Bayesian inference of multiscale diffusion processes

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1 Introduction

Let (Ω, \mathcal{A}, P) be a probability space and consider the scalar Ornstein–Uhlenbeck process

$$dX_t(\omega, a) = -aX_t(\omega, a) dt + \sqrt{2\Sigma} dW_t(\omega),$$

$$X_0(\omega, a) = x \in \mathbb{R}.$$
(1)

where a is an unknown parameter with true value $a^{\dagger} \in \mathbb{R}^{+}$ and $\Sigma \in \mathbb{R}$ is fixed. Moreover, we consider the initial condition $x \in \mathbb{R}$ to be deterministic and independent of a. Let us define the forward mapping $\mathcal{G} \colon \Omega \times \mathbb{R} \to \mathbb{R}^{N}$ as

$$\mathcal{G}(\omega, a) \mapsto \mathcal{X}_N = \{X_{t_j}(\omega, a)\}_{j=1}^N, \tag{2}$$

for a sequence of time instants t_j defined as $t_j = jh$, for h > 0 and for j = 1, ..., N, $t_N = T$. We are given a set of observations $\mathcal{Y}_N \in \mathbb{R}^n$ of the process X_t as

$$\mathcal{Y}_N = \mathcal{G}(\omega^{\dagger}, a^{\dagger}) + \eta,$$

where η is an additive Gaussian source of noise distributed as $\eta \sim \mathcal{N}(0, \sigma_{\eta}^2 I_N)$, where I_d is the identity in d dimensions, and $\omega^{\dagger} \in \Omega$ is a fixed event. As in (2), we consider $\mathcal{Y}_N = \{Y_{t_j}(\omega, a)\}_{j=1}^N$. In the following, we denote by $\mathcal{N}(x; \mu, \sigma^2)$ the density of a Gaussian random variable of mean μ and variance σ^2 evaluated at a point x, i.e.,

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{\frac{(x-\mu)^2}{2\sigma^2}\right\}.$$

Fixed a Gaussian prior $p(a) = \mathcal{N}(a; 0, \sigma_a^2)$ on the drift coefficient, our goal is to compute the posterior distribution $p(a \mid \mathcal{Y}_N)$ of the parameter given the observations in a Bayesian framework. First, we apply Bayes' rule to obtain

$$p(a, \mathcal{X}_N \mid \mathcal{Y}_N) \propto p(a, \mathcal{X}_N) p(\mathcal{Y}_N \mid a, \mathcal{X}_N)$$

$$\propto p(a) p(\mathcal{X}_N \mid a) p(\mathcal{Y}_N \mid a, \mathcal{X}_N),$$

which, thanks to the observation model and to the Markov property of X_t , can be written as

$$p(a, \mathcal{X}_N \mid \mathcal{Y}_N) \propto p(a) \, p(\mathcal{X}_N \mid a) \prod_{j=1}^N p(Y_{t_j} \mid X_{t_j}, a)$$

$$= p(a) \prod_{j=1}^N p(X_{t_j} \mid X_{t_{j-1}}, a) \prod_{j=1}^N p(Y_{t_j} \mid X_{t_j}, a)$$
(3)

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Then, in order to obtain the marginal posterior of the parameter, one has to integrate out \mathcal{X}_N and get the posterior distribution of the parameter

$$p(a \mid \mathcal{Y}_N) \propto \int p(a, \mathcal{X}_N \mid \mathcal{Y}_N) \, \mathrm{d}\mathcal{X}_N$$

Let us compute the terms in (3) separately. First, the prior is given by $p(a) = \mathcal{N}(a; 0, \sigma_a^2)$. Then, for the likelihood term we have $p(Y_{t_j} \mid X_{t_j}, a) = \mathcal{N}(X_{t_j}; Y_{t_j}, \sigma_\eta^2)$. Finally, due to the distribution of the OU process we get

$$p(X_{t_i} \mid X_{t_{i-1}}, a) = \mathcal{N}(X_{t_i}; e^{-ah}X_{t_{i-1}}, a^{-1}\Sigma(1 - e^{-2ah})).$$

For h small enough, we can consider the transition probability of the Euler–Maruyama method applied to (1), which reads

$$p(X_{t_i} \mid X_{t_{i-1}}, a) = \mathcal{N}(X_{t_i}; (1 - ah)X_{t_{i-1}}, 2\Sigma h),$$

which is a good approximation of the true transition probability and allows for a simpler treatment.

Analytical posterior for the drift coefficient

Noiseless observations

We consider

$$dX_t = -a\nabla V(X_t) dt + \sqrt{2\beta^{-1}} dW_t(\omega),$$

$$X_0 = x \in \mathbb{R},$$

and an EM sequence $\mathcal{X} = \{X_n\}_{n=0}^N$ with time step h. The approximated MLE $\hat{a}_{N,h}$ for a is given by

$$\hat{a}_{N,h} = -\frac{\sum_{n=0}^{N-1} \langle \nabla V(X_n), X_{n+1} - X_n \rangle}{\sum_{n=0}^{N-1} \left| \nabla V(X_n) \right|^2 h}.$$

In the Bayesian framework, if no noise is added to the observations \mathcal{X} and for a prior $a \sim \mu_0$ with density P(a) we have

$$P(a \mid \mathcal{X}) \propto P(\mathcal{X} \mid a) P(a)$$
.

Let us consider $\mu_0 = \mathcal{U}(A)$, where $A = \{\text{admissible values for } a\}$. Then, maximising $P(a \mid \mathcal{X})$ is equivalent to maximising $P(\mathcal{X} \mid a)$ and therefore the MAP estimator $\tilde{a}_{N,h}$ is equal to the MLE estimator $\hat{a}_{N,h}$. For a Gaussian prior $\mu_0 = \mathcal{N}(\mu_a, \sigma_a^2)$, we get

$$\tilde{a}_{N,h} = -\frac{\sigma_a^2 \beta \sum_{n=0}^{N-1} \langle \nabla V(X_n), X_{n+1} - X_n \rangle + \mu_a}{\sigma_a^2 \beta \sum_{n=0}^{N-1} |\nabla V(X_n)|^2 h - 1}.$$

Hence, in the limit $N \to \infty$, we have, independently of μ_a and σ_a ,

$$\lim_{N\to\infty} \tilde{a}_{N,h} = \lim_{N\to\infty} \hat{a}_{N,h}.$$

Noisy observations

We first state a known result on Gaussian densities we will employ extensively in the computations below.

Lemma 1. Let
$$p(x) = \mathcal{N}(x; \mu_p, \sigma_p^2)$$
 and $q(x) = \mathcal{N}(x; \mu_q, \sigma_q^2)$. Then

$$p(x)q(x) = Z \mathcal{N}(x; \mu_{pq}, \sigma_{pq}^2),$$

where

$$\mu_{pq} = \frac{\mu_p \sigma_q^2 + \mu_q \sigma^2}{\sigma_p^2 + \sigma_q^2}, \quad \sigma_{pq}^2 = \frac{\sigma_p^2 \sigma_q^2}{\sigma_p^2 + \sigma_q^2},$$

and where

$$Z = \mathcal{N}(\mu_p; \mu_q, \sigma_p^2 + \sigma_q^2).$$

Proof. Find a reliable reference.

Moreover, we will use the relation valid for any $c \in \mathbb{R}$

$$\mathcal{N}(cx; \mu, \sigma^2) = \frac{1}{c} \mathcal{N}(x; c^{-1}\mu, c^{-2}\sigma^2). \tag{4}$$

In the following, we omit all constants which are independent of \mathcal{X}_N and a. Let us compute the posterior for one single observation Y_{t_1} , where $t_1 = h$. In this case, the transition probability is given by $p(X_{t_1} \mid X_{t_0}, a) = \mathcal{N}(X_{t_1}; (1-ah)X_{t_0}, 2\Sigma h)$, and the observation likelihood is $p(Y_{t_1} \mid X_{t_1}, a) = \mathcal{N}(Y_{t_1}; X_{t_1}, 2\sigma_{\eta}^2)$, which by symmetry can be rewritten as $p(Y_{t_1} \mid X_{t_1}, a) = \mathcal{N}(X_{t_1}; Y_{t_1}, 2\sigma_{\eta}^2)$. Thanks to Lemma 1 we have

$$\mathcal{N}(X_{t_1}; (1-ah)X_{t_0}, 2\Sigma h) \, \mathcal{N}(X_{t_1}; Y_{t_1}, \sigma_n^2) = Z_0(a) \, \mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2),$$

where μ_1 and σ_1^2 are given by

$$\mu_1 = \frac{(1 - ah)X_{t_0}\sigma_\eta^2 + 2Y_{t_1}\Sigma h}{2\Sigma h + \sigma_\eta^2},$$

$$\sigma_1^2 = \frac{2\Sigma h\sigma_\eta^2}{2\Sigma h + \sigma_\eta^2},$$

and where $Z_0(a)$ reads

$$Z_0(a) = \mathcal{N}((1 - ah)X_{t_0}; Y_{t_1}, \sigma_n^2 + 2\Sigma h),$$

which can be rewritten using (4) as

$$Z_0(a) = \frac{1}{1 - ah} \mathcal{N}\left(X_{t_0}; (1 - ah)^{-1} Y_{t_1}, (1 - ah)^{-2} (\sigma_{\eta}^2 + 2\Sigma h)\right)$$
 (5)

In general, in the following we will write

$$\begin{split} \mu_j &= \frac{(1-ah)X_{t_{j-1}}\sigma_\eta^2 + 2Y_{t_j}\Sigma h}{2\Sigma h + \sigma_\eta^2},\\ \sigma_j^2 &= \frac{2\Sigma h\sigma_\eta^2}{2\Sigma h + \sigma_\eta^2}, \end{split}$$

and

$$Z_{j}(a) = \mathcal{N}((1 - ah)X_{t_{j}}; Y_{t_{j+1}}, \sigma_{\eta}^{2} + 2\Sigma h)$$

$$= \frac{1}{1 - ah} \mathcal{N}(X_{t_{j}}; (1 - ah)^{-1}Y_{t_{j+1}}, (1 - ah)^{-2}(\sigma_{\eta}^{2} + 2\Sigma h)).$$

Finally, we get

$$p(a \mid \mathcal{Y}_1) = \int p(a, \mathcal{X}_N \mid \mathcal{Y}_N) \, d\mathcal{X}_N$$

$$\propto \int p(a) \, p(X_{t_1} \mid X_{t_0}, a) \, p(Y_{t_1} \mid X_{t_0}, a) \, dX_{t_1}$$

$$= p(a) \, Z_0(a) \int \mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) \, dX_{t_1} = p(a) \, Z_0(a),$$

and the marginal posterior on the drift coefficient is therefore given in closed form. Let us now consider a second observation Y_{t_2} at time $t_2 = 2h$. In this case and thanks to the computations above, we have

$$p(a \mid \mathcal{Y}_2) \propto p(a) Z_0(a) \int \mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) Z_1(a) \mathcal{N}(X_{t_2}; \mu_2, \sigma_2^2) dX_{t_2} dX_{t_1}.$$
 (6)

Let us compute the product $\mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) Z_1(a)$. Thanks to the relation (5), we have

$$\mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) Z_1(a) \propto \frac{1}{1 - ah} \mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) \mathcal{N}(X_{t_1}; (1 - ah)^{-1} Y_{t_2}, (1 - ah)^{-2} (\sigma_\eta^2 + 2\Sigma h)),$$

which gives thanks to Lemma 1

$$\mathcal{N}(X_{t_1}; \mu_1, \sigma_1^2) Z_1(a) \propto \widetilde{Z}_1(a) \mathcal{N}(X_{t_1}; \widetilde{\mu}_1, \widetilde{\sigma}_1^2),$$

where

$$\tilde{\mu}_1 = \frac{\mu_1 (1 - ah)^{-2} (\sigma_{\eta}^2 + 2\Sigma h) + (1 - ah)^{-1} Y_{t_2} \sigma_1^2}{\sigma_1^2 + (1 - ah)^{-2} (\sigma_{\eta}^2 + 2\Sigma h)},$$

$$\tilde{\sigma}_1^2 = \frac{\sigma_1^2 (1 - ah)^{-2} (\sigma_{\eta}^2 + 2\Sigma h)}{\sigma_1^2 + (1 - ah)^{-2} (\sigma_{\eta}^2 + 2\Sigma h)},$$

and where

$$\widetilde{Z}_1(a) = \frac{1}{1 - ah} \mathcal{N}(\mu_1; (1 - ah)^{-1} Y_{t_2}, \sigma_1^2 + (1 - ah)^{-2} (\sigma_\eta^2 + 2\Sigma h))$$

Replacing back into (6), one gets

$$p(a \mid \mathcal{Y}_2) \propto p(a) Z_0(a) \widetilde{Z}_1(a) \int \mathcal{N}(X_{t_1}; \tilde{\mu}_1, \tilde{\sigma}_1^2) \int \mathcal{N}(X_{t_2}; \mu_2, \sigma_2^2) dX_{t_2} dX_{t_1}$$

= $p(a) Z_0(a) \widetilde{Z}_1(a)$.

A recursive argument gives now the following result.

Theorem 1. Maybe The posterior distribution on the drift coefficient corresponding to N observations is given by

$$p(a \mid \mathcal{Y}_N) \propto p(a) Z_0(a) \prod_{j=1}^{N-1} \widetilde{Z}_j(a).$$

NO!

Proof. The result is obtained through an inductive argument. In particular, we first show

$$p(a, \mathcal{X}_N \mid \mathcal{Y}_N) \propto p(a) Z_0(a) \left(\prod_{j=1}^{N-1} \widetilde{Z}_j(a) \right) \mathcal{N}(X_{t_N}; \mu_N, \sigma_N^2) \prod_{j=1}^{N-1} \mathcal{N}(X_{t_j}; \widetilde{\mu}_j, \widetilde{\sigma}_j^2).$$
 (7)

The base cases N=1 and N=2 are treated above. Let us suppose the equality above to be true for \mathcal{X}_{N-1} and \mathcal{Y}_{N-1} . Then

$$\begin{split} p(a, \mathcal{X}_{N} \mid \mathcal{Y}_{N}) &\propto p(a) \prod_{j=1}^{N} p(X_{t_{j}} \mid X_{t_{j-1}}, a) \prod_{j=1}^{N} p(Y_{t_{j}} \mid X_{t_{j}}, a) \\ &= p(a, \mathcal{X}_{N-1} \mid \mathcal{Y}_{N-1}) \, p(X_{t_{N}} \mid X_{t_{N-1}}) \, p(Y_{t_{N}} \mid X_{t_{N}}, a) \\ &\propto p(a) \, Z_{0}(a) \Big(\prod_{j=1}^{N-2} \widetilde{Z}_{j}(a) \Big) \, \mathcal{N}(X_{t_{N-1}}; \mu_{N-1}, \sigma_{N-1}^{2}) \prod_{j=1}^{N-2} \mathcal{N}(X_{t_{j}}; \widetilde{\mu}_{j}, \widetilde{\sigma}_{j}^{2}) \\ &\times Z_{N-1}(a) \, \mathcal{N}(X_{t_{N}}; \mu_{N}, \sigma_{N}^{2}). \end{split}$$

Computations similar to the case N=2 lead to

$$Z_{N-1}(a)\mathcal{N}(X_{t_{N-1}};\mu_{N-1},\sigma_{N-1}^2) = \widetilde{Z}_{N-1}(a)\mathcal{N}(X_{t_{N-1}};\widetilde{\mu}_{N-1},\widetilde{\sigma}_{N-1}^2),$$

which shows (7). Let us now remark that for each j, \tilde{Z}_j depends only on μ_j , which in turn depends

only on $X_{t_{i-1}}$. Hence,

$$\begin{split} \frac{p(a\mid\mathcal{Y}_N)}{p(a)\,Z_0(a)} &\propto \int \Big(\prod_{j=1}^{N-1} \widetilde{Z}_j(a)\Big) \,\mathcal{N}(X_{t_N};\mu_N,\sigma_N^2) \prod_{j=1}^{N-1} \mathcal{N}(X_{t_1};\tilde{\mu}_j,\tilde{\sigma}_j^2) \,\mathrm{d}\mathcal{X}_N \\ &= \int \cdots \int \Big(\prod_{j=1}^{N-1} \widetilde{Z}_j(a)\Big) \prod_{j=1}^{N-1} \mathcal{N}(X_{t_j};\tilde{\mu}_j,\tilde{\sigma}_j^2) \int \mathcal{N}(X_{t_N};\mu_N,\sigma_N^2) \,\mathrm{d}X_{t_N} \,\mathrm{d}\mathcal{X}_{N-1} \\ &= \int \cdots \int \Big(\prod_{j=1}^{N-1} \widetilde{Z}_j(a)\Big) \prod_{j=1}^{N-2} \mathcal{N}(X_{t_j};\tilde{\mu}_j,\tilde{\sigma}_j^2) \int \mathcal{N}(X_{t_{N-1}};\tilde{\mu}_{N-1},\tilde{\sigma}_{N-1}^2) \,\mathrm{d}X_{t_{N-1}} \,\mathrm{d}\mathcal{X}_{N-2} \\ &= \int \cdots \int \Big(\prod_{j=1}^{N-2} \widetilde{Z}_j(a)\Big) \prod_{j=1}^{N-3} \mathcal{N}(X_{t_j};\tilde{\mu}_j,\tilde{\sigma}_j^2) \int \widetilde{Z}_{N-1}(a) \,\mathcal{N}(X_{t_{N-2}};\tilde{\mu}_{N-2},\tilde{\sigma}_{N-1}^2) \,\mathrm{d}X_{t_{N-2}} \,\mathrm{d}\mathcal{X}_{N-3} \end{split}$$

The recursion looks worse than I thought.

2 Particle Markov Chain Monte Carlo

The Particle Markov Chain Monte Carlo methods (PMCMC) [1] offer

References

[1] C. Andrieu, A. Doucet, and R. Holenstein, *Particle Markov chain Monte Carlo methods*, J. R. Stat. Soc. Ser. B. Stat. Methodol., (2010), pp. 269 – 342.