Bayesian inference for discretely observed diffusion processes

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Van Dantzig Seminar

Estimating parameters of a discretely observed diffusion process

Diffusion process X

$$\mathrm{d}X_t = b_\theta(t, X_t)\,\mathrm{d}t + \sigma_\theta(t, X_t)\,\mathrm{d}W_t, \quad X_0 = u,$$

with transition densities $p(s, x; t, y)$
Discrete observations

$$X_{t_i} = x_i, \quad 0 = t_0 < t_1 < \cdots < t_n.$$

- Bayesian estimate for parameter θ with prior $\pi_0(\theta)$.
- Likelihood is intractable (product of transition densities)
- Continuous time likelihood known in closed form (Girsanov's theorem)

Computational approach

Data Augmentation (DA): Sample from the joint posterior of missing data and parameter.

1. Sample diffusion bridges conditional on $\{X_{t_i} = x_i\}$ and θ (this gives "complete", latent data);
2. Sample from θ conditional on the complete data.

Can use an accept/reject or Metropolis-Hastings step.

Rough outline:

- Simulation of diffusion bridges
- If unknown parameters are in the diffusion coefficient, DA does not work
- Example
- When and how to discretize

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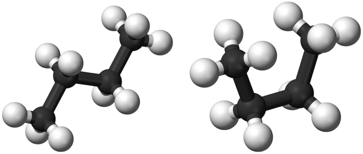
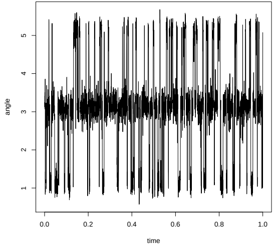
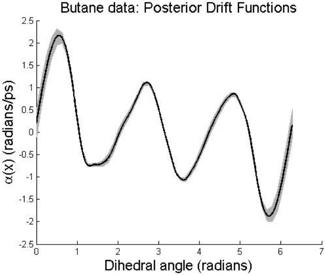
Examples: Butane dihedral angle, Pokern (2007)

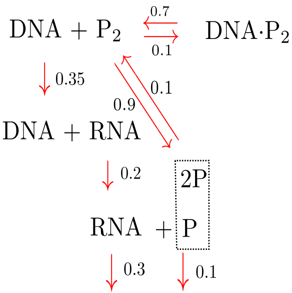


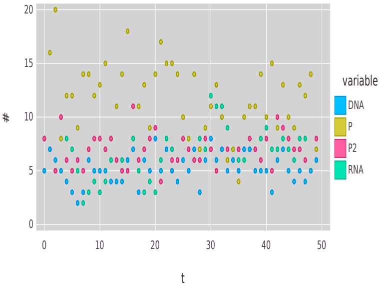




$$\mathrm{d}X_t = \sum_{i=1}^{J} \theta_i \psi_i(X_t)\,\mathrm{d}t + \mathrm{d}W_t$$

Chemical reaction network, Golightly and Wilkinson (2010)





$$dX_t = Sh_\theta(X_t)\,dt + S\,\mathrm{diag}(\sqrt{h_\theta(X_t)})\,dW_t$$

Intuition: Diffusion bridge

Two processes with equivalent distributions $\mathbb{P}$ and $\mathbb{W}$

- Diffusion process X with $\sigma \equiv 1$ starting in u
- Brownian motion W starting in u

Brownian motion W conditional on $W_T = v$: Brownian bridge.

The two conditional distributions $\mathbb{P}^\star$ and $\mathbb{W}^\star$ given $X_T = v$ resp. $W_T = v$ are equivalent

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{W}} = \frac{p(0,u;T,v)}{\phi(0,u;T,v)} \frac{\mathrm{d}\mathbb{P}^\star}{\mathrm{d}\mathbb{W}^\star}$$

with p and ϕ denoting the transition densities.

Works only if σ is constant. More general bridge proposals X° are needed,

$$\frac{\mathrm{d}\mathbb{P}^\star}{\mathrm{d}\mathbb{P}^\circ}(X^\circ) = C\Psi(X^\circ)$$

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Diffusion bridges

Bridge from $(0, u)$ to (T, v)

$$\mathrm{d}X_t^\star = b^\star(t, X_t^\star)\,\mathrm{d}t + \sigma(t, X_t^\star)\,\mathrm{d}W_t, \quad X_0^\star = u$$

with drift ($a = \sigma\sigma'$)

$$b^\star(t,x) = b(t,x) + a(t,x)\underbrace{\nabla_x \log p(t,x;T,v)}_{r(t,x;T,v)}.$$

- Delyon & Hu, Durham & Gallant: Proposals X° of the form

$$dX_t^\circ = \left(\lambda b(t, X_t^\circ) + \frac{v - X_t^\circ}{T - t}\right)\mathrm{d}t + \sigma(t, X_t^\circ)\,\mathrm{d}W_t, \quad X_0^\circ = u.$$

  $\lambda \in \{0, 1\}$.
- Beskos & Roberts: rejection sampling algorithm for obtaining bridges without discretisation error.

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Bridge from $(0, u)$ to (T, v)

$$\mathrm{d}X_t^\circ = b^\circ(t, X_t^\circ)\,\mathrm{d}t + \sigma(t, X_t^\circ)\,\mathrm{d}W_t, \quad X_0^\circ = u$$

with drift

$$b^\circ(t, x) = b(t, x) + a(t, x)\underbrace{\nabla_x \log \tilde{p}(t, x; T, v)}_{\tilde{r}(t, x; T, v)}.$$

Take $\tilde{p}$ the transition density of

$$\mathrm{d}\tilde{X}_t = \left(\tilde{\beta}(t) + \tilde{B}(t)\tilde{X}_t\right)\,\mathrm{d}t + \tilde{\sigma}(t)\,\mathrm{d}W_t.$$

If $\tilde{a}(T) = a(T, v)$ (and a few more conditions), then

$$\frac{\mathrm{d}\mathbb{P}^\star}{\mathrm{d}\mathbb{P}^\circ}(X^\circ) = \frac{\tilde{p}(0, u; T, v)}{p(0, u; T, v)}\Psi(X^\circ)$$

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where Ψ is tractable.

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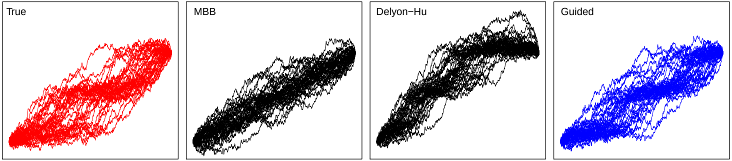
An example

Example: Simulate X given that $X_0 = 0$ and $X_1 = \pi/2$.

$$\mathrm{d}X_t = (2 - 2\sin(8X_t))\,\mathrm{d}t + \tfrac{1}{2}\,\mathrm{d}W_t$$



Guided proposal from

$$\mathrm{d}\tilde{X}_t = 1.34\,\mathrm{d}t + \frac{1}{2}\,\mathrm{d}W_t.$$

yielding

$$\mathrm{d}X_t^\circ = \left(2 - 2\sin(8X_t^\circ) + \frac{\pi/2 - X_t^\circ}{1-t} - 1.34\right)\mathrm{d}t + \frac{1}{2}\,\mathrm{d}W_t, \quad X_0^\circ = 0.$$

Finding good proposals

- Cross entropy method (previous example)
- Local linearizations (chemical reaction network example)
- Substituting space dependence for time dependence (next slide)

Substituting space dependence for time dependence

$$\mathrm{d}X_t = -\sin(X_t)\,\mathrm{d}t, \quad X_0 = \pi/2$$
$$\mathrm{d}\tilde{X}_t = -\operatorname{sech}(t)\,\mathrm{d}t, \quad \tilde{X}_0 = \pi/2$$

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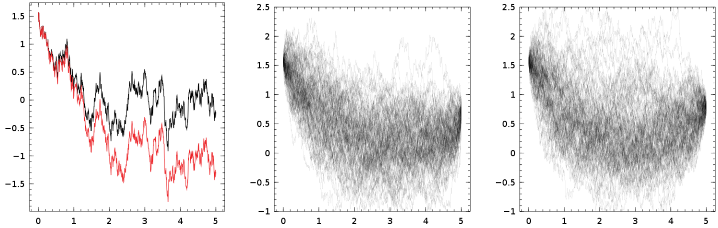

Sample of X and $\tilde{X}$ (black, red) X° $X^\star$.

Updating bridges

- Use a Metropolis-Hastings step with independent proposals from X°.
- Assume one bridge with $X^\circ_0 = u$, $X^\circ_T = v$.
- Sample proposal process X°. Accept proposal X° with probability $\min(1, A)$

$$A = \frac{\Psi(X^\circ)}{\Psi(X^\star)}$$

else retain current process $X^\star$.

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Parameters in the diffusion coefficient: DA does not work

Toy example from Roberts and Stramer (2001).

Consider the diffusion generated by the SDE

$$\mathrm{d}X_t = \theta\,\mathrm{d}W_t, \qquad X_0 = 0$$

X_1 is observed. θ unknown.

Intuitive argument why DA fails:

- Initialize θ by θ_0 and simulate a bridge $X^\star$ in continuous time.
- $X^\star$ has quadratic variation θ_0, so any new iterate for θ must be θ_0.

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Reparametrisation

- Let Z° be a Wiener process. We have

$$\mathrm{d}X_t^\circ = (b_\theta + a_\theta \tilde{r}_\theta)(t, X_t^\circ)\,\mathrm{d}t + \sigma_\theta(t, X_t^\circ)\,\mathrm{d}Z_t^\circ.$$

  We write

$$X^\circ = g(\theta, Z^\circ).$$

- Similarly

$$X^\star = g(\theta, Z^\star)$$

  by taking

$$Z_t^\star = W_t + \int_0^t \sigma_\theta'(s, X_s^\star)\,(r_\theta(t, X_t^\star) - \tilde{r}_\theta(s, X_s^\star))\,\mathrm{d}s$$

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Reparametrisation

Key idea: Sample from θ conditional on $(X_0 = u, X_T = v, Z^\star)$ instead of θ conditional on $(X_0 = u, X_T = v, X^\star)$.

Notation:

Process	$Z^\star \xrightarrow{g(\theta,\cdot)} X^\star$		$Z^\circ \xrightarrow{g(\theta,\cdot)} X^\circ$	
Law	$\mathbb{Q}^\star_\theta$	$\mathbb{P}^\star_\theta$	$\mathbb{Q}^\circ$	$\mathbb{P}^\circ_\theta$

Metropolis-Hastings step: Propose a value θ° from some proposal distribution $q(\cdot \mid \theta)$ and accept the proposal with probability $\min(1, A)$, where

$$A = \underbrace{\frac{\pi_0(\theta^\circ)}{\pi_0(\theta)}}_{\text{prior ratio}} \underbrace{\frac{p_{\theta^\circ}(0,u;T,v)}{p_\theta(0,u;T,v)} \frac{\mathrm{d}\mathbb{Q}^\star_{\theta^\circ}}{\mathrm{d}\mathbb{Q}^\star_\theta}(Z^\star)}_{\text{likelihood ratio}} \underbrace{\frac{q(\theta \mid \theta^\circ)}{q(\theta^\circ \mid \theta)}}_{\text{proposal ratio}}.$$

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Algorithm

1. **Update** $Z^\star \mid (\theta, X_{t_i} = x_{i,1\le i\le n})$. Independently, for $1 \le i \le n$ do
   1.1 Sample a Wiener process Z_i°.
   1.2 Sample $U \sim \mathcal{U}(0,1)$. Compute

$$A_1 = \frac{\Psi_\theta(g(\theta, Z_i^\circ))}{\Psi_\theta(g(\theta, Z_i^\star))}.$$

Set

$$Z_i^\star := \begin{cases} Z_i^\circ & \text{if} \quad U \le A_1 \\ Z_i^\star & \text{if} \quad U > A_1 \end{cases}.$$

2. **Update** $\theta \mid (Z^\star, X_{t_i} = x_{i,1\le i\le n})$.
   2.1 Sample $\theta^\circ \sim q(\cdot \mid \theta)$.
   2.2 Sample $U \sim \mathcal{U}(0,1)$. Compute

$$A_2 = \prod_{i=1}^{n} \frac{\tilde{p}_{\theta^\circ}(t_{i-1}, x_{i-1}; t_i, x_i)}{\tilde{p}_\theta(t_{i-1}, x_{i-1}; t_i, x_i)} \frac{\Psi_{\theta^\circ}(g(\theta^\circ, Z_i^\star))}{\Psi_\theta(g(\theta, Z_i^\star))} \frac{q(\theta \mid \theta^\circ)}{q(\theta^\circ \mid \theta)} \frac{\pi_0(\theta^\circ)}{\pi_0(\theta)}$$

Set

$$\theta := \begin{cases} \theta^\circ & \text{if} \quad U \le A_2 \\ \theta & \text{if} \quad U > A_2 \end{cases}.$$

Repeat steps (1) and (2).

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   1.1 Sample a Wiener process Z_i°.
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$$A_1 = \frac{\Psi_\theta(g(\theta, Z_i^\circ))}{\Psi_\theta(g(\theta, Z_i^\star))}.$$

   Set

$$Z_i^\star := \begin{cases} Z_i^\circ & \text{if} \quad U \le A_1 \\ Z_i^\star & \text{if} \quad U > A_1 \end{cases}.$$

2. **Update** $\theta \mid (Z^\star, X_{t_i} = x_{i,1 \le i \le n})$**.**
   2.1 Sample $\theta^\circ \sim q(\cdot \mid \theta)$.
   2.2 Sample $U \sim \mathcal{U}(0,1)$. Compute

$$A_2 = \prod_{i=1}^{n} \frac{\tilde{p}_{\theta^\circ}(t_{i-1}, x_{i-1}; t_i, x_i)}{\tilde{p}_\theta(t_{i-1}, x_{i-1}; t_i, x_i)} \frac{\Psi_{\theta^\circ}(g(\theta^\circ, Z_i^\star))}{\Psi_\theta(g(\theta, Z_i^\star))} \frac{q(\theta \mid \theta^\circ)}{q(\theta^\circ \mid \theta)} \frac{\pi_0(\theta^\circ)}{\pi_0(\theta)}$$

   Set

$$\theta := \begin{cases} \theta^\circ & \text{if} \quad U \le A_2 \\ \theta & \text{if} \quad U > A_2 \end{cases}.$$

Repeat steps (1) and (2).

Algorithm

1. **Update** $Z^\star \mid (\theta, X_{t_i} = x_{i,1\le i\le n})$**.** Independently, for $1 \le i \le n$ do
   1.1 Sample a Wiener process Z_i°.
   1.2 Sample $U \sim \mathcal{U}(0,1)$. Compute
   $$A_1 = \frac{\Psi_\theta(g(\theta, Z_i^\circ))}{\Psi_\theta(g(\theta, Z_i^\star))}.$$
   Set
   $$Z_i^\star := \begin{cases} Z_i^\circ & \text{if} \quad U \le A_1 \\ Z_i^\star & \text{if} \quad U > A_1 \end{cases}.$$
2. **Update** $\theta \mid (Z^\star, X_{t_i} = x_{i,1\le i\le n})$**.**
   2.1 Sample $\theta^\circ \sim q(\cdot \mid \theta)$.
   2.2 Sample $U \sim \mathcal{U}(0,1)$. Compute
   $$A_2 = \prod_{i=1}^{n} \frac{\tilde{p}_{\theta^\circ}(t_{i-1}, x_{i-1}; t_i, x_i)}{\tilde{p}_\theta(t_{i-1}, x_{i-1}; t_i, x_i)} \frac{\Psi_{\theta^\circ}(g(\theta^\circ, Z_i^\star))}{\Psi_\theta(g(\theta, Z_i^\star))} \frac{q(\theta \mid \theta^\circ)}{q(\theta^\circ \mid \theta)} \frac{\pi_0(\theta^\circ)}{\pi_0(\theta)}$$
   Set
   $$\theta := \begin{cases} \theta^\circ & \text{if} \quad U \le A_2 \\ \theta & \text{if} \quad U > A_2 \end{cases}.$$

Repeat steps (1) and (2).

Numerical example: Data

Prokaryotic auto-regulation example, Golightly and Wilkinson (2010)

Markov chain modelling quantities of $(\mathrm{RNA}, \mathrm{P}, \mathrm{P}_2, \mathrm{DNA})$ at integer times

Numerical example: SDE

Chemical Langevin equation. Diffusion approximation of the Markov chain

$$\mathrm{d}X_t = Sh_\theta(X_t)\,\mathrm{d}t + S\,\mathrm{diag}(\sqrt{h_\theta(X_t)})\,\mathrm{d}W_t$$

driven by a $\mathbb{R}^8$-valued Brownian motion, where

$$S = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 2 & 0 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$h_\theta(x) = \mathrm{diag}(\theta) \cdot [x_3 x_4, K - x_4, x_4, x_1, \tfrac{1}{2} x_2(x_2 - 1), x_3, x_1, x_2]'$$

Numerical example: Proposals

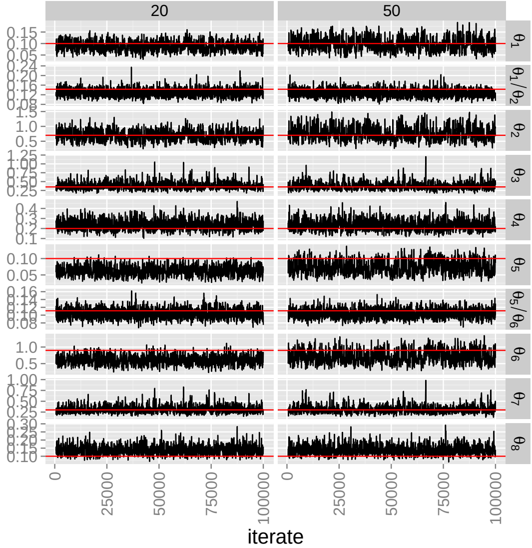
Linearization of drift

$\bar{h}_\theta(x) = \text{diag}(\theta) \cdot [c_1 + \lambda_1 x_3 + \gamma_1 x_4, K - x_4, x_4, x_1, c_2 + \lambda_2 x_2, x_3, x_1, x_2]'$

Choose $\tilde{B}_\theta$ and $\tilde{\beta}_\theta$ such that

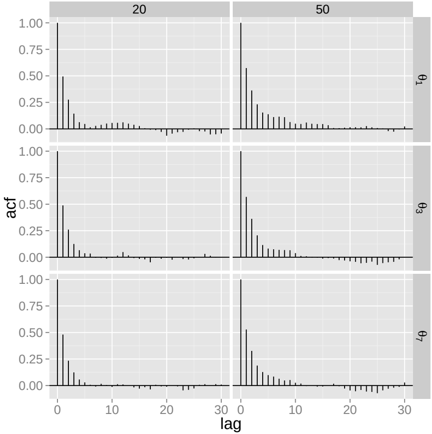
$$\tilde{B}_\theta x + \tilde{\beta}_\theta = S\bar{h}_\theta(x)$$

Numerical example: Results



Iterates of the MCMC chain for $m = 20, 50$ interpolated points

Numerical example: Results



ACF plots of the thinned samples of θ_1, θ_3, θ_7 (taking every 50th iterate after burn in).

Summary

Data augmentation for discretely observed diffusion processes

Non-constant and unknown σ: two challenges

- Finding good proposals for the conditional process
- Overcoming dependence between missing data and parameter

Both can be addressed using guided proposals

- Proposal bridges which take drift into account
- Guided proposals provide a natural reparametrization to decouple parameter and latent path

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Remarks

Overcoming singularities in the drift

Scaling and time change

$$U_s = \mathrm{e}^{s/2}(v - X^\circ_{T(1-\mathrm{e}^{-s})})$$

If the target is a Brownian motion, the proposal process U discretized on an equidistant grid and simulated using vanilla Euler scheme coincides with the scaled and time changed Brownian bridge (up to a small error)

Remarks

Determining $\tilde{B}$ and $\tilde{\beta}$

- Sometimes there a natural linearizations of the drift
- Adaptive proposals minimizing cross-entropy.