Likelihood Inference for SDE-models

with applications in Biology and Geophysics

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Likelihood function for discrete time observations

$$dX_t = b(X_t;\theta)dt + \sigma(X_t;\theta)dW_t \qquad \theta \in \Theta \subseteq \mathbb{R}^p$$

X, b and W d-dimensional, σ $d \times d$-matrix

Data: $X_{t_0}, \cdots, X_{t_n}$, $0 = t_0 < \cdots < t_n$

Likelihood-function:

$$L_n(\theta) = \prod_{i=1}^{n} p(\Delta_i, X_{t_{i-1}}, X_{t_i};\theta), \qquad \Delta_i = t_i - t_{i-1}$$

$$X_\Delta \mid X_0 = x \sim p(\Delta, x, \cdot\,;\theta)$$

Bayesian estimation for diffusion processes

$$dX_t = \alpha(X_t; \theta)dt + \sigma(X_t)dW_t$$

Data: $D = (X_{t_0}, \ldots, X_{t_n}), \quad t_0 = 0$

Partial observation of $\mathbf{X}_{t_n} = (X_t)_{0 \le t \le t_n}$

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Gibbs sampler

1. Draw θ from the prior distribution
2. Simulate a sample path $\mathbf{X}_{t_n}$ conditionally on θ and D
3. Draw θ conditionally on $\mathbf{X}_{t_n}$ and D
4. GO TO 2

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Diffusion bridge: A solution of the SDE in the interval $[0, T]$ such that $X_0 = a$ and $X_T = b$ is called an (a, b, T)-bridge.

Assume that the process X is ergodic

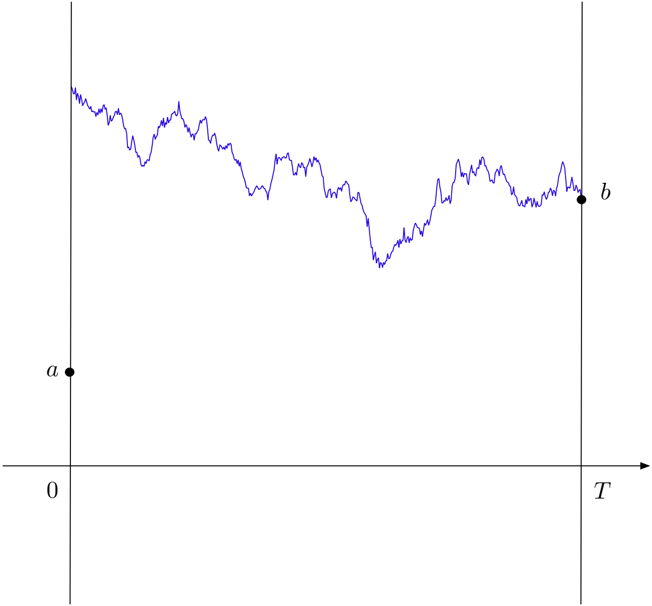
Simple bridge simulation: Bladt and Sørensen (Bernoulli 2014, 2021)

Diffusion bridge simulation

An incomplete list of other papers

- Durham and Gallant (2002)
- Delyon and Hu (2006)
- Beskos, Papaspiliopoulos and Roberts (2006, 2007)
- Golightly and Wilkinson (2008)
- Hairer, Stuart and Voss (2009)
- Chen and Huang (2013)
- Pollock, Johansen and Roberts (2016)
- Schauer, van der Meulen and van Zanten (2017)
- van der Meulen and Schauer (2017)
- Whitaker, Golightly, Boys and Sherlock (2017)

1D Diffusion bridge simulation



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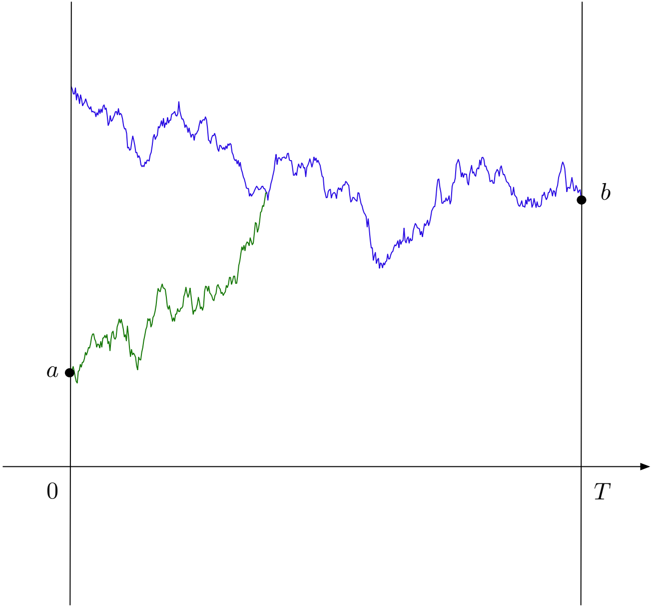

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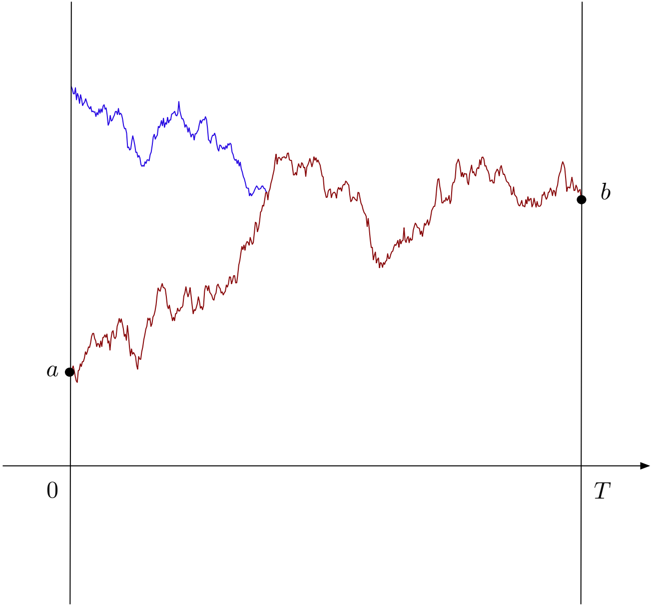

Approximate diffusion bridge simulation

$$dX_t^i = \alpha(X_t^i)dt + \sigma(X_t^i)dW_t^i, \quad X_0^1 = a \quad \text{and } X_0^2 = b$$

W^1 and W^2 independent standard Wiener processes

Define $\tau = \inf\{0 \le t \le T | X_t^1 = X_{T-t}^2\}$ $(\inf \emptyset = +\infty)$ and

$$Z_t = \begin{cases} X_t^1 & \text{if } 0 \le t \le \tau \\ X_{T-t}^2 & \text{if } \tau < t \le T. \end{cases}$$

Theorem

The distribution of $\{Z_t\}_{0 \le t \le T}$ conditional on the event $\{\tau \le T\}$ equals the distributions of an (a, b, T)-bridge conditional on the event that the bridge is hit by an independent stationary diffusion with the same stochastic differential equation as X.

Approximate diffusion bridge simulation

$$Z_t = \begin{cases} X'_t & \text{if } 0 \le t \le \tau \\ \bar{X}_t & \text{if } \tau < t \le T, \end{cases}$$

Theorem

The density of Z on the canonical space $C_{a,b}([0,T])$:

$$f_{appr}(x) = f(x)\pi_T(x)/\pi_T$$

- $C_{a,b}([0,T])$: the continuous functions on $[0,T]$ from a to b
- f is the density of an (a,b,T)-diffusion bridge
- $\pi_T(x)$: probability that the sample path x is hit by an independent stationary diffusion
- π_T: probability that an (a,b,T)-diffusion bridge is hit by an independent stationary diffusion

Metropolis-Hastings algorithm: exact bridge

Simulate an initial approximate (a, b, T)-diffusion bridge, $X^{(0)}$, set k = 1.

(1) Propose a new sample paths by simulating an approximate (a, b, T)-diffusion bridge $X^{(k)}$

(2) Accept the proposed diffusion bridge with probability

$$\min\left(1, \frac{f(X^{(k)})f_{appr}(X^{(k-1)})}{f(X^{(k-1)})f_{appr}(X^{(k)})}\right) = \min\left(1, \frac{\pi_T(X^{(k-1)})}{\pi_T(X^{(k)})}\right)$$

Otherwise $X^{(k)} = X^{(k-1)}$

(3) Set $k = k + 1$ and GO TO (1)

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But we do not know $\pi_T(x)$

But we can simulate

Pseudo-marginal MH-algorithm, Andrieu and Roberts (2009)

For a given $x \in C_{a,b}([0, T])$, define a random variable S as follows:

Simulate a sequence, $Y^{(1)}, Y^{(2)}, \ldots$, of independent stationary diffusions, until a sample path is obtained that intersects x

$$S = \min\{i : Y^{(i)} \text{ intersects } x\}.$$

$$E(S) = 1/\pi_T(x).$$

Pseudo-marginal Metropolis-Hastings algorithm: exact bridge

Metropolis-Hastings Markov chain with state $(X^{(k)}, S^{(k)})$.

Simulate an initial approximate (a, b, T)-diffusion bridge, $X^{(0)}$, and an associated $S^{(0)}$ (with $x = X^{(0)}$), and set k = 1.

(1) Propose a new sample paths by simulating an approximate (a, b, T)-diffusion bridge, $X^{(k)}$, and an associated $S^{(k)}$ (with $x = X^{(k)}$)

(2) Accept the proposed $(X^{(k)}, S^{(k)})$ with probability

$$\min\left(1, \frac{S^{(k)}}{S^{(k-1)}}\right)$$

Otherwise $X^{(k)} = X^{(k-1)}$ and $S^{(k)} = S^{(k-1)}$

(3) Set $k = k + 1$ and GO TO (1)

Multivariate diffusions and bridge simulation without discretization error

Simulation of multivariate diffusions:

Bladt, Finch and Sørensen (2016, 2021)

Uses methods from the literature on coupling of diffusion processes (Lindvall and Rogers, 1986, Chen and Li, 1089)

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Diffusion bridge simulation without discretization error:

The confluent diffusion bridge sampler, by Jenkins, Pollock, Roberts and Sørensen (2021), combines two approaches

- The simple sampler of Bladt and Sørensen (2014, 2021)
- The exact and ε-strong simulation of unconditioned diffusions of Pollock, Johansen and Roberts (2016)

to obtain a sampler without discretisation error with a computing time that is linear in T

Hyperbolic diffusion

$$dX_t = -\frac{\alpha X_t}{\sqrt{1+\|X_t\|^2}}dt + dW_t, \quad \alpha > 0$$

Data: $D = (X_{t_0}, \ldots, X_{t_n}), \quad t_0 = 0$

Partial observation of $\mathbf{X}_{t_n} = (X_t)_{0 \le t \le t_n}$

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1. Draw α from the prior distribution
2. Simulate a sample path $\mathbf{X}_{t_n}$ conditionally on α and D
3. Draw α conditionally on $\mathbf{X}_{t_n}$ and D
4. GO TO 2

Hyperbolic diffusion

Likelihood function based on $\mathbf{X}_{t_n}$

$$L^c(\alpha) = \exp\left(\alpha H_{t_n} - \frac{1}{2}\alpha^2 B_{t_n}\right),$$

$$H_t = \sqrt{1 + \|X_0\|^2} - \sqrt{1 + \|X_t\|^2} + \int_0^t \frac{1 + \frac{1}{2}\|X_s\|^2}{(1 + \|X_s\|^2)^{3/2}} ds$$

$$B_t = \int_0^t \frac{\|X_s\|^2}{1 + \|X_s\|^2} ds$$

Exponential family of processes in the sense of Küchler & Sørensen (1997)

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Exponential family of processes in the sense of Küchler & Sørensen (1997)

Conjugate prior: $N_+(\bar{\alpha}, \sigma^2)$

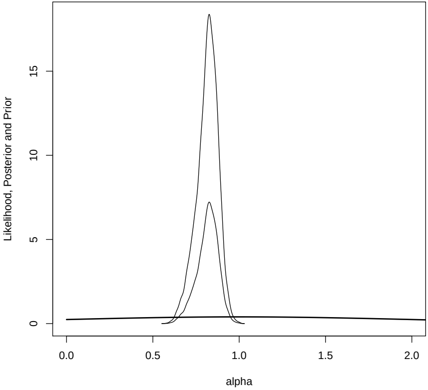
Posterior distribution: $N_+((H_{t_n} + \bar{\alpha}/\sigma^2)/(B_{t_n} + \sigma^{-2}), (B_{t_n} + \sigma^{-2})^{-1})$

Hyperbolic diffusion

$t_i = i, \ \ i = 0, \dots, 1000$

$\alpha = 0.8$ Prior: $N_+(1,1)$ 5000 iterations of the Gibbs sampler

Approximative bridge simulation



Stochastic differential equation with mixed effects

Baltazar-Larios, Bladt and Sørensen (2023)

$$dX_t^i = d_{\alpha,a_i}(X_t^i)dt + \sigma_{\beta,b_i}(X_t^i)dW_t^i, \quad i = 1, \ldots, N$$

$\sigma_{\beta,b}(x) > 0$ for all x, β, b, X^i ergodic

W^i, $i = 1, \cdots, N$, independent standard Wiener processes

Random effect: $(a_i, b_i) \sim p_\gamma(a, b)$, $i = 1, \ldots, N$,
independent random vectors

Parameters: α, β, γ

Data:

$$X_{\text{obs}} = (X_{\text{obs}}^1, \ldots, X_{\text{obs}}^N)$$

$$X_{\text{obs}}^i = (X_{t_1^i}^i, \ldots, X_{t_{n_i}^i}^i), \quad t_1^i < t_2^i < \ldots < t_{n_i}^i, \quad i = 1, \ldots, N$$

Lamperti transformation

$$dX_t^i = d_{\alpha,a_i}(X_t^i)dt + \sigma_{\beta,b_i}(X_t^i)dW_t^i, \quad i = 1, \ldots, N$$

$$Y_t^i = h_{\beta,b_i}(X_t^i) \qquad\qquad h_{\beta,b}(x) = \int_{x^*}^{x} \frac{1}{\sigma_{\beta,b}(u)} du$$

By Ito's formula:

$$dY_t^i = \mu_{\alpha,\beta,a_i,b_i}(Y_t^i)dt + dW_t^i,$$

where

$$\mu_{\alpha,\beta,a_i,b_i}(y) = \frac{d_{\alpha,a_i}(h_{\beta,b_i}^{-1}(y))}{\sigma_{\beta,b_i}(h_{\beta,b_i}^{-1}(y))} - \frac{1}{2}\sigma'_{\beta,b_i}\left(h_{\beta,b_i}^{-1}(y)\right)$$

with $\sigma'_{\beta,b_i}(x) = \partial_x \sigma_{\beta,b_i}(x)$

The probability measures corresponding to continuous time observation of Y are equivalent, and an explicit likelihood function is given by Girsanov

Data augmentation

The data X_{obs} can be thought of as a partial observation of a “full” data set $(X_{\text{obs}}, X_{\text{mis}})$

The “missing” data are $X_{\text{mis}} = (X^1_{\text{mis}}, \ldots, X^N_{\text{mis}})$ with

$$X^i_{\text{mis}} = \{Y^{*ij}_t,\ t \in [t^i_{j-1}, t^i_j],\ j = 2, \ldots, n_i,\ a_i, b_i\}.$$

$$Y^{*ij}_t = Z^{i,j}_t - \ell^i_{\beta,b_i}(t), \quad t \in [t^i_{j-1}, t^i_j]$$

$$\ell^i_{\beta,b}(t) = \frac{(t^i_j - t)h_{\beta,b}(X^i_{t^i_{j-1}}) + (t - t^i_{j-1})h_{\beta,b}(X^i_{t^i_j})}{t^i_j - t^i_{j-1}}, \qquad t \in [t^i_{j-1}, t^i_j]$$

Conditionally on X^i_{obs} and a_i, b_i,

$$Z^{i,j}_t,\ \ j = 2, \ldots, n_i,\ i = 1, \ldots, N$$

are independent $(t^i_{j-1}, h_{\beta,b_i}(X^i_{t^i_{j-1}}), t^i_j, h_{\beta,b_i}(X^i_{t^i_j}))$-bridges for the diffusion Y^i

Likelihood function for the augmented data set

$$L(\alpha,\beta,\gamma; X_{\text{obs}}, X_{\text{mis}}) = \prod_{i=1}^{N} L_i(\alpha,\beta; X^i_{\text{obs}}, X^i_{\text{mis}}) \prod_{i=1}^{N} p_\gamma(a_i, b_i)$$

where

$$\log L_i(\alpha,\beta; X^i_{\text{obs}}, X^i_{\text{mis}}) = H_{\alpha,\beta,a_i,b_i}(X^i_{t^i_n}) - H_{\alpha,\beta,a_i,b_i}(X^i_{t^i_1})$$

$$-\sum_{j=2}^{n_i} \left[\frac{(h_{\beta,b_i}(X^i_{t^i_j}) - h_{\beta,b_i}(X^i_{t^i_{j-1}}))^2}{2(t^i_j - t^i_{j-1})} + \log(\sigma_{\beta,b_i}(X^i_{t^i_j})) + \frac{1}{2}\int_{t^i_{j-1}}^{t^i_j} \phi_{\alpha,\beta,a_i,b_i}(Y^{*ij}_s + \ell^i_{\beta,b_i}(s))ds \right]$$

with

$$H_{\alpha,\beta,a,b}(x) = \int_{x^*}^{x} \frac{d_{\alpha,a}(u)}{\sigma^2_{\beta,b}(u)} du - \tfrac{1}{2}\log(\sigma_{\beta,b}(x))$$

$$\phi_{\alpha,\beta,a,b}(y) = \mu'_{\alpha,\beta,a,b}(y) + \mu_{\alpha,\beta,a,b}(y)^2$$

Girsanov plus Roberts and Stramer (2001)

Gibbs sampler

Specify a prior distribution $\pi(\alpha, \beta, \gamma)$

1. Draw (α, β, γ) from the prior distribution π

2. Conditionally on γ, draw (a_i, b_i) from p_γ, independently for $i = 1, \ldots, N$

3. Simulate independent sample paths Y^{*ij} conditionally on $\alpha, \beta, a_i, b_i, X^i_{\text{obs}}$ for $j = 2, \ldots, n_i,\ i = 1, \ldots, N$

4. Draw (a_i, b_i) conditionally on $\alpha, \beta, \gamma, X^i_{\text{obs}}, Y^{*i2}, \ldots, Y^{*in_i}$, independently for $i = 1, \ldots, N$
   Conditional density $\propto$
   $L_i(\alpha, \beta, \gamma; X^i_{\text{obs}}, Y^{*i2}, \ldots, Y^{*in_i}, a_i, b_i) p_\gamma(a_i, b_i)$

5. Draw (α, β, γ) given X_{mis} and X_{obs}
   Conditional density $\propto \pi(\alpha, \beta, \gamma) \cdot L(\alpha, \beta, \gamma; X_{\text{obs}}, X_{\text{mis}})$

6. GO TO 3

Ornstein-Uhlenbeck with mixed effects

$$dX_t^i = -a_i X_t^i dt + \beta dW_t^i, \qquad a_i \sim \text{exponential}(\gamma), \;\; i = 1, \ldots, N, \qquad \beta > 0$$

Parameters: γ, β

Data:

$X_{\text{obs}} = (X_{\text{obs}}^1, \ldots, X_{\text{obs}}^N)$

$X_{\text{obs}}^i = (X_{t_1}^i, \ldots, X_{t_n}^i), \;\; t_1 < t_2 < ... < t_n, \;\; i = 1, \ldots, N$

Prior:

γ and β are independent

$$\gamma \sim \Gamma(\nu, \lambda^{-1}), \;\; \eta = \beta^{-2} \sim \Gamma(\kappa, \delta^{-1})$$

The continuous time full model is an exponential family of processes in the sense of Küchler & Sørensen (1997)

Gibbs sampler

1. Draw (γ, η) from the prior distribution

2. $a_i \sim \text{exponential}(\gamma)$, $i = 1, \ldots, N$

3. Simulate independent sample paths Y^{*ij} conditionally on $\eta, a_i, X^i_{\text{obs}}$ for $j = 2, \ldots, n,\ i = 1, \ldots, N$

4. $a_i \sim N_+((A_i - \gamma)/B_i, B_i^{-1})$ independently for $i = 1, \ldots, N$
$A_i = A(X^i_{\text{obs}}, \eta),\ B_i = B(X^i_{\text{obs}}, Y^{*i}, \eta)$

5. $\gamma \sim \Gamma(\nu + N, (\lambda + a.)^{-1})$

6. $\eta \sim c\eta^{(n.-N)/2+\kappa-1} e^{-\eta(E_1+\delta)} \cdot e^{\sqrt{\eta}E_2+\eta E_3}$
$E_1 = E_1(X_{\text{obs}}),\ E_k = E_k(X_{\text{obs}}, Y^*, a_1, \ldots a_N),\ k = 2, 3$

7. GO TO 3

Membrane potential data

Data from Picchini, De Gaetano and Ditlevsen (2010):

Membrane potential of a single neuron measured every 0.15 ms

N = 109 interspike intervals, n = 1116

Model:

$$dX_t^i = (a_i - \alpha X_t^i)dt + \beta dW_t^i, \qquad a_i \sim N(\mu, \sigma^2), \;\; i = 1, \ldots, N,$$

Parameters: μ, $\sigma^2 > 0$, $\alpha > 0$, $\beta > 0$

Prior:

μ, σ^2, α and β are independent

$$\mu \sim N(1,1), \;\; \tau^2 = \sigma^{-2} \sim \text{exponential}(1)$$

$$\alpha \sim \text{exponential}(1), \qquad \eta = \beta^{-1} \sim \text{exponential}(1)$$

Membrane potential data

Gibbs sampler: 5000 iterations (burn-in = 4000)

Posterior distribution:

Parameter	mean	0.025-quantile	0.975-quantile
α	16.82	16.58	17.02
β	0.013513	0.013510	0.0103516
μ	0.174	0.172	0.176
σ	0.0584	0.0580	0.0593

Integrated diffusions

Baltazar-Larios and Sørensen (2010)

$$dX_t = b(X_t;\theta)dt + \sigma(X_t;\theta)dW_t, \quad X_0 \sim \nu_\theta$$

X ergodic with stationary density function ν_θ

Data:

$$\begin{aligned} Y_i &= \int_{t_{i-1}}^{t_i} X_s\,ds + Z_i, \quad i = 1,\ldots,n, \quad t_0 = 0, \quad Z_i \sim N(0,\tau^2) \text{ independent} \\ X_{\text{obs}} &= (Y_1,\ldots,Y_n) \end{aligned}$$

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Examples: Ice-core data (paleoclimate), integrated realized volatility, molecular dynamics, harmonic oscillator

$$dV_t = -(\alpha_1 P_t + \alpha_2 V_t)dt + \sigma dW_t, \qquad P_t = \int_0^t V_s ds$$

$$Y_i = P_{t_i} - P_{t_{i-1}} + Z_i$$

Integrated diffusions

Baltazar-Larios and Sørensen (2010)

$$dX_t = b(X_t;\theta)dt + \sigma(X_t;\theta)dW_t, \quad X_0 \sim \nu_\theta$$

X ergodic with stationary density function ν_θ

Data:

$$\begin{aligned} Y_i &= \int_{t_{i-1}}^{t_i} X_s\,ds + Z_i, \quad i=1,\ldots,n, \quad t_0=0, \quad Z_i \sim N(0,\tau^2) \text{ independent} \\ X_{\text{obs}} &= (Y_1,\ldots,Y_n) \end{aligned}$$

Likelihood function conditional on the diffusion process:

$$\prod_{i=1}^{n} \varphi\left(Y_i; \int_{t_{i-1}}^{t_i} X_s\,ds,\ \tau^2\right), \quad \varphi \text{ Gaussian density function}$$

Data augmentation: $Y_{\text{mis}} = \{X_t \,:\, 0 \le t \le t_n\}$?

Likelihood function for the augmented data set

$$dX_t = b(X_t;\theta)dt + \sigma(X_t;\theta)dW_t, \qquad X_0 \sim \nu_\theta$$

Lamperti transform:

$$U_t = h_\theta(X_t) \qquad\qquad h_\theta(x) = \int_{x^*}^{x} \frac{1}{\sigma(y;\theta)} dy$$

$$Y_i = \int_{t_{i-1}}^{t_i} h_\theta^{-1}(U_s)\, ds + Z_i, \qquad i = 1, \ldots, n$$

Data augmentation: $Y_{\text{mis}} = \{U_t \;:\; 0 \leq t \leq t_n\}$

$$\log L\left(\theta, \tau^2\,; Y_1, \ldots, Y_n, (U_t, t \in [0, t_n])\right) =$$

$$\sum_{i=1}^{n} \log \varphi \left(Y_i\,; \int_{t_{i-1}}^{t_i} h_\theta^{-1}(U_t)\, dt,\ \tau^2 \right) + H_\theta(U_{t_n}) - H_\theta(U_0) - \tfrac{1}{2} \int_0^{t_n} \phi_\theta(U_t) dt$$

EM algorithm

$(\hat{\theta}, \hat{\tau}^2)$ initial value of the parameter vector

(1) (E–step) Generate sample paths of $X^{(k)}$, $k = 1, \ldots, M$ conditional on $Y_1, \ldots, Y_n$ using the parameter value $(\hat{\theta}, \hat{\tau}^2)$, and calculate

$$g(\theta, \tau) = \frac{1}{M - M_0} \sum_{k=M_0+1}^{M} \log L \left(\theta, \tau\, ; Y_1, \ldots, Y_n, (h_{\hat{\theta}}(X_t^{(k)}), t \in [0, t_n]) \right)$$

(burn-in period M_0)

(2) (M–step) $(\hat{\theta}, \hat{\tau}^2) = \operatorname{argmax} g(\theta, \tau)$

(3) GO TO (1)

Conditional diffusion simulation

Chib, Pitt & Shephard (2006)

Simulate a stationary sample path of $X^{(0)}$ in $[0, t_n]$ and set $\ell = 1$

(1) Set $k_0 = 0$ and $i = 1$

(2) Draw $k_i \sim Poisson(\lambda) + 1$, if $\sum_{j=1}^{i} k_j \geq n$ set $k_i = n$, $K = i$ and stop, else set $i = i + 1$ and repeat 2

(3) For $j = 1, \ldots, K$ simulate independent $(X^{(\ell-1)}_{t_{k_{j-1}}}, X^{(\ell-1)}_{t_{k_j}}, t_{k_j} - t_{k_{j-1}})$-bridges $B^{(\ell,j)}$ conditional on $Y_{t_{k_{j-1}}+1}, \ldots, Y_{t_{k_j}}$ and set

$$X^{(\ell)}_t = B^{(\ell,j)}_{t-t_{k_{j-1}}} \quad \text{for } t \in [t_{k_{j-1}}, t_{k_j}],\ j = 1, \ldots, K$$

(4) Set $\ell = \ell + 1$ and GO TO (1)

Conditional bridge simulation

The following Metropolis-Hastings algorithm simulates the $(X^{(\ell-1)}_{t_{k_{j-1}}}, X^{(\ell-1)}_{t_{k_j}}, t_{k_j} - t_{k_{j-1}})$-bridge $B^{(\ell,j)}$ conditional on $Y_{k_{j-1}} + 1, \ldots, Y_{k_j}$:

(1) Simulate an initial $(X^{(\ell-1)}_{t_{k_{j-1}}}, X^{(\ell-1)}_{t_{k_j}}, t_{k_j} - t_{k_{j-1}})$-diffusion bridge, $B^{(\ell,j,0)}$, and set k = 1.

(2) Propose a new sample path by sampling a $(X^{(\ell-1)}_{t_{k_{j-1}}}, X^{(\ell-1)}_{t_{k_j}}, t_{k_j} - t_{k_{j-1}})$-diffusion bridge $B^{(\ell,j,k)}$

(3) Accept the proposed diffusion bridge with probability

$$\min\left(1, \prod_{i=k_{j-1}+1}^{k_j} \frac{\varphi\left(Y_i;\ \int_{t_{i-1}}^{t_i} B^{(\ell,j,k)}_{t-t_{k_{j-1}}}\,dt,\ \tau^2\right)}{\varphi\left(Y_i;\ \int_{t_{i-1}}^{t_i} B^{(\ell,j,k-1)}_{t-t_{k_{j-1}}}\,dt,\ \tau^2\right)}\right).$$

Otherwise $B^{(\ell,j,k)} = X^{(\ell,j,k-1)}$

(4) Set $k = k + 1$ and GO TO (2)

Integrated square root process: simulation study

$$dX_t = (\alpha - \beta X_t)dt + \sigma\sqrt{X_t}dW_t$$

$\alpha = 0.5 \quad \beta = 0.2 \quad \sigma = 0.5 \quad \tau^2 = 1.25$

$Y_i, \quad t_i = i, \quad i = 1\ldots, 1500$

$M = 10000, \quad M_0 = 1000$

1000 simulated datasets

Average of parameter estimates:

λ	α	β	σ	τ^2
30	0.4802	0.2056	0.4787	1.2432
20	0.4727	0.2043	0.4698	1.2406
10	0.4587	0.1965	0.4609	1.2287

Ice core data

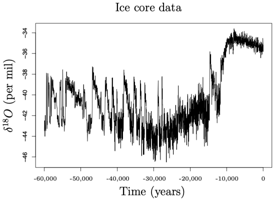


Figure 6.1: $\delta^{18}O$-values integrated over 20 years intervals obtained from ice core data from the Greenland ice-sheet.

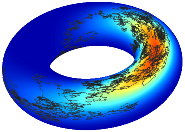
Model:
$$dX_t = -\alpha X_t dt + \sigma dW_t$$

EM-algorithm: $M = 10000$, $M_0 = 1000$ $\lambda = 20$

Parameter	[-10000,0]	[-30000,-10000]	[-60000,-30000]
α^{-1}	205.3	669.8	321.1
σ	0.0303	0.1167	0.1395
$\sigma/\sqrt{2\alpha}$	0.307	2.136	1.767
τ^2	0.1063	0.6967	0.2260

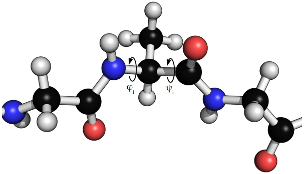
Ditlevsen, Ditlevsen and Andersen (2002)

Model of protein structure evolution

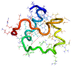


García-Portugués and Sørensen (2023)

Dihedral angles (ϕ, ψ)



A simplified representation of a protein of size N is



$$= ((\boldsymbol{\phi}, \boldsymbol{\psi}), \mathbf{a}, \mathbf{s}) \in \underbrace{\mathbb{T}^{2N}}_{\text{dihedral angles}} \times \underbrace{\{1, \ldots, 20\}^{N}}_{\text{amino acids}}$$

The stochastic process (ϕ_t, ψ_t) must be *ergodic, time-reversible and reasonably tractable*

New circular diffusions

$f : \mathbb{R} \to \mathbb{R}^+$ is a differentiable **circular** probability density:

(*i*) $f(x + 2k\pi) = f(x)$ and (*ii*) $\int_0^{2\pi} f(\theta)\,\mathrm{d}\theta = 1$, for any $x \in \mathbb{R}$ and $k \in \mathbb{Z}$

$F(x) = \int_0^x f(\theta)\,\mathrm{d}\theta,\ x \in \mathbb{R},$ is a one-to-one map $\mathbb{R} \to \mathbb{R}$

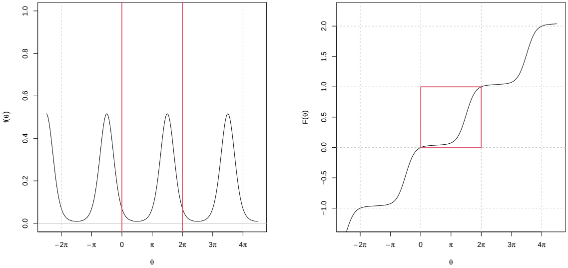


Figure: Circular pdf f (left) and its cdf F (rigth), with extensions from $[0, 2\pi)$ (red boundaries) to $\mathbb{R}$.

New circular diffusions

Define $\Theta_t = F^{-1}(\sigma W_t + F(\theta_0)) \mod 2\pi, \; t > 0,$

where W is a standard Wiener process, $\sigma > 0$ and $\theta_0 \in [0, 2\pi)$

Proposition

1. $\{\Theta_t\}$ solves the SDE

$$\mathrm{d}\Theta_t = -\frac{\sigma^2 f'(\Theta_t)}{2f(\Theta_t)^3}\mathrm{d}t + \frac{\sigma}{f(\Theta_t)}\mathrm{d}W_t$$

   on the circle $\mathbb{T}^1 := [0, 2\pi)$, with 0 and 2π identified

2. $\{\Theta_t\}$ is time-reversible and ergodic with stationary density f

3. For $t > 0$ and $\theta_1, \theta_2 \in \mathbb{T}^1$, the transition density of $\{\Theta_t\}$ is

$$p_t(\theta_2 \,|\, \theta_1) = 2\pi f_{\mathrm{WN}}\left(2\pi F(\theta_2); 2\pi F(\theta_1), 4\pi^2 t\sigma^2\right) f(\theta_2),$$

   where $f_{\mathrm{WN}}\left(\theta; \mu, \sigma^2\right) = \sum_{k\in\mathbb{Z}} \phi_{\sigma^2}(\theta - \mu + 2k\pi)$ is the **wrapped normal** density function, with $\phi_{\sigma^2}(\cdot)$ denoting the density of $\mathcal{N}(0, \sigma^2)$

$$\Theta_{t_2} \,|\, \Theta_{t_1} = \theta_1 \sim p_{t_2 - t_1}(\cdot \,|\, \theta_1), \;\; t_2 > t_1 \geq 0$$

Example: a von Mises diffusion

The von Mises distribution has the density function

$$f_{\mathrm{vM}}(\theta;\mu,\kappa) = (2\pi I_0(\kappa))^{-1}\exp\{\kappa\cos(\theta-\mu)\},\ \ \mu\in\mathbb{T}^1,\ \kappa>0$$

The von Mises diffusion solves the SDE

$$\mathrm{d}\Theta_t = \frac{\sigma^2\kappa\sin(\Theta_t-\mu)}{2\exp\{2\kappa\cos(\Theta_t-\mu)\}}\mathrm{d}t + \frac{\sigma}{\exp\{\kappa\cos(\Theta_t-\mu)\}}\mathrm{d}W_t$$

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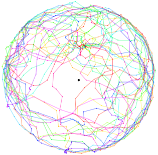
The von Mises diffusion solves the SDE

$$\mathrm{d}\Theta_t = \frac{\sigma^2\kappa\sin(\Theta_t-\mu)}{2\exp\{2\kappa\cos(\Theta_t-\mu)\}}\mathrm{d}t + \frac{\sigma}{\exp\{\kappa\cos(\Theta_t-\mu)\}}\mathrm{d}W_t$$

Experiment: Assessing directionality of ants movement. An ant in a circular container, movement tracked for 2 x 10 minutes



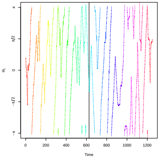


Figure: Ant, recorded track, and the track's angles

Experiment: assessing directionality of ants movement

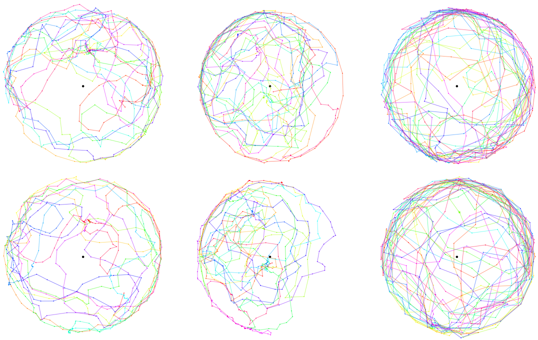


Figure: Rows: “exploration” and “revisit” stages. Columns: three most active ants

Same directional behaviour in “exploration” and “revisit” stages?

$$\mathcal{H}_0 : \xi_{\text{exp.}} = \xi_{\text{rev.}} \text{ vs. } \mathcal{H}_1 : \xi_{\text{exp.}} \neq \xi_{\text{rev.}}, \quad \xi = (\mu, \kappa, \sigma)$$

Ant 1, 2, 3 homogeneity p-values: 0.1394, 1.4×10^{-14}, 9.1×10^{-12}