

Learning Shape Trends: Parameter Estimation in Diffusions on Shape Manifolds

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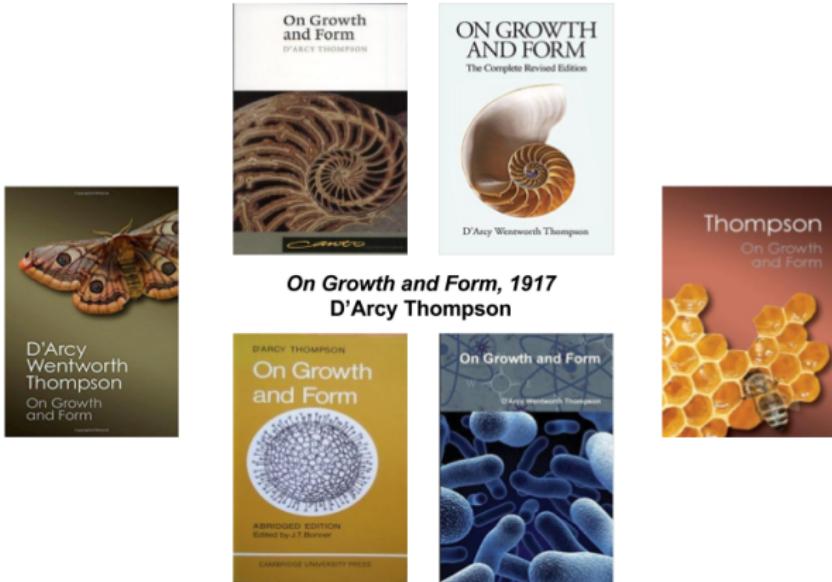
Joint work with Laurent Younes, Johns Hopkins University

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Alfred P. Sloan
FOUNDATION

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 deformable landmarks
- 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) [9]
- noise estimation in diffusions (Sommer'15, Arnaudon'16)[1],[?]

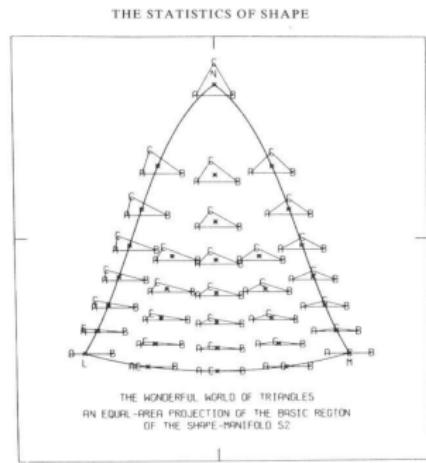


Figure 5.1 The spherical blackboard, showing 32 triangles located according to their shapes

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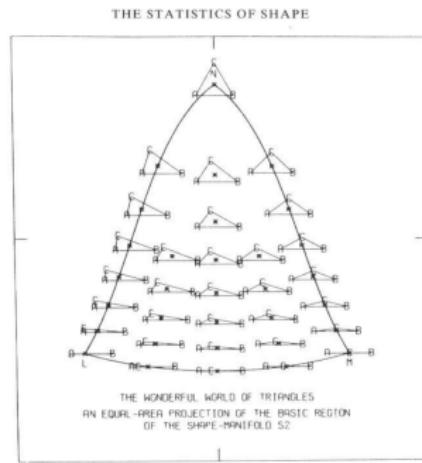
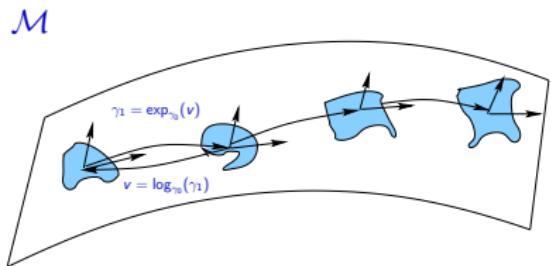


Figure 5.1 The spherical blackboard, showing 32 triangles located according to their shapes

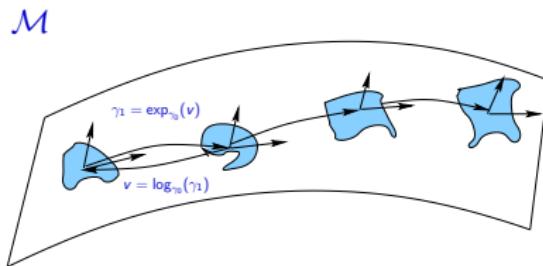
We focus on learning trends in diffusion processes on the Riemannian manifold of deformable landmarks.

The Shape Manifold



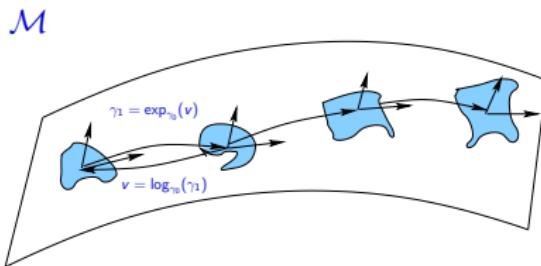
- The *shape manifold* \mathcal{M} consists of simple closed plane curves γ
 - here $\gamma = \{x_1, \dots, x_m \in \mathbb{R}^2, x_i \neq x_j \text{ when } i \neq j\}$

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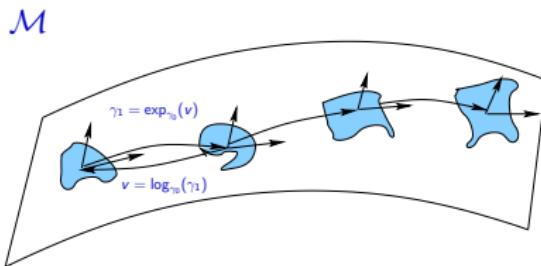
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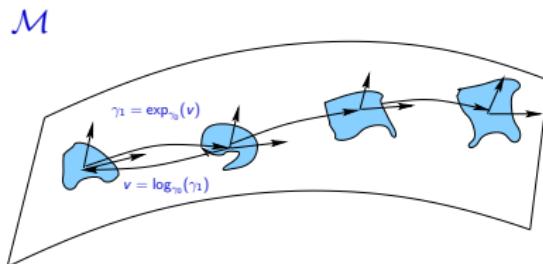
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 - can be computed by solving a system of ODE's
- *Logarithm map:* $v = \log_{\gamma_0}(\gamma_1)$
 - we assume it exists locally

Diffusion Models

Noise Models:

Random perturbations → random walk → Brownian motion

Brownian motion is not informative!

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Diffusion Models:

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

unknown parameters

↙

Stratonovich Equations on Manifolds

Let $\{A, B_1, \dots, B_n\}$ 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, \dots, E_n .

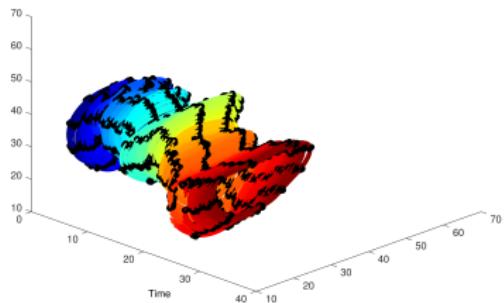
Generating Brownian motion on \mathcal{M}

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

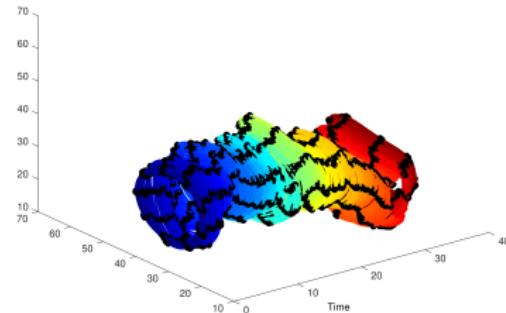
where $\{\varepsilon_k\}_{k=1}^n \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$.

Driftless Diffusion

Brownian Motion



Brownian Motion



Constant drift

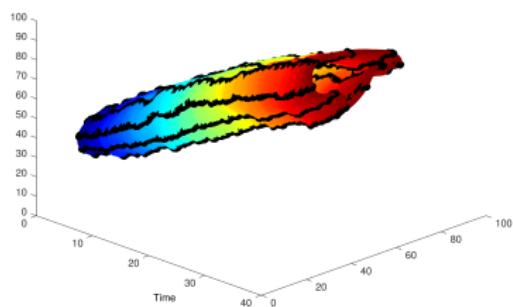
Constant with respect to the \mathbf{K} basis

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

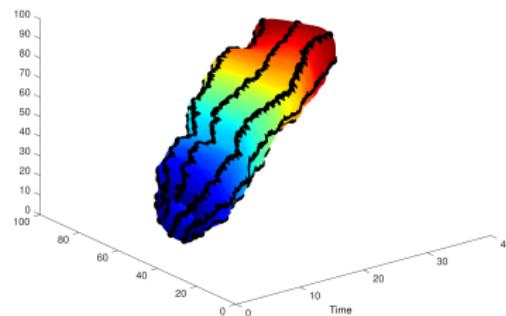
Note: the drift will not be constant wrt to other bases.

Constant Drift Diffusion

Constant Drift



Constant Drift



Mean-reverting Drift

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

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

Let μ be a template shape.

Mean-reverting process on \mathcal{M}

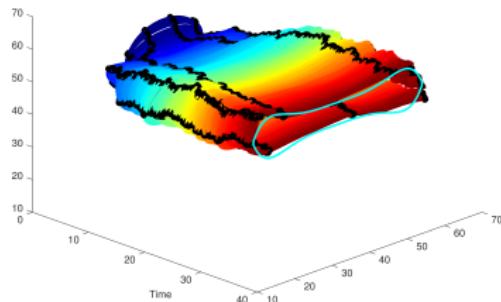
$$d\gamma_t = -\theta \nabla_{\gamma_t} dist(\gamma_t, \mu) + dW_t$$

Instead of Riemannian distance we use:

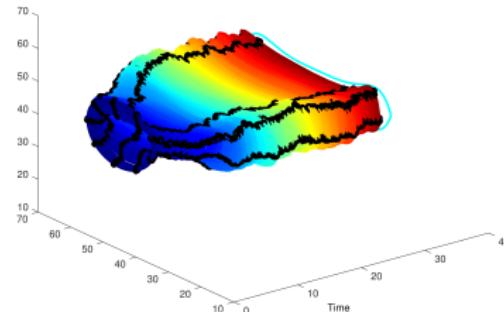
$$dist(X_t, \mu) = \text{area of mismatch of the two shapes}$$

Mean-reverting drift diffusion

Ornstein-Uhlenbeck Drift

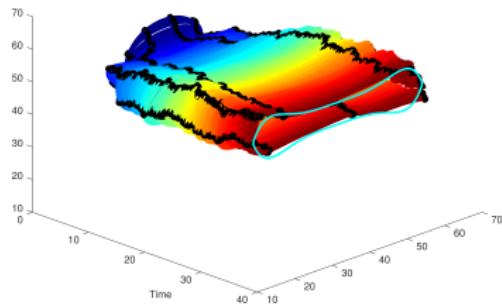


Ornstein-Uhlenbeck Drift

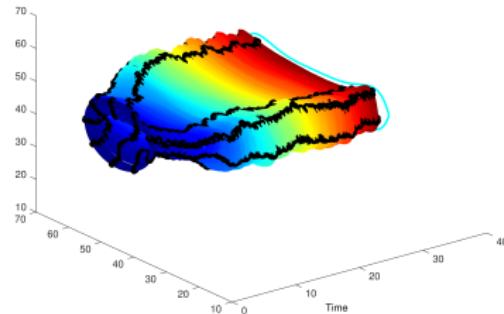


Mean-reverting drift diffusion

Ornstein-Uhlenbeck Drift



Ornstein-Uhlenbeck Drift



This model can be generalized for multiple templates μ_1, \dots, μ_p :

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

Length-Area Drift

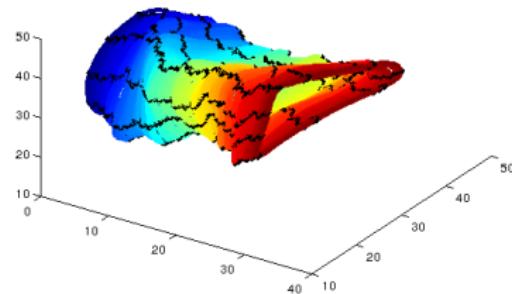
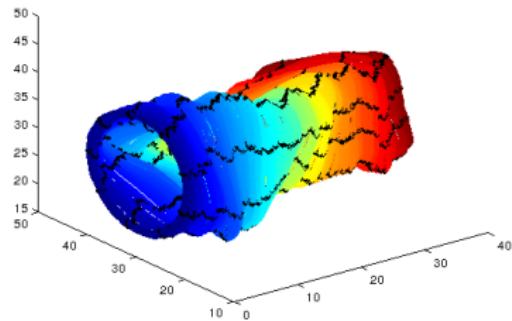
Suppose we don't have μ but only estimates for its length L_μ and area A_μ .

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: $\gamma_{t_0}, \dots, \gamma_{t_n}$.

We would like to maximize the joint likelihood:

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

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:

- ➊ pick a base process which does not depend on the parameters
 - driftless process

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- ② calculate the likelihood ratio of the diffusion with respect to the base process
 - Girsanov formula

Likelihood-ratio Parameter Estimation [7, 8]

Idea:

- ① pick a base process which does not depend on the parameters
 - driftless process
- ② calculate the likelihood ratio of the diffusion with respect to the base process
 - 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 :

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

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

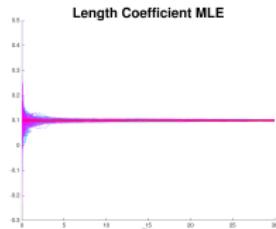
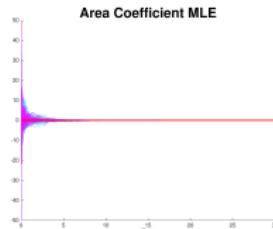
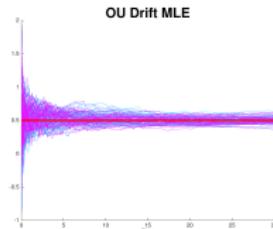
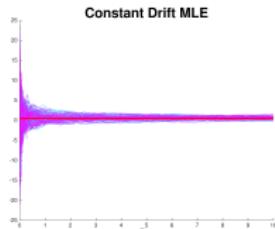
$$\begin{bmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \end{bmatrix} = \left(\sum_{i=1}^{N-1} M_i dt \right)^{-1} b,$$

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

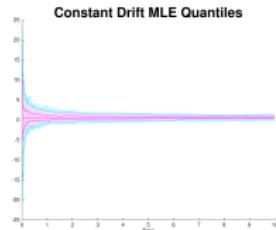
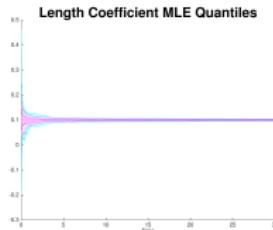
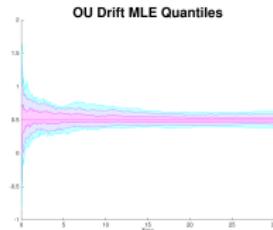
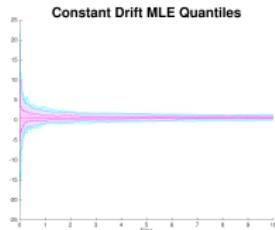
$$b = \begin{bmatrix} \sum_{i=1}^{N-1} \langle \nabla|L(\gamma_i) - L|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \\ \sum_{i=1}^{N-1} \langle \nabla|A(\gamma_i) - A|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \end{bmatrix}.$$

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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