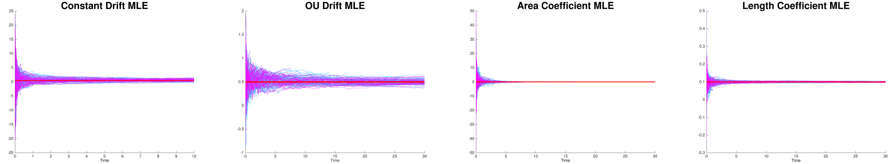
$$\begin{bmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \end{bmatrix} = \left(\sum_{i=1}^{N-1} M_i dt \right)^{-1} b,$$

where M_i - the Grammian matrix of $\nabla|L(\gamma_i) - L|^2$ and $\nabla|A(\gamma_i) - A|^2$, and

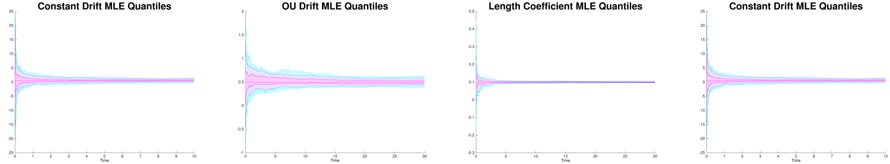
$$b = \begin{bmatrix} \sum_{i=1}^{N-1} \langle \nabla |L(\gamma_i) - L|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \\ \sum_{i=1}^{N-1} \langle \nabla |A(\gamma_i) - A|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \end{bmatrix}.$$

Likelihood-ratio Estimates

Independent ML Estimates



MLE Quantiles
(0.01,0.05, 0.25, 0.75,0.95,0.99)



Future Directions and Open Problems

Applications:

- parameter estimation from sparse observations
  - EM formulation to treat the missing observations
  - importance sampling approximation of the expectation step
- including higher order shape terms: e.g. curvature, torsion
- considering the distance to several template shapes - regression
- testing for different model parameters
- classification of time series

Theory:

- properties of diffusion models
  - long-term behavior
  - ergodicity
- extension to infinite dimensions: curves and surfaces
- properties of the estimators

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