Sampling Conditioned Hypoelliptic Diffusions

Jochen Voss

University of Leeds

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Joint work with Martin Hairer and Andrew Stuart
Outline

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Sampling on Path Space
The solution of an SDE, e.g. of the form
\[
dX_t = b(X_t)\, dx + a(X_t) \, dW_t \quad \forall \, t \in [0, T],
\]
defines a probability distribution \( \mu \) on the space \( C([0, T], \mathbb{R}^d) \).

**Idea.** Use a MCMC method, i.e. find a stochastic process \( x \) with values in \( C([0, T], \mathbb{R}^d) \) whose stationary distribution coincides with the target distribution \( \mu \). Assuming ergodicity, we can probe all statistical properties of \( \mu \) using ergodic averages:
\[
\int_{C([0,T],\mathbb{R}^d)} f(x) \, d\mu(x) = \lim_{S \to \infty} \frac{1}{S} \int_0^S f(x_\tau) \, d\tau.
\]

This point of view is particularly useful, if there are additional contraints on the solution \( X \) which destroy the basic Markovian structure of the process. Example: sampling bridges with \( X(0) = a \) and \( X(T) = b \).
basic example: sampling Brownian bridges

The stochastic heat equation

$$\partial_\tau x(\tau, t) = \partial^2_t x(\tau, t) + \sqrt{2} \partial_\tau w(\tau, t)$$

with Dirichlet boundary conditions

$$x(\tau, 0) = 0, \quad x(\tau, T) = 0$$

has the distribution of a Brownian bridge on $[0, T]$ as its stationary distribution.

- $\partial_\tau w$ is space-time white noise
- $t \in [0, T]$ is physical time ("space" of the SPDE, time of the Brownian bridge)
- $\tau \in [0, \infty)$ is algorithmic time (time of the SPDE)
One can obtain results like the following:

**Theorem 1.** Let $X$ be the solution of

$$dX_t = f(X_t) \, dt + dW_t, \quad X(0) = 0, \, X(T) = 0.$$ 

Then the stationary distribution of

$$\partial_\tau x(\tau, t) = \partial_t^2 x(\tau, t) - \left( ff' + \frac{1}{2} f'' \right)(x) + \sqrt{2} \partial_\tau w(\tau, t)$$

with Dirichlet boundary conditions

$$x(\tau, 0) = 0, \quad x(\tau, T) = 0$$

coincides with the distribution of $X$ on $C([0, 1], \mathbb{R})$.

The result needs (among other assumptions) that $f$ is a gradient.
Main Result
We consider hypoelliptic diffusions of the form

\[ m\ddot{X}_t = F(X_t) - \dot{X}_t + \sqrt{2/\beta} \dot{W}_t \]

where \( X_t \in \mathbb{R}^d \) for \( t \in [0, T] \), \( F : \mathbb{R}^d \to \mathbb{R}^d \), \( \beta > 0 \) and \( \dot{W} \) is white noise. This could, for example, describe a physical system with friction and noise.

**Example.** We can consider the case \( F = -V' \) where \( V \) is a double-well potential:

\[ V(x) = (x-1)^2(x+1)^2 \quad \forall x \in \mathbb{R}. \]

Depending on the amount of noise, the system exhibits metastable behaviour.
\[ m\ddot{X}_t = F(X_t) - \dot{X}_t + \sqrt{2/\beta} \dot{W}_t \quad X_0 = 0 \]
Sometimes we want to simulate the dynamics of the system conditioned on certain events.

**Examples.**

- We can study the transitions between meta-stable states by simulating paths conditioned on a transition happening.
- In signal processing we want to find the conditional distribution of the system given (noisy) observations.

**Problem.** How can we sample from the distribution $\mu$ of

$$m \ddot{X}_t = F(X_t) - \dot{X}_t + \sqrt{2/\beta} \dot{W}_t,$$

conditioned on $X_0 = x_-$ and $X_T = x_+$?
\[ m\ddot{X}_t = F(X_t) - \dot{X}_t + \sqrt{2/\beta} \dot{W}_t \quad X_0 = -1, \quad X_{1000} = +1 \]
Main Result

**Theorem 2.** Let $x : \Omega \times \mathbb{R}_+ \to C([0, T], \mathbb{R}^d)$ be the solution of

$$
\partial_\tau x(\tau, t) = \mathcal{L}(x(\tau, t) - \bar{x}(t)) + \mathcal{N}(x) + \sqrt{2} \partial_\tau w(\tau, t)
$$

where $\mathcal{L} = -\frac{\beta}{2}(m^2 \partial^4_t - \partial^2_t)$ with certain boundary conditions,

$$
\mathcal{N}_k(x) = -\frac{\beta}{2} F_i(x) \partial_k F_i(x) + \frac{m\beta}{2} \partial_t x_i \partial_t x_j \partial^2_{ij} F_k(x)
$$

$$
- \frac{\beta}{2} \partial_t x_j (\partial_j F_k(x) - \partial_k F_j(x))
$$

$$
+ \frac{m\beta}{2} \partial^2_t x_j (\partial_j F_k(x) + \partial_k F_j(x))
$$

$$
+ \frac{m\beta}{2} (F_k(x-) \partial_t \delta_0 - F_k(x+) \partial_t \delta_T)
$$

and $w$ is a cylindrical Wiener process. Then, in stationarity, the distribution of $t \mapsto x(\tau, t)$ coincides with the target distribution $\mu$. 
Remarks about the Proof
As usual, we can rewrite the second order SDE as a system of first order SDEs. Let \( q_t = X_t \) and \( p_t = m \dot{X}_t \), then

\[
\begin{align*}
 dq_t &= \frac{1}{m} p_t \, dt, \quad q_0 = x_- \\
 dp_t &= -\frac{1}{m} p_t \, dt + F(q) \, dt + \sqrt{2/\beta} \, dW_t, \quad p_0 \sim \mathcal{N}(0, \frac{m}{\beta}).
\end{align*}
\]

**Remark.** \( q \) is a deterministic function of \( p \). Using this function we can solve the second equation to get \( p \). Finally we can compute \( q \) from \( p \).
The linear case \((F = 0)\)

For \(F = 0\), the hypoelliptic SDE simplifies to

\[ m\ddot{X}_t = -\dot{X}_t + \sqrt{2/\beta}\dot{W}_t. \]

Since this equation is linear, \(X\) is a Gaussian process and its distribution is completely characterised by the mean \(\bar{x}\) and the covariance operator \(C\).

**Lemma.** Let \(\mathcal{L}\) be a linear, negative, self-adjoint operator on \(L^2([0, T], \mathbb{R}^d)\) such that \(C = -\mathcal{L}^{-1}\) is trace class and let \(\bar{x} \in L^2([0, T], \mathbb{R}^d)\). Then

\[ \partial_\tau x(\tau, t) = \mathcal{L}(x - \bar{x})\,d\tau + \sqrt{2}\partial_\tau w(\tau, t) \]

has stationary distribution \(\mathcal{N}(\bar{x}, C)\).

In our situation we get \(\mathcal{L} = -\frac{\beta}{2}(m^2\partial_t^4 - \partial_t^2)\) (with certain boundary conditions).
The non-linear case ($F \neq 0$)

**Lemma (on $\mathbb{R}^n$).** Let $\mu, \nu$ be probability distributions. Assume that $\nu$ is the stationary distribution of

$$dz(\tau) = Lz(\tau) \, d\tau + \sqrt{2} \, dw(\tau).$$

and that $\frac{d\mu}{d\nu} = \varphi$. Then

$$dx(\tau) = Lx(\tau) \, d\tau + \nabla \log \varphi(x(\tau)) + \sqrt{2} \, dw(\tau)$$

has stationary distribution $\mu$.

The result can be carried over to infinite dimensional situations by finite dimensional approximation.

**Note.** Since the equation for $z$ is linear, we know $\nu = \mathcal{N}(0, -L^{-1})$. 
In our case:

- \( \nu \) is the target distribution with \( F = 0 \),
- \( \mu \) is the target distribution with \( F \neq 0 \).

Girsanov's formula gives

\[
\varphi(q) = \exp \left( \sqrt{\frac{\beta}{2}} \int_0^T \langle F(q(t)), dW(t) \rangle - \frac{\beta}{4} \int_0^T |F(q(t))|^2 \, dt \right).
\]

The (variational) derivative of \( \varphi \) is given by

\[
D \log \varphi(q) h = \frac{m\beta}{2} \left( F_k(q_+) h'_k(T) - F_k(q_-) h'_k(0) \right) \\
- \frac{\beta}{2} \int_0^T \left( F_i \partial_k F_i - m\dot{q}_i \dot{q}_j \partial_{ij}^2 F_k \\
+ \dot{q}_j (\partial_j F_k - \partial_k F_j) - m\ddot{q}_j (\partial_j F_k + \partial_k F_j) \right) h_k(t) \, dt \\
= \langle \mathcal{N}(q), h \rangle.
\]
Remarks.

- Existence of local solution follows from the fact that the non-linearity $\mathcal{N}$ is a Lipschitz function from $H^{3/2+\epsilon}$ to $H^{-3/2-\epsilon}$ (for good enough $F$). One can get the required a-priori bounds to prove the existence of global solutions. The most “dangerous” term in the non-linearity is

$$\partial_t^2 x_j \left( \partial_j F_k(x) + \partial_k F_j(x) \right).$$

- Differently from the earlier result (for first order SDEs), we do not require the drift $F$ to be a gradient.
Conclusion

- The method provides a generic framework to derive sampling equations, many applications are possible (e.g. nonlinear filtering).
- Different from the first-order SDE case, we do not require a gradient structure.
- Interesting problems in the theory of the method, implementation, and applications.

References

- M. Hairer, A.M. Stuart and J. Voss, *Sampling Conditioned Diffusions*. Pages 159–186 in Trends in Stochastic Analysis, Cambridge University Press, vol. 353 of London Mathematical Society Lecture Note Series, 2009.
- M. Hairer, A.M. Stuart and J. Voss, *Sampling Conditioned Hypoelliptic Diffusions*. To appear in the Annals of Applied Probability, 2010.