Bayesian nonparametric inference for diffusion models with discrete sampling

Delft University of Technology

Jakob Söhl
joint work with Richard Nickl
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Diffusion Markov Processes

Consider a process \((X_t : t \geq 0)\) that solves the stochastic differential equation
\[
\text{d}X_t = b(X_t) \text{d}t + \sigma(X_t) \text{d}W_t, \quad t \geq 0.
\]
Here \(b\) is a drift coefficient, \(\sigma\) the diffusion coefficient, \((W_t)_{t \geq 0}\) Brownian motion.

Under mild assumptions on \((\sigma, b)\), \((X_t : t \geq 0)\) is a unique Markov process with transition densities \(p_{t,\sigma b}(x, y)\) describing the operator
\[
\mathbb{E}_{\sigma b}[f(X_{t+s})|X_s = x] = \int_Y f(y) p_{t,\sigma b}(x, y) \text{d}y =: P_t f(x), \quad f \in \mathcal{C}_b(Y), \quad s \geq 0.
\]
Applications

→ Diffusion models are ubiquitous in modern science: They serve as fundamental building blocks in the modelling of dynamic phenomena in
  • physics, biology, geosciences
  • evolutionary dynamics and life sciences
  • engineering
  • economics & finance

They are closely related to stochastic models that model a dynamical system by some differential operator $L$ that propagates the system state perturbed with statistical noise.


→ Often the parameters $(\sigma, b)$ are unknown and one wants to infer their values from some form of sample of the diffusion.
An idealised assumption would be to observe an entire trajectory \((X_t : 0 \leq t \leq T)\), up to time \(T\). Inference on \(b\) becomes possible as \(T \to \infty\). (Note that \(\sigma\) is known in this case.)

More realistic: discrete observations \(X_0, X_\Delta, X_{2\Delta}, \ldots, X_{n\Delta}\) of the continuous process, where \(\Delta\) is the ‘observation distance’.

- **High-frequency observations**: \(\Delta \to 0\) and \(n\Delta = T \to \infty\)
- **Low-frequency observations**: \(\Delta > 0\) fixed as \(n \to \infty\).

The high-frequency regime asymptotically reflects the ‘continuous data’ setting. Low-frequency is harder.
Some Spectral Theory

When the diffusion is restricted to a regular compact space by reflection, say $[0, 1]$ for simplicity, the transition operator $P_t$ coincides with the action of the semigroup $(e^{tL} : t \geq 0)$ on $L^2(\mu)$ where the infinitesimal generator

$$L = L_{\sigma b} = b(x) \frac{d}{dx} + \frac{\sigma(x)^2}{2} \frac{d^2}{dx^2}$$

admits (subject to suitable boundary conditions) a discrete spectrum of eigenfunctions $u_k : k = 0, 1, 2, \ldots$ with eigenvalues $\lambda_k \in [-Ck^2, -C'k^2]$, $k \geq 1$. Here $\mu$ is the invariant density of the Markov process. We deduce the expansion

$$p_{t, \sigma b}(x, y) = \sum_k e^{\lambda_k t} u_k(x) u_k(y) \mu(y), \quad x, y \in [0, 1].$$

→ In the case of a scalar diffusion reflected at $\{0, 1\}$ the boundary conditions are of von Neumann type ($u'_k(0) = u'_k(1) = 0$). If $b = 0$ and $\sigma = 1$ we have reflected Brownian motion. Dirichlet conditions correspond to killed Brownian motion.
Frequentist Estimation at Low Frequency

- In a seminal paper, Gobet, Hoffmann & Reiβ (2004) studied the above model in the nonparametric setting. They started from the spectral identities

\[
\sigma^2 = \frac{2\lambda_1 \int_0^\cdot u_1 \, d\mu}{u_1' \mu}, \quad b = \lambda_1 \frac{u_1 u_1' \mu - u_1'' \int_0^\cdot u_1 \, d\mu}{(u_1')^2 \mu}.
\]

While estimation of \( \mu \) is straightforward, recovery of the first eigen-pair \((u_1, \lambda_1)\) requires estimation of the entire transition operator \( P \). GHR show that this can be done empirically in a minimax optimal way, with resulting \( L^2 \)-convergence rates

\[
n^{-s/(2s+3)} \quad \text{for} \quad \sigma^2
\]

and

\[
n^{-\left(s-1\right)/(2s+3)} \quad \text{for} \quad b
\]

whenever, for \( C \)-Hölder or Sobolev space, \((\sigma, b)\) belongs to \( \Theta_s = \{ \| \sigma \|_{C^s} + \| b \|_{C^{s-1}} \leq B, \sigma \geq c > 0 \} \). These rates reveal an ill-posed nonlinear inverse problem of order 1 and 2.
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\]

- While estimation of \( \mu \) is straightforward, recovery of the first eigen-pair \((u_1, \lambda_1)\) requires estimation of the entire transition operator \(P_\Delta\). GHR show that this can be done empirically in a minimax optimal way, with resulting \(L^2\)-convergence rates

\[
n^{-s/(2s+3)} \text{ for } \sigma^2 \text{ and } n^{-(s-1)/(2s+3)} \text{ for } b
\]

whenever, for \(C^s\) a \(s\)-Hölder or Sobolev space,

\[
(\sigma, b) \in \Theta_s = \{\|\sigma\|_{C^s} + \|b\|_{C^{s-1}} \leq B, \sigma \geq c > 0\}.
\]

These rates reveal an ill-posed nonlinear inverse problem of order 1 and 2.
From a Bayesian perspective it is natural to put a prior \( \Pi \) on the pair \((\sigma, b)\). The resulting posterior distribution is obtained from Bayes’ formula. For instance if the process is started in equilibrium, \( X_0 \sim \mu \sigma b \), then

\[
d\Pi((\sigma, b)|X_0, X_\Delta, \ldots X_{n\Delta}) = \frac{\mu \sigma b(X_0) \prod_{i=1}^{n} p_{\Delta, \sigma b}(X_{(i-1)\Delta}, X_{i\Delta}) \, d\Pi(\sigma, b)}{\int \mu \sigma b(X_0) \prod_{i=1}^{n} p_{\Delta, \sigma b}(X_{(i-1)\Delta}, X_{i\Delta}) \, d\Pi(\sigma, b)}.
\]

Direct evaluation is out of reach, since the transition probabilities depend in an analytically intractable, non-linear way on \( \sigma, b \).
Papaspiliopoulos, Pokern, Roberts & Stuart (2012) showed how one can sample from the posterior distribution when $\sigma = 1$ (or parametric) and the prior on $b$ comes from a Gaussian process. One uses conjugacy under continuous sampling, combined with a ‘latent’ variables sampling idea.

Can this ‘work’, particularly if the prior only models the regularity of $\sigma, b$ – so is ignorant of the ‘inverse problem’? The same question can be asked about many similar Bayesian ‘solutions’ of inverse problems (Stuart (2010)).
Frequentist Posterior Contraction Rates for Inverse Problems

• Following the program of van der Vaart, Ghosal et al., one can ask whether the posterior distribution contracts about the ‘true value’ \((\sigma_0, b_0)\) at the right rate. Do we have, for large enough \(M > 0\) that

\[
\Pi \left( (\sigma, b) : n^{s/(2s+3)} \| \sigma - \sigma_0 \| + n^{(s-1)/(2s+3)} \| b - b_0 \| > M \| X_0, \ldots, X_n \Delta \right) \to 0
\]

in \(P_{\sigma_0 b_0}\)-probability as \(n \to \infty\)?
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\]

in \(\mathbb{P}_{\sigma_0 b_0}\)-probability as \(n \rightarrow \infty\)?

- For general linear inverse problems

\[
Y = Af + \epsilon; \quad A : \mathbb{H}_1 \rightarrow \mathbb{H}_2 \text{ linear, compact,}
\]

with Gaussian white noise \(\epsilon\), results are available: see Knapik, van der Vaart & van Zanten (2011), Agapiou, Larsson & Stuart (2013) for the Gaussian conjugate setting, and Ray (2013) for a general approach.
Bayesian Estimation for Low-Frequency Observations

For nonlinear settings, very little is known. Particularly in the diffusion model with low-frequency observations only consistency in a weak topology (with $\sigma = 1$ known) has been proved so far (van der Meulen & van Zanten, 2013).

There are extensions to multidimensional diffusions (Gugushvili & Spreij, 2014) and to jump diffusions (Koskela, Spano & Jenkins, 2015).

All three papers assume $\sigma = 1$ known and show consistency in a weak topology.
Wavelet Series Priors I

\( \psi_{lk} \) boundary corrected Daubechies wavelets, \( 0 < \alpha < \beta < 1, \)
\( \mathcal{I} = \{(l, k) : \psi_{lk} \text{ supported in } [\alpha, \beta]\} \)

Model diffusion coefficient \( \sigma \) by

\[
\log(\sigma^{-2}(x)) = \sum_{(l, k) \in \mathcal{I}} \frac{2^{-l(s+1/2)}}{l^2} u_{lk} \psi_{lk}(x), \quad u_{lk} \sim \text{iid } U(-B, B).
\]

Comments:

- Could replace uniform distributions \( U(-B, B) \) by any distribution with bounded support and density bounded away from zero.
- Could truncate sum in \( l \) at \( L_n \rightarrow \infty \) sufficiently fast.
- By connection between Hölder norms and wavelet series \( \log(\sigma^{-2}) \) is modelled as typical \( s \)-Hölder smooth function (with a ‘convenient’ log-factor).
Wavelet Series Priors II

Model invariant density $\mu$ through

$$H(x) = \sum_{(l,k)\in I} \frac{2^{-(l(s+3)/2)}}{l^2} \bar{u}_{lk} \psi_{lk}(x), \quad \bar{u}_{lk} \sim \text{iid} \ U(-B, B),$$

$$\mu = e^H / \int e^H.$$

Drift coefficient $b$ indirectly given by

$$2b = (\sigma^2)' + \sigma^2 (\log \mu)'.$$

Overall Prior is given by $\Pi = \mathcal{L}(\sigma^2, ((\sigma^2)' + \sigma^2 H')/2)$.

Comments:

- Priors on $b$, $\sigma^2$ are not independent.
- Invariant density is modelled explicitly.
Assumptions on $\sigma_0$ and $\mu_0$

We define the Hölder-type space

$$C^t([0, 1]) := \left\{ f \in C([0, 1]) : \| f \|_{C^t} < \infty \right\}, \quad \text{where}$$

$$\| f \|_{C^t} := \sum_{k=0}^{\lfloor t \rfloor} \| D^k f \|_{\infty} + \sup_{h > 0} \sup_{x \in [0, 1]} \frac{|D\lfloor t \rfloor f(x + h) - D\lfloor t \rfloor f(x)|}{h^{t - \lfloor t \rfloor} \log(1/h)^{-2}}.$$

Assume diffusion coefficient $\sigma_0 \in C^s$ is of form

$$\log \sigma_0^{-2}(x) = \sum_{(l,k) \in I} \tau_{lk} \psi_{lk}(x), \quad x \in [0, 1], \quad \text{with } 2^{l(s+1/2)} l^2 |\tau_{lk}| \leq B.$$

Assume invariant density $\mu_0 \in C^{s+1}$ is of form

$$\log \mu_0(x) = \sum_{(l,k) \in I} \nu_{lk} \psi_{lk}(x), \quad x \in [0, 1], \quad \text{with } 2^{l(s+3/2)} l^2 |\nu_{lk}| \leq B.$$
**Contraction Theorem**

For $s \geq 2$ we define $\Theta_s$ by

$$\left\{ (\sigma, b) : \|\sigma\|_{C^s} \leq D, \|b\|_{C^{s-1}} \leq D, \inf_x \sigma(x) \geq d, \text{ boundary conditions} \right\}$$

**Theorem**

$(X_t : t \geq 0)$ reflected diffusion with $(\sigma_0, b_0) \in \Theta_s$. $\sigma_0$ and $\mu_0$ as above. $\Pi$ wavelet series prior. Then for all $0 < \alpha < \beta < 1$ there exists $\gamma > 0$ such that in the $L^2([\alpha, \beta])$-norm

$$\Pi \left( (\sigma, b) : \frac{n^s}{2s+3} \|\sigma^2 - \sigma_0^2\|_{L^2} > \log \gamma n \quad \text{or} \quad \frac{n^{s-1}}{2s+3} \|b - b_0\|_{L^2} > \log \gamma n \right| X_0, \ldots, X_{n\Delta} \right) \to 0$$

in $\mathbb{P}_{\sigma_0 b_0}$-probability for $\Delta > 0$ fixed and $n \to \infty$. 
The contraction theorem shows that the posterior distribution contracts about the true parameters at the minimax rate within $\log n$ factors.

Note that the above prior does not require knowledge of the ‘inverse problem’ at all, in particular not the singular value decomposition of the operator.

Bayes formula gives a (near-) optimal solution of this ill-posed non-linear inverse problem. It illustrates the power of the Bayesian approach to inverse problems.
Comments on the Conditions

- The additional logarithmic factor in the definition of $C^s$ might change the minimax rate by a logarithmic factor $(\log n)^\eta$, $\eta > 0$.

- The assumption $\mu_0 \in C^{s+1}$ is restricting $(\sigma_0, b_0)$ beyond having to lie in $\Theta_s$. As the lower bounds by GHR are for $\mu_0 \equiv 1 \in C^{s+1}$ this does not affect the minimax rates.

- $\mu_0$ assumed to be in $C^{s+1}$ and $\mu$ modelled explicitly since information theoretic distance involves the term $\|\mu - \mu_0\|_{L^2}$. 

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General Contraction Theorem

The basic strategy follows Ghosal, Ghosh & van der Vaart (2000)

Small ball probability condition: $C, L, r$ constants so that

$$
\Pi(B_{\epsilon_n}, r) \geq e^{-Cn\epsilon_n^2},
$$

and $\Pi(B \setminus B_n) \leq Le^{-(C+4)n\epsilon_n^2}$ for some sequence $B_n \subseteq B$

Tests: Sequence of tests $\Psi_n \equiv \Psi(X_0, \ldots, X_{n\Delta})$ and of metrics $d_n$ such that for $M > 0$ large enough,

$$
E_{\sigma_0 b_0}[\Psi_n] \to n \to \infty \ 0, \quad \sup_{(\sigma, b) \in B_n: d_n((\sigma, b), (\sigma_0, b_0)) \geq M\epsilon_n} E_{\sigma b}[1 - \Psi_n] \leq Le^{-(C+4)n\epsilon_n^2}.
$$

Give posterior contraction: Then the posterior $\Pi(\cdot | X_0, \ldots, X_{n\Delta})$ satisfies

$$
\Pi((\sigma, b): d_n((\sigma, b), (\sigma_0, b_0)) > M\epsilon_n | X_0, \ldots, X_{n\Delta}) \to 0
$$

in $\mathbb{P}_{\sigma_0 b_0}$-probability, as $n \to \infty$. 

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Small Ball Probability Condition

$\mathcal{B} \subseteq \Theta$ with a $\sigma$-field $\mathcal{S}$, $\Pi$ prior distribution on $\mathcal{S}$, $(\sigma_0, b_0) \in \Theta$, $\varepsilon_n \to 0$, $\sqrt{n \varepsilon_n} \to \infty$, and $C, r$ fixed constants

Suppose $\Pi$ satisfies

$$\Pi(B_{\varepsilon_n, r}) \geq e^{-C n \varepsilon_n^2},$$

where

$$B_{\varepsilon, r} = \left\{ (\sigma, b) \in \mathcal{B} : \text{KL}((\sigma_0, b_0), (\sigma, b)) \leq \varepsilon^2, \right.$$ \begin{align*}
\text{Var}_{\sigma_0 b_0} \left( \log \frac{p_{\sigma b}(\Delta, X_0, X_\Delta)}{p_{\sigma_0 b_0}(\Delta, X_0, X_\Delta)} \right) &\leq 2 \varepsilon^2, \right. \\
\text{KL}(\mu_{\sigma_0 b_0}, \mu_{\sigma b}) &\leq r, \text{Var}_{\sigma_0 b_0} \left( \log \frac{\mu_{\sigma b}(X_0)}{\mu_{\sigma_0 b_0}(X_0)} \right) \leq 2 r \left\}. \right.$$
Bound on Information Theoretic Distance

Information theoretic distance

$$KL((\sigma_0, b_0), (\sigma, b)) := \mathbb{E}_{\sigma_0 b_0} \left[ \log \left( \frac{p_{\sigma_0 b_0}(\Delta, X_0, X_\Delta)}{p_{\sigma b}(\Delta, X_0, X_\Delta)} \right) \right],$$

$p_{\sigma b}$ transition density, expectation $\mathbb{E}_{\sigma_0 b_0}$ w.r.t. stationary distribution

Need good bound on KL:

$$KL((\sigma_0, b_0), (\sigma, b)) \lesssim \|p_{\sigma b} - p_{\sigma_0 b_0}\|^2_{L^2} \lesssim \|P_\Delta^{\sigma b} - P_\Delta^{\sigma_0 b_0}\|^2_{HS} \lesssim \|e^{\Delta/L_{\sigma b}^{-1}} - e^{\Delta/L_{\sigma_0 b_0}^{-1}}\|^2_{HS} \lesssim \|L_{\sigma b}^{-1} - L_{\sigma_0 b_0}^{-1}\|^2_{HS},$$

where $P_\Delta^{\sigma b}$ transition operator and $L_{\sigma b}$ infinitesimal generator.
Bound on Information Theoretic Distance II

Inverse of infinitesimal generator

\[ L_{\sigma b}^{-1} f(x) = \int K_{\sigma b}(x, z)f(z)\mu_0(z)\,dz \]

Bound distance between integral kernels

\[ KL(((\sigma_0, b_0), (\sigma, b))) \lesssim \|L_{\sigma b}^{-1} - L_{\sigma_0 b_0}^{-1}\|_{HS}^{2} \]

\[ \lesssim \int \int (K_{\sigma b} - K_{\sigma_0 b_0})^2(x, z)\mu_0(x)\mu_0(z)\,dx\,dz \]

\[ \lesssim \|\mu_{\sigma b} - \mu_{\sigma_0 b_0}\|_{L^2([0,1])}^2 + \left\| \frac{1}{\sigma^2} - \frac{1}{\sigma_0^2} \right\|_{(B_{1\infty}^1)^*}^2 + \|b - b_0\|_{(B_{1\infty}^2)^*}^2, \]

with dual spaces of Besov spaces \( B_{1\infty}^1 \) and \( B_{1\infty}^2 \).
Concentration of Frequentist Estimators and Tests

- A Birgé-Le Cam Hellinger testing theory like the one used in Ghosal, Ghosh, van der Vaart, is not available for (non-linear) inverse problems.

- Instead we use a ‘concentration of measure approach’ to such tests, put forward in Giné & Nickl (2011). In the present setting, for $\hat{\sigma}$ and $\hat{b}$ estimators by Gobet, Hoffmann & Reiß (2004) we can prove:

**Theorem**

There exists $R > 0$ such that for $n$ large enough we have uniformly over $\Theta_s$, $s \geq 2$,

$$
P \left( \| \hat{\sigma}^2 - \sigma^2 \|_{L^2([\alpha, \beta])} \geq R n^{-s/(2s+3)} \quad \text{or} \quad \| \hat{b} - b \|_{L^2([\alpha, \beta])} \geq R n^{-(s-1)/(2s+3)} \right) \leq \exp \left( -D n^{1/(2s+3)} \right).
$$

This means exponential concentration of $\hat{\sigma}^2$ and $\hat{b}$ at minimax rates $n^{-s/(2s+3)}$ and $n^{-(s-1)/(2s+3)}$, respectively.
Concentration Inequality

Bernstein-type inequality

There exists $\kappa > 0$ such that for all reflected diffusions
\[ \mathrm{d}X_t = b(X_t) \, \mathrm{d}t + \sigma(X_t) \, \mathrm{d}W_t, \quad t \in [0, \infty) \] with $(\sigma, b) \in \Theta := \Theta_2$ and arbitrary initial distribution, $\forall f : [0, 1] \to \mathbb{R}$ bounded, $\forall x > 0$ and $\forall n \in \mathbb{N}$,
\[
\mathbb{P} \left( \left| \sum_{j=0}^{n-1} (f(X_{j\Delta}) - \mathbb{E}_\mu[f]) \right| > x \right) \leq \kappa \exp \left( -\frac{1}{\kappa} \min \left( \frac{x^2}{n \| f \|_{L^2(\mu)}^2}, \frac{x}{\log(n) \| f \|_{\infty}} \right) \right).
\]
Concentration Inequality for Suprema of Empirical Processes

Class of functions $\mathcal{F} = \{ f_i : i \in I \}$ with $0 \in \mathcal{F}$ and $\dim I = d$

$$V^2 = \kappa n \sup_{f \in \mathcal{F}} \| f \|_{L^2(\mu)}^2$$ and $$U = \kappa \log n \sup_{f \in \mathcal{F}} \| f \|_{\infty}$$

**Theorem**

For $\tilde{\kappa} = 18$ and for all $x \geq 0$ we have

$$\mathbb{P} \left( \sup_{f \in \mathcal{F}} \left| \sum_{j=0}^{n-1} (f(X_{j\Delta}) - \mathbb{E}_\mu[f]) \right| \geq \tilde{\kappa} \left( V \sqrt{d + x} + U(d + x) \right) \right) \leq 2\kappa e^{-x}.$$ 

Follows from chaining and previous concentration inequality.

Using duality arguments from Giné & Nickl (2011) this gives deviation bounds for the estimation errors of frequentist estimators of $\sigma^2$, $b$.

Lessons for General Non-Linear Inverse Problems $Y = Af + \epsilon$

Bayesian methods for inverse problems should work in principle. Proving that may be quite difficult though!

Two key modifications of the standard Ghosal-Ghosh-van der Vaart approach are required:

- If $A$ is the operator to invert (possibly after linearisation), one needs to show that the information distance is bounded above by $\|Af\|$ where $\| \cdot \|$ would be the information distance when $A = Id$. This allows to take ‘faster’ $\epsilon_n$-sequences in the small ball computations. In our case the main contribution is to achieve this by considering negative Besov norms on $(\sigma, b)$.

- In absence of robust Hellinger tests, one can show that for a large support set in the prior a frequentist estimator that solves the inverse problem admits tight sub-Gaussian exponential concentration bounds on its estimation error, which can be used in the construction of tests. In our case we had to derive new concentration inequalities for samples means of discretely sampled diffusions.
References


Thank you for your attention!