

Learning Shape Trends: Parameter Estimation in Diffusions on Shape Manifolds

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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 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]

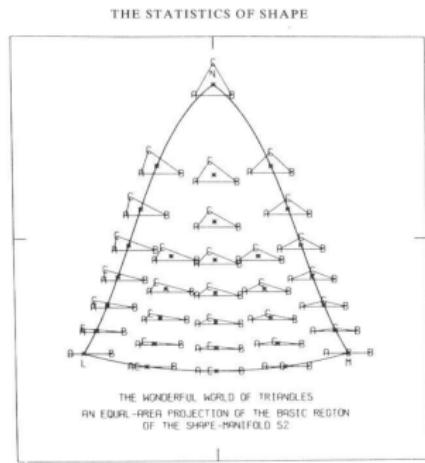


Figure 5.1 The spherical blackboard, showing 32 triangles located according to their shapes

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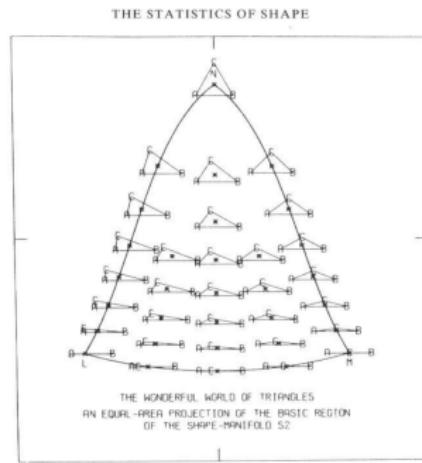
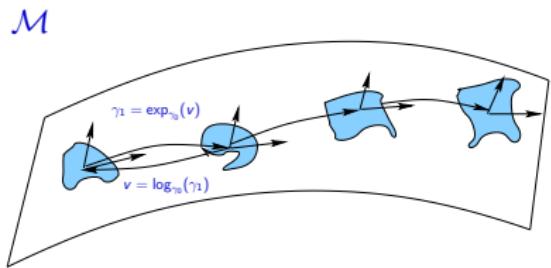


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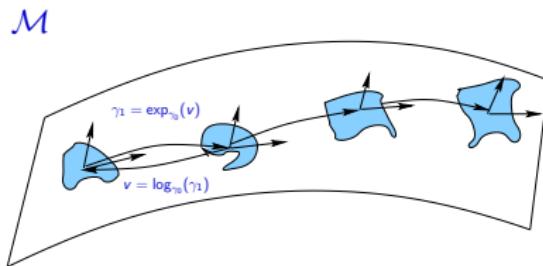
We focus on learning trends in diffusion processes on the Riemannian manifold of discretized contours.

The Shape Manifold



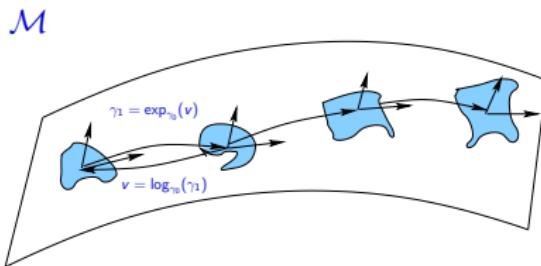
- The *shape manifold* \mathcal{M} consists of simple closed plane curves γ
 - here $\gamma = \{x_1, \dots, x_m \in \mathbb{R}^2, x_i \neq x_j \text{ when } i \neq j\}$

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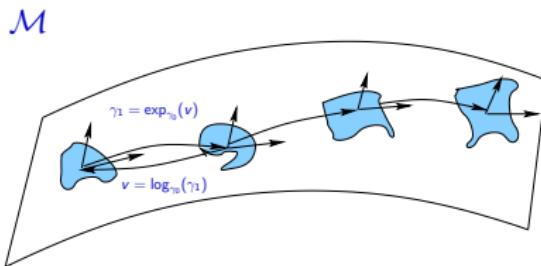
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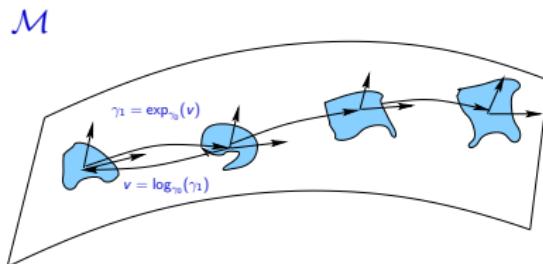
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- *Logarithm map:* $v = \log_{\gamma_0}(\gamma_1)$
 - we assume it exists locally

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 .

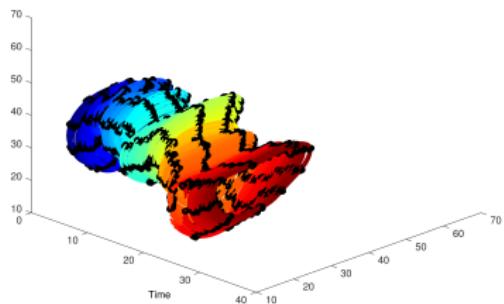
Generating Brownian motion on \mathcal{M}

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

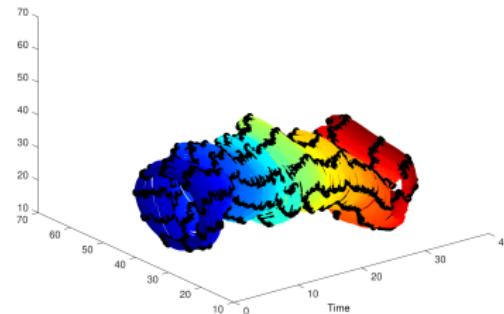
where $\{\varepsilon_k\}_{k=1}^n \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$.

Driftless Diffusion

Brownian Motion



Brownian Motion



Constant drift

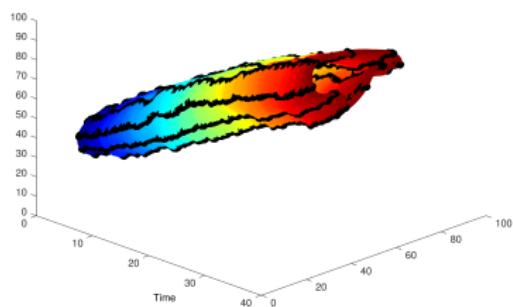
Constant with respect to the \mathbf{K} basis

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

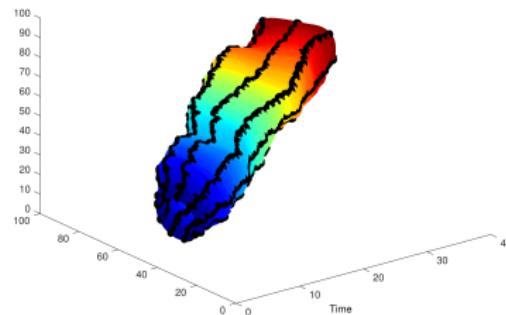
Note: the drift will not be constant wrt to other bases.

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}

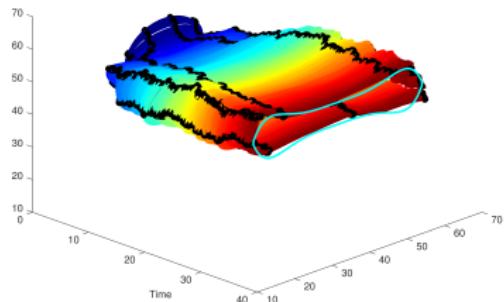
$$d\gamma_t = -\theta \nabla_{\gamma_t} dist(\gamma_t, \mu) + dW_t$$

Instead of Riemannian distance we use:

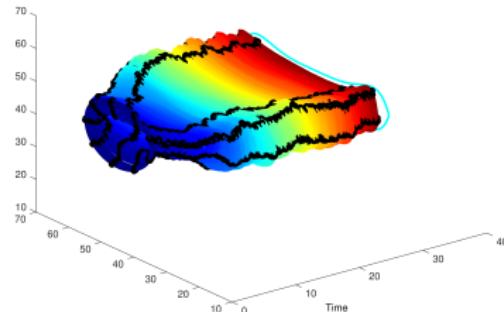
$$dist(X_t, \mu) = \text{area of mismatch of the two shapes}$$

Mean-reverting drift diffusion

Ornstein-Uhlenbeck Drift

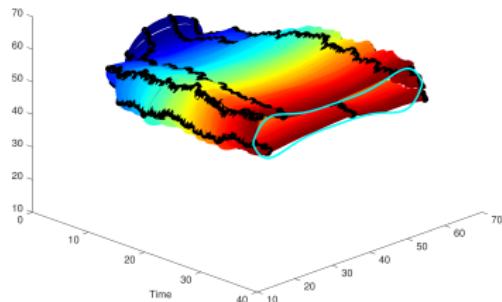


Ornstein-Uhlenbeck Drift

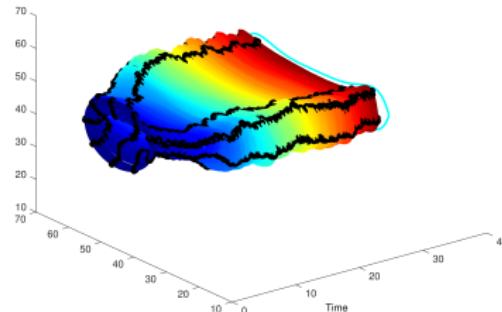


Mean-reverting drift diffusion

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

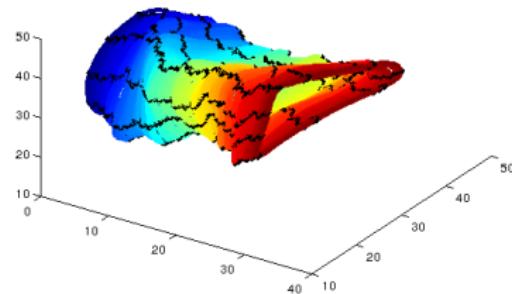
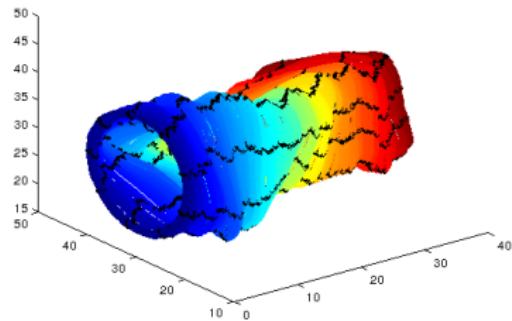
Suppose we don't have μ but only estimates for its length L_μ and area A_μ .

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

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Idea:

- ① pick a base process which does not depend on the parameters
 - 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 :

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

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

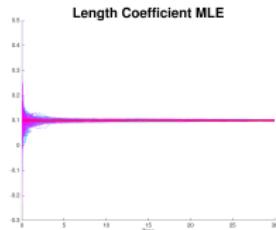
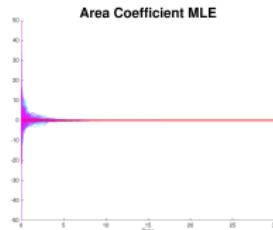
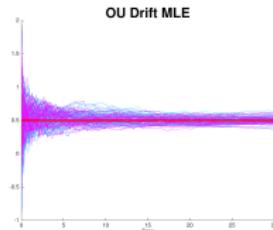
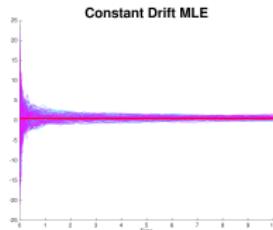
$$\begin{bmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \end{bmatrix} = \left(\sum_{i=1}^{N-1} M_i dt \right)^{-1} b,$$

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

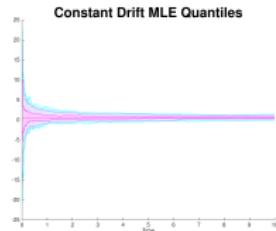
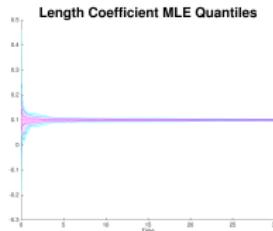
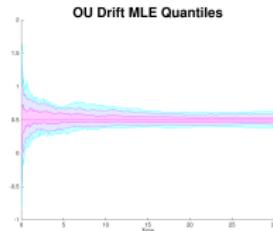
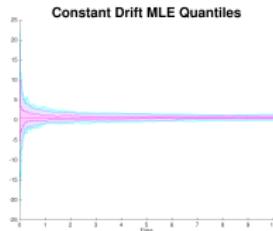
$$b = \begin{bmatrix} \sum_{i=1}^{N-1} \langle \nabla|L(\gamma_i) - L|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \\ \sum_{i=1}^{N-1} \langle \nabla|A(\gamma_i) - A|^2, \log(\gamma_i, \gamma_{i+1}) \rangle \end{bmatrix}.$$

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

-  Alexis Arnaudon, Darryl D. Holm, Akshay Pai, and Stefan Sommer.
A stochastic large deformation model for computational anatomy.
arXiv:1612.05323, 2016.
-  FrankG. Ball, IanL. Dryden, and Mousa Golalizadeh.
Brownian motion and Ornstein-Uhlenbeck processes in planar shape space.
Methodology and Computing in Applied Probability, 10(1):1–22, 2008.
-  Ya. I. Belopolskaya and Yu. L. Dalecky.
Stochastic Equations and Differential Geometry.
Springer, 1990.
-  K.D. Elworthy.
Stochastic Differential Equations on Manifolds.
Cambridge University Press, 1982.
-  Ulf Grenander, Anuj Srivastava, and Sanjay Saini.
Characterization of biological growth using iterated diffeomorphisms.
IEEE International Symposium on Biological Imaging, pages 1136–1139, 2006.
-  D.G. Kendall.
The diffusion of shape.
Advances in Applied Probability, 9(3):428–430, 1977.
-  R. S. Lipster and A. N. Shiryaev.
Statistics of Random Processes I. General Theory.
Springer-Verlag, 1977.
-  R. S. Lipster and A. N. Shiryaev.
Statistics of Random Processes II. Applications.
Springer-Verlag, 1977.
-  Stefan Sommer.
Anisotropic distributions on manifolds: Template estimation and most probable paths.
International Conference on Information Processing in Medical Imaging, 9123:193–204, 2015.