ESTIMATING SMALL PROBABILITIES FOR LANGEVIN DYNAMICS

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Abstract. The problem of estimating small transition probabilities for overdamped Langevin dynamics is considered. A simplification of Girsanov’s formula is obtained in which the relationship between the infinitesimal generator of the underlying diffusion and the change of probability measure corresponding to a change in the potential energy is made explicit. From this formula an asymptotic expression for transition probability densities is derived. Separately the problem of estimating the probability that a small noise Langevin process escapes a potential well is discussed.

1. Introduction

Let $X_t$ be a stochastic process in $\mathbb{R}^d$ satisfying the stochastic differential equation

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

(1)

This is the overdamped Langevin equation. Formally, $X_t$ is a time homogeneous Itô process [1] with conservative drift and constant diffusion. Intuitively, $X_t$ represents the dynamics of large particles interacting through the potential energy $V$, with additional “random” motion driven by collisions with many small particles. The overdamped Langevin equation can be viewed as a simplification of the well-known (second order) Langevin equation, which models the dynamics of a system of particles in contact with a heat bath at positive temperature $T = (k_B\beta)^{-1}$. The overdamped version is obtained from a scaling limit of the Langevin equation in which a damping constant tends to infinity [2], [3]. The overdamped Langevin equation can then be viewed as approximating the high friction limit of the Langevin equation, in which no acceleration takes place. In this paper small transition probabilities on the process (1) are considered.

A useful estimate of a small probability should have an error which is much smaller than the probability itself. Unfortunately, standard Monte Carlo sampling techniques are often not useful in this sense. This is because for a fixed number of samples, as the probability $p$ being estimated approaches zero, the variance of the standard Monte Carlo estimate of $p$ is nearly proportional to $p$. The error, represented by the standard deviation, is then nearly proportional to $\sqrt{p} \gg p$.

Small probabilities of the process (1) have been studied in the large $\beta$ limit in the context of Freidlin-Wentzell theory [4]. In particular, the asymptotic behavior of probabilities as $\beta \to \infty$ satisfy a large deviations principle (LDP) [5]. Though the LDP by itself says nothing about probabilities at a fixed $\beta$, the Freidlin-Wentzell theory has

\footnotesize

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recently been used in conjunction with optimal control theory to construct Monte Carlo
importance sampling schemes that are asymptotically optimal (as $β \to ∞$) in various
senses \[6\], \[7\], \[8\]. Such schemes reduce the variance of standard Monte Carlo estimates
by sampling with a measure under which the relevant event is more probable; samples are
then multiplied by an appropriate factor depending on this measure. In general asymptot-
ically optimal schemes of this sort are adaptive, with an evolving change of measure
requiring significant computation at each time step. By contrast, non-adaptive schemes,
for which the change of measure is fixed and impact on computation time is negligible,
generally are not asymptotically optimal (see, however, \[9\]).

Introduced below is a non-adaptive importance sampling scheme for estimating the
probability that a Langevin process escapes a potential well in the large $β$ regime. Though
the analysis here is restricted to the overdamped case \(1\), the scheme can equally be used
with the second order Langevin equation. It is shown to be asymptotically optimal in
certain cases, and to exhibit very good (if not optimal) performance more generally. Estimates
on its effectiveness at finite $β$ and asymptotically as $β \to ∞$ are given. Separately,
an asymptotic expansion for transition probability densities as $t \to 0$ is proved.

The organization of the paper is as follows. Background and notation are discussed
and a change in measure formula is proved in Section 2 below. In Section 3 an asymptotic
expression for transition probabilities is proved. In Section 4 importance sampling and
the problem of estimating the probability that the process \(1\) has exited a potential well
are discussed. In Section 5 a one-dimensional numerical example is provided.

2. Background, notation and change of measure

Here the well-known relationship between stochastic differential equations (SDEs) and
partial differential equations (PDEs) is briefly reviewed. The discussion here is focused
on the Langevin SDE

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

Here $W_t$ is a $d$-dimensional Wiener process, and $V : \mathbb{R}^d \to \mathbb{R}$ is called the potential. Throughout it is assumed that $V \in C^2_b(\mathbb{R}^d)$; that is, $V$ is bounded together with its (con-
tinuous) first and second order partial derivatives. Under these conditions \(2\) has unique
strong solutions for every initial condition as well as transition probability densities \[10\].

The Langevin SDE has infinitesimal generator $L_V$ defined by

\[
L_V f(x) = \lim_{t \to 0} \frac{\mathbb{E}_x[f(X_t) - f(x)]}{t}
\]

for $f \in C^2_b(\mathbb{R}^d)$. Here $\mathbb{E}_x$ denotes expectation with respect to the initial condition $X_0 = x$. From Itô’s lemma and the dominated convergence theorem, one finds that

\[
L_V = -\nabla V \cdot \nabla + \beta^{-1} \Delta
\]

The operator $L_V$ is closely related to probabilities of the process \(2\). In particular, let $p_t(x, y)$ be the probability density that $X_t = y$ given that $X_0 = x$. (By the Markov
property of the process \(2\) this determines all the transition probability densities.) If
the second order partial derivatives of $V$ are all Lipschitz continuous, then for fixed $x$,
\( p_t(x, y) \) satisfies the PDE
\[
\frac{\partial}{\partial t} p_t(x, y) = L^*_{V} p_t(x, y)
\] (4)
This is the Fokker-Planck equation \([11]\). Here the operator
\[
L^*_{V} = \nabla \cdot (\nabla V) + \beta^{-1} \Delta
\]
is formally adjoint to \( L_{V} \) and in \((4)\) is assumed to act only on the \( y \)-component of \( p_t(x, y) \). In principle by numerically solving the Fokker-Planck equation one obtains the transition probability densities, but this is impractical when the dimension \( d \) is large.

Let \( \mathbb{P} \) be the reference probability measure under which \( X_t \) satisfies
\[
dX_t = -\nabla V(X_t) \, dt + \sqrt{2\beta^{-1}} \, dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T
\]
One might ask how the measure \( \mathbb{P} \) changes if \( V \) is replaced by another potential \( \tilde{V} \). In general this question is answered by Girsanov’s theorem \([11], [12]\). However, the special structure of the overdamped Langevin equation allows for a useful simplification to the well-known Girsanov formula. In fact in Theorem 2.1 below it is shown that the change in probability measure has a simple relationship with the infinitesimal generators \( L_{V} \) and \( L_{\tilde{V}} \):

**Theorem 2.1.** Assume \( V, \tilde{V} \in C^2_b(\mathbb{R}^d) \). Let \( \tilde{\mathbb{P}} \) be the reference measure under which \( X_t \) satisfies
\[
dX_t = -\nabla \tilde{V}(X_t) \, dt + \sigma \, d\tilde{W}_t, \quad X_0 = x_0, \quad 0 \leq t \leq T
\]
where \( \sigma = \sqrt{2\beta^{-1}} \) and \( \tilde{W}_t \) is a \( d \)-dimensional Wiener process. Define \( \mathbb{P} \) by
\[
\frac{d\mathbb{P}}{d\tilde{\mathbb{P}}} = \exp \left[ \sigma^{-2} \left( \int_0^T \nabla (V(X_s) - \tilde{V}(X_s)) \cdot \nabla \tilde{V}(X_s) \, ds \right) \right]
\] (5)
where \( L \) is given by \((3)\). Then under \( \mathbb{P} \), \( X_t \) satisfies
\[
dX_t = -\nabla V(X_t) \, dt + \sigma \, dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T
\]
where \( W_t \) is a \( d \)-dimensional \( \mathbb{P} \)-Wiener process.

**Remark 2.2.** In the above, \( L_0 \equiv \beta^{-1} \Delta \).

**Proof.** Let \( U = \tilde{V} - V \), and define \( \mathbb{P} \) by
\[
\frac{d\mathbb{P}}{d\tilde{\mathbb{P}}} = \exp \left[ \sigma^{-1} \int_0^T \nabla U(X_s) \cdot d\tilde{W}_s - \frac{\sigma^{-2}}{2} \int_0^T \nabla U(X_s) \cdot \nabla U(X_s) \, ds \right]
\] (6)
By Girsanov’s theorem, under \( \mathbb{P} \) the process \( X_t \) satisfies
\[
dX_t = -\nabla V(X_t) \, dt + \sigma \, dW_t, \quad X_0 = x_0, \quad t \in [0, T]
\]
By Itô’s lemma, under \( \tilde{\mathbb{P}} \),
\[
dU(X_s) = \nabla U(X_s) \cdot dX_s + \frac{1}{2} dX'_s \nabla^2 U(X_s) dX_s \tag{7}
\]
\[
= -\nabla U(X_s) \cdot \nabla \tilde{V}(X_s) ds + \sigma \nabla U(X_s) \cdot d\tilde{W}_s + \frac{\sigma^2}{2} \Delta U(X_s) ds \tag{8}
\]
where \( \nabla^2 U \) denotes the Hessian matrix of \( U \), and \( dX'_s \) is the transpose of \( dX_s \). Rearranging, multiplying by \( \sigma^{-2} \), and using the integral form of (7)-(8), this becomes
\[
\sigma^{-1} \int_0^T \nabla U(X_s) \cdot d\tilde{W}_s \tag{9}
\]
\[
= \sigma^{-2} [U(X_T) - U(x_0)] + \sigma^{-2} \int_0^T \nabla U(X_s) \cdot \nabla \tilde{V}(X_s) ds - \frac{1}{2} \int_0^T \Delta U(X_s) ds \tag{10}
\]
Substituting (9)-(10) into (6) and simplifying,
\[
\frac{d\mathbb{P}}{d\mathbb{P}^\text{ref}} = \exp \left[ \sigma^{-1} \int_0^T \nabla U(X_s) \cdot d\tilde{W}_s - \frac{\sigma^{-2}}{2} \int_0^T \nabla U(X_s) \cdot \nabla U(X_s) ds \right] \tag{11}
\]
\[
= \exp \left[ \sigma^{-2} \left( U(X_T) - U(x_0) + \int_0^T \left( \nabla \tilde{V} \cdot \nabla \tilde{V} - \nabla \tilde{V} \cdot \nabla \tilde{V} - \sigma^2 \Delta U \right) (X_s) ds \right) \right] \tag{12}
\]
By comparing (11)-(12) with (5), the result follows. \( \Box \)

Although Girsanov’s formula and Itô’s lemma can be used with any Itô process \( \Pi \), in the proof of Theorem 2.1 the assumptions that the change in drift (here \( \nabla \tilde{V} - \nabla V \)) is conservative and that the diffusion matrix (here \( \sigma I_d \)) is a constant multiple of the identity matrix are essential. The result can be generalized slightly:

**Theorem 2.3.** Assume \( V \in C^2_b(\mathbb{R}^d) \) and \( F: \mathbb{R}^d \to \mathbb{R}^d \) is Lipschitz continuous. Let \( \mathbb{P}^\text{pref} \) be the reference measure under which \( X_t \) satisfies
\[
dX_t = F(X_t) dt + \sigma dW_t^\text{ref}, \quad X_0 = x_0, \quad 0 \leq t \leq T
\]
where \( W_t^\text{ref} \) is a \( d \)-dimensional Wiener process and \( \sigma > 0 \). Define \( \mathbb{P} \) by
\[
\frac{d\mathbb{P}}{d\mathbb{P}^\text{ref}} = \exp \left[ \sigma^{-2} \left( V(x_0) - V(X_T) + \int_0^T (L_V - L_0 + 2L^\text{ref}) V(X_s) ds \right) \right]
\]
where
\[
L^\text{ref} = F \cdot \nabla + \frac{\sigma^2}{2} \Delta
\]
is the infinitesimal generator of the reference process. Then under \( \mathbb{P} \), \( X_t \) satisfies
\[
dX_t = -\nabla V(X_t) dt + F(X_t) dt + \sigma dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T
\]
where \( W_t \) is a \( d \)-dimensional \( \mathbb{P} \)-Wiener process.
The proof of Theorem 2.3 is similar to that of Theorem 2.1 and is therefore omitted.

Note that much intuition can be gained out of a simple inspection of the formula (5). For example if $T, \delta$ are small and

$$A = \{X : X_T \in B_\delta(y)\}$$

where $B_\delta(y)$ is a ball of radius $\delta$ around $y$, then

$$\mathbb{P}(A) \approx \exp \left[ \sigma^{-2} \left( V(x_0) - V(y) - \left[ \tilde{V}(x_0) - \tilde{V}(y) \right] \right) \right] \tilde{\mathbb{P}}(A) \quad (13)$$

In particular, if $\tilde{V} = 0$ then the probability on the right hand side of (13) can be written as an integral of a Gaussian density; this suggests an estimate of asymptotic transition probabilities which is pursued in the next section.

3. Asymptotic transition probabilities

Consider the transition probability density $p_t(x, y)$ of the process

$$dX_t = -\nabla V(X_t) \, dt + \sigma \, dW_t \quad (14)$$

Recall $p_t(x, y)$ is the conditional probability density that $X_t = y$ given that $X_0 = x$. Notice that if $V = 0$ in (14) then $X_t = \sigma W_t$ and

$$p_t(x, y) = (2\pi \sigma^2 (t - s))^{-d/2} \exp \left( -\frac{|y - x|^2}{2\sigma^2 (t - s)} \right)$$

In the following theorem Theorem 2.1 is used to estimate transition probability densities for a generic potential.

**Theorem 3.1.** Assume $V \in C^2_b(\mathbb{R}^d)$ and $(L_V + L_0)V$ is Lipschitz continuous with Lipschitz constant $K$. Let $p_t(x, y)$ be the transition probability density of the process (14). Define

$$\psi_{x,y}(r) = (1 - r)x + ry$$

Then for any $\delta > 0$,

$$p_t(x, y) \geq \left( \exp \left[ \sigma^{-2} \left( V(x) - V(y) + \frac{t}{2} \int_0^1 (L_V + L_0)V(\psi_{x,y}(r)) \, dr - M_1 \delta t \right) \right] - M_2 \gamma(\delta, t) \right) \rho_t(y - x)$$

and

$$p_t(x, y) \leq \left( \exp \left[ \sigma^{-2} \left( V(x) - V(y) + \frac{t}{2} \int_0^1 (L_V + L_0)V(\psi_{x,y}(r)) \, dr + M_1 \delta t \right) \right] + M_2 \gamma(\delta, t) \right) \rho_t(y - x)$$
where
\[
M_1 = \frac{1}{2} \sqrt{dK} \\
M_2 = 2d \exp \left( \sigma^{-2} \left[ V(x) - V(y) + \frac{t}{2} \sup |(L_V + L_0)V| \right] \right) \\
\gamma(\delta, t) = \exp \left( -\frac{2\delta^2}{\sigma^2 t} \right) \\
\rho_t(x) = (2\pi\sigma^2 t)^{-d/2} \exp \left( -\frac{|x|^2}{2\sigma^2 t} \right)
\]

In particular, as \( t \to 0^+ \),
\[
p_t(x, y) = \left( \exp \left[ \sigma^{-2} \left( V(x) - V(y) + \frac{t}{2} \int_0^1 (L_V + L_0)V(\psi_{x,y}(r)) dr \right) \right] + O(t^{\alpha+1}) \right) \rho_t(y - x)
\]
for any \( \alpha \in (0, \frac{1}{2}) \).

**Remark 3.2.** Note that \( \rho_t(y - x) \) is the transition probability density of the process \( \sigma W_t \).

Theorem 3.1 can be seen a a first-order correction to transition probability densities when a conservative drift is added to the process
\[
dX_t = \sigma \, dW_t
\]
as in (14). The term in parentheses in (16) gives the correction corresponding to the addition of the drift \(-\nabla V\). Note that when \( t \) is small, the correction is dominated by the term \( \exp[\sigma^{-2}(V(x) - V(y))] \), which depends only on the change in potential energy from \( x \) to \( y \).

Using Theorem 2.3, the asymptotic result of Theorem 3.1 can be generalized as follows:

**Theorem 3.3.** Let \( L^{\text{ref}} \) and \( p^{\text{ref}}_t(x, y) \) be the infinitesimal generator and transition probability density of the reference process
\[
dX_t = F(X_t) \, dt + \sigma \, dW_t
\]
where \( W_t \) is a \( d \)-dimensional Wiener process and \( F : \mathbb{R}^d \to \mathbb{R}^d \) is Lipschitz continuous. Assume \( V \in C^2_b(\mathbb{R}^d) \) and \( (L_V - L_0 + 2L^{\text{ref}})V \) is bounded and Lipschitz continuous. Let \( p_t(x, y) \) be the transition probability density of the process
\[
dX_t = -\nabla V(X_t) \, dt + F(X_t) \, dt + \sigma \, dW_t
\]
and define
\[
\psi_{x,y}(r) = (1 - r)x + ry
\]
Then as $t \to 0^+$,

$$p_t(x, y) = \left( \exp \left[ \sigma^{-2} \left( V(x) - V(y) + \frac{t}{2} \int_0^1 (L_V - L_0 + 2L_{ref}) V(\psi_{x,y}(r)) \, dr \right) \right] + O(t^{\alpha+1}) \right) p_{ref}^t(x, y)$$

for any $\alpha \in (0, \frac{1}{2})$.

The proof of Theorem 3.1 is a consequence of Theorem 2.1 and the following lemmas:

**Lemma 3.4.** Let $\mathbb{P}$ be the measure under which $X_t$ satisfies

$$dX_t = \sigma \, dW_t, \quad X_0 = x$$

where $W_t$ is a $d$-dimensional Wiener process. Fix $t > 0$, $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$, $y = (y_1, y_2, \ldots, y_d) \in \mathbb{R}^d$, and $\delta > 0$. Define

$$N_{\delta,t}^{x,y}(r) = \prod_{k=1}^d \left( 1 - \frac{r}{t} \right) x_k + \frac{r}{t} y_k - \delta, \left( 1 - \frac{r}{t} \right) x_k + \frac{r}{t} y_k + \delta$$

Then

$$\mathbb{P} \left( X_r \in N_{\delta,t}^{x,y}(r), \ 0 \leq r \leq t \bigg| X_t = y \right) \geq 1 - 2d \exp \left( -\frac{2\delta^2}{\sigma^2 t} \right)$$

**Proof.** With $X_t^k$ the $k$th component of $X_t$, a well-known formula of Siegmund ([13], [14]) leads to

$$\mathbb{P} \left( X_r^k < \left( 1 - \frac{r}{t} \right) x_k + \frac{r}{t} y_k + \delta, \ 0 \leq r \leq t \bigg| X_t^k = y_k \right)$$

$$= 1 - \exp \left( -\frac{2\delta^2}{\sigma^2 t} \right)$$

$$= \mathbb{P} \left( X_r^k > \left( 1 - \frac{r}{t} \right) x_k + \frac{r}{t} y_k - \delta, \ 0 \leq r \leq t \bigg| X_t^k = y_k \right)$$

The result follows by subadditivity. \qed

**Lemma 3.5.** Assume $G : \mathbb{R}^d \to \mathbb{R}$ is Lipschitz continuous with Lipschitz constant $K_G$. Fix $t > 0$, $x, y \in \mathbb{R}^d$ and $\delta > 0$. If $X_r \in N_{\delta,t}^{x,y}(r)$ for all $r \in [0, t]$ then

$$\left| \int_0^t G(X_r) \, dr - t \int_0^1 G((1 - r)x + ry) \, dr \right| \leq \sqrt{d} \delta K_G t$$
Proof. Note that if $X_r \in N_{x,y}^r(r)$ for all $r \in [0,t]$, then
\begin{align*}
\left| \int_0^t G(X_r) \, dr - t \int_0^1 G((1-r)x + ry) \, dr \right| &= \left| \int_0^t G(X_r) \, dr - \int_0^t G \left( \left(1 - \frac{r}{t} \right)x + \frac{ry}{t} \right) \, dr \right| \\
&\leq \int_0^t \left| G(X_r) - G \left( \left(1 - \frac{r}{t} \right)x + \frac{ry}{t} \right) \right| \, dr \\
&\leq \int_0^t \sqrt{d_\delta K_G} \, dr \\
&= \sqrt{d_\delta K_G} t
\end{align*}

\[ \square \]

Proof of Theorem 3.1. Let $\tilde{P}$ be the reference measure under which $X_t$ satisfies
\[ dX_t = \sigma d\tilde{W}_t, \quad X_0 = x, \quad 0 \leq t \leq T \]
where $\tilde{W}_t$ is a $d$-dimensional Wiener process, and let $\tilde{E}$ be the corresponding expectation. For $y = (y_1, y_2, ..., y_d) \in \mathbb{R}^d$ and $h > 0$ define
\[ S_{y,h} = \prod_{k=1}^d [y_k, y_k + h) \]

Using Theorem 2.1 with $\tilde{V} = 0$ yields
\[ \tilde{P}(X_t \in S_{y,h}) = \tilde{E} \left[ \exp \left( \sigma^{-2} \left( V(x) - V(X_t) + \frac{1}{2} \int_0^t (L_V + L_0) V(X_r) \, dr \right) \right) 1_{\{X_t \in S_{y,h}\}} \right] \]
such that under $\tilde{P}$, $X_t$ satisfies
\[ dX_t = -\nabla V(X_t) \, dt + \sigma dW_t, \quad X_0 = x, \quad 0 \leq t \leq T \]
with $W_t$ a $d$-dimensional $P$-Wiener process. Now
\[ \frac{\tilde{P}(X_t \in S_{y,h})}{h^d} = \frac{\tilde{E} \left[ \exp \left( \sigma^{-2} \left( V(x) - V(X_t) + \frac{1}{2} \int_0^t (L_V + L_0) V(X_r) \, dr \right) \right) 1_{\{X_t \in S_{y,h}\}} \right]}{\tilde{P}(X_t \in S_{y,h})} \cdot \tilde{P}(X_t \in S_{y,h}) \tag{20} \]

Taking limits in (20)-(21) as $h \to 0$ gives
\[ p_t(x,y) = \tilde{E} \left[ \exp \left( \sigma^{-2} \left( V(x) - V(y) + \frac{1}{2} \int_0^t (L_V + L_0) V(X_r) \, dr \right) \right) \right| X_t = y \] $p_t(y - x)$

The first statement of the theorem follows from Lemmas 3.4-3.5 with $G = (L_V + L_0)V$. The last statement follows by taking $\delta = t^\alpha$. $\square$
The proof of Theorem 3.3, which is omitted, is similar to the proof of Theorem 3.1 and relies on the fact that the exit probabilities of the pinned diffusion of Lemma 3.4 retain the same asymptotics as $t \to 0$ with the addition of a drift $F$ (see Theorem 2.1 of [13]).

4. IMPORTANCE SAMPLING AND EXITING A WELL

Here the problem of estimating a small escape probability $P(A)$ of the process (1) is considered. In standard Monte Carlo, one estimates $P(A)$ by taking the average number of samples, out of some total $N$, for which the event $A$ is observed. More precisely, the standard Monte Carlo approximation of $P(A)$ is

$$
\Theta \equiv \frac{1}{N} \sum_{n=1}^{N} 1^n_A
$$

(22)

where $1^n_A$ are i.i.d. random variables with the same distribution (under $P$) as the indicator function $1_A$. This estimate has expected value

$$
E(\Theta) = P(A)
$$

and variance

$$
\text{Var}(\Theta) = \frac{\text{Var}(1_A)}{N}
$$

where

$$
\text{Var}(1_A) = P(A) - P(A)^2
$$

(23)

The relative error of $\Theta_N$ is its standard deviation divided its expected value:

$$
\text{Relative Error}(\Theta) \equiv \frac{\sqrt{\text{Var}(\Theta)}}{P(A)} = \frac{1}{\sqrt{N}} \sqrt{\frac{P(A)}{P(A)^2} - 1}
$$

The relative error blows up for fixed $N$ as $P(A) \to 0$, making the estimate (22) useless for a fixed computational effort if $P(A)$ is very small.

An alternative to standard Monte Carlo sampling is importance sampling (see e.g. [16], [17]), in which one chooses another probability measure $\tilde{P}$ for sampling. One then estimates $P(A)$ by taking the average number of samples (out of $N$) for which $A$ has occurred, such that each sample is weighted by the factor $dP/d\tilde{P}$. More precisely, an unbiased importance sampling estimator for $P(A)$ is

$$
\tilde{\Theta} \equiv \frac{1}{N} \sum_{n=1}^{N} \left( \frac{dP}{d\tilde{P}} 1^n_A \right)
$$

(24)

where $1^n_A$ are i.i.d. random variables with the same distribution (under $\tilde{P}$) as $1_A$. Here $P$ must be absolutely continuous with respect to $\tilde{P}$. $\tilde{\Theta}$ is called unbiased because

$$
P(A) = E[1_A] = E \left[ \frac{dP}{d\tilde{P}} 1_A \right]
$$

which implies

$$
P(A) = E[\Theta] = E \left[ \tilde{\Theta} \right]
$$
where $\tilde{E}$ is the expectation corresponding to $\tilde{P}$. To optimally reduce the number of samples necessary to achieve a given error, one wants to minimize the variance

$$\text{Var}(\Theta) = \frac{1}{N} \text{Var} \left( \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right)$$

subject to constraints of feasibility. Here

$$\text{Var} \left( \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right) = \tilde{E} \left[ \left( \frac{d\mathbb{P}}{d\tilde{P}} \right)^2 1_A \right] - \mathbb{P}(A)^2 = \tilde{E} \left[ \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right] - \mathbb{P}(A)^2 \quad (25)$$

One would hope, for instance, that the variance is greatly reduced compared with standard Monte Carlo, that is,

$$\frac{\text{Var}(\tilde{\Theta})}{\text{Var}(\Theta)} = \frac{\text{Var} \left( \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right)}{\text{Var}(1_A)} \leq C << 1 \quad (26)$$

Another important quantity is the relative error

$$\text{Relative Error}(\tilde{\Theta}) \equiv \sqrt{\frac{\text{Var}(\tilde{\Theta})}{\mathbb{P}(A)}} = \frac{1}{\sqrt{N}} \sqrt{\frac{\tilde{E} \left( \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right)}{\mathbb{P}(A)^2}} - 1 \quad (27)$$

To minimize the relative error, one wants to minimize the quantity

$$\Lambda \equiv \frac{\tilde{E} \left( \frac{d\mathbb{P}}{d\tilde{P}} 1_A \right)}{\mathbb{P}(A)^2} \quad (28)$$

In general it is very difficult to prove an inequality like (26), or useful bounds on (27)-(28), outside of certain asymptotic regimes. Examined below is the small noise regime of the overdamped Langevin equation, defined by

$$dX^\epsilon_t = -\nabla V(X^\epsilon_t) \, dt + \sqrt{\epsilon} \, dW_t \quad (29)$$

where $\epsilon$ is a small parameter. The small noise regime can be thought of as a nearly deterministic version of the SDE, where the dynamics are dominated by the potential energy and diffusive effects are small.

In the below the reduction in variance from using (24) instead of (22) for estimating probabilities in the small noise regime of the overdamped Langevin SDE is considered. Though the analysis is restricted to the small noise overdamped Langevin equation, the method itself is applicable to the second-order Langevin equation. The scheme involves only changes in measure $\mathbb{P} \to \tilde{\mathbb{P}}$ corresponding to a fixed change in the potential $V \to \tilde{V}$. That is, the sampling measure $\tilde{\mathbb{P}}$ will correspond to the process

$$dX^\epsilon_t = -\nabla \tilde{V}(X^\epsilon_t) \, dt + \sqrt{\epsilon} \, d\tilde{W}_t, \quad X_0 = x_0, \quad 0 \leq t \leq T \quad (29)$$

whereas the target measure $\mathbb{P}$ will correspond to

$$dX^\epsilon_t = -\nabla V(X^\epsilon_t) \, dt + \sqrt{\epsilon} \, dW_t, \quad X_0 = x_0, \quad 0 \leq t \leq T \quad (30)$$

Here and throughout the dependence of $\mathbb{P}$ and $\tilde{\mathbb{P}}$ on $\epsilon$ is suppressed. In Theorem \[4.2\] it is shown that for estimating the probability of escaping a potential well, an exponential reduction in variance (compared to standard Monte Carlo) can be achieved simply by
taking a sampling potential \( \tilde{V} \) which reduces the depth of the well. The magnitude of the reduction in variance is closely related to the difference \( V(x_0) - \tilde{V}(x_0) \). The scheme allows for the well to be “inverted,” and in fact in Theorem 4.3 it is shown that under certain conditions this creates an \textit{asymptotically optimal} reduction in variance, in the sense that \[ \lim_{\epsilon \to 0} \epsilon \log \Lambda = 0 \] (31)

The limit in (31) is optimal because for any \( P, \tilde{P}, \) and \( A \), Jensen’s inequality and (25) imply \( \Lambda \geq 1 \).

Below \( \Lambda_\epsilon \) is written for \( \Lambda \) defined in (28), and \( \Theta_\epsilon, \tilde{\Theta}_\epsilon \) are written for \( \Theta, \tilde{\Theta} \) defined in (22), (24), to emphasize the dependence of these objects on \( \epsilon \). Events of the following type will be considered:

**Definition 4.1.** Let \( D \subset \mathbb{R}^d \) be a bounded open set such that \( \partial D \) is a simple closed curve, and define

\[ \mathcal{A}_\epsilon \equiv \{ X_\epsilon : X_T \notin D \} \]

The following is the main result of this section.

**Theorem 4.2.** Assume \( V \in C^2_b(\mathbb{R}^d), \tilde{V} \in C^2_b(\mathbb{R}^d) \), such that:

(i) \( V(x_0) < \tilde{V}(x_0) \)

(ii) \( |\nabla \tilde{V}(x)| \leq |\nabla V(x)| \) for all \( x \in D \)

(iii) \( \tilde{V}(x) = V(x) \) for all \( x \notin D \)

and define

\[ M = \frac{1}{2} \sup_{x \in D} \left( \Delta V(x) - \Delta \tilde{V}(x) \right) \]

Let \( \tilde{P} \) be the reference measure under which \( X_T^\epsilon \) satisfies (29), and define \( P \) as in (5). (The dependence of \( P \) and \( \tilde{P} \) on \( \epsilon \) is suppressed.) Then under \( P, X_T^\epsilon \) satisfies (30). If

\[ \tilde{V}(x_0) - V(x_0) \geq \epsilon TM \]

then

\[ \frac{\text{Var}(\Theta_\epsilon)}{\text{Var}(\tilde{\Theta}_\epsilon)} \leq e^{\epsilon^{-1}(V(x_0)-\tilde{V}(x_0))+TM} \]

Furthermore

\[ \lim_{\epsilon \to 0} \epsilon \log \Lambda_\epsilon \leq V(x_0) - \tilde{V}(x_0) + I_V(x_0) \] (32)

where

\[ I_V(x_0) \equiv \inf \left\{ \frac{1}{2} \int_0^T \left| \dot{\phi}(t) + \nabla V(\phi(t)) \right|^2 dt : \phi \in H^1_{x_0,T}, \phi(T) \notin D \right\} \] (33)

with

\[ H^1_{x_0,T} \equiv \left\{ \phi : [0, T] \to \mathbb{R}^d : \phi(t) = x_0 + \int_0^t \dot{\phi}(s) ds, \int_0^T |\dot{\phi}(t)|^2 dt < \infty \right\} \]
Proof. By Theorem 2.1 and assumptions (ii)-(iii),
\[
\mathbb{E} \left[ \frac{dP}{d\tilde{P}} 1_{A_\epsilon} \right] \leq e^{-\epsilon \left( V(x_0) - \tilde{V}(x_0) \right) + TM \mathbb{P}(A_\epsilon)}
\] (34)

Using assumption (i), choose \( \epsilon > 0 \) so that
\[
\tilde{V}(x_0) - V(x_0) \geq \epsilon TM
\]

Then from (23), (25) and (26),
\[
\frac{\text{Var}(\Theta_\epsilon)}{\text{Var}(\Theta_\epsilon)} = \frac{\text{Var}\left( \frac{dP}{d\tilde{P}} 1_{A_\epsilon} \right)}{\text{Var}(1_{A_\epsilon})} \leq \frac{\mathbb{E}\left[ \frac{dP}{d\tilde{P}} 1_{A_\epsilon} \right]}{\mathbb{P}(A_\epsilon)}
\] (35)

Comparing with (34) with (35),
\[
\frac{\text{Var}(\Theta_\epsilon)}{\text{Var}(\Theta_\epsilon)} \leq e^{-\epsilon \left( V(x_0) - \tilde{V}(x_0) \right) + TM}
\]

From Definition 4.1 and continuity of \( \nabla V \) it follows that \( A_\epsilon \) is a continuity set \([5]\) with respect to the rate function
\[
\phi \mapsto \begin{cases} 
\frac{1}{2} \int_0^T \left| \dot{\phi}(t) + \nabla V(\phi(t)) \right|^2 dt, & \phi \in H^1_{x_0,T} \\
\infty, & \phi \notin H^1_{x_0,T}
\end{cases}
\]

Therefore
\[
\lim_{\epsilon \to 0} \epsilon \log \mathbb{P}(A_\epsilon) = -I_V(x_0)
\]

A simple calculation now leads to (32). \( \square \)

Theorem 4.2 shows that by choosing an sampling potential \( \tilde{V} \) which reduces the depth of the potential well around \( x_0 \) and which agrees with \( V \) outside the well, the probability that the process (30) is outside the well at time \( T \) can be estimated with an exponentially reduced variance compared to standard Monte Carlo. The variance is reduced by a factor proportional to
\[
\exp \left[ \epsilon^{-1} \left( V(x_0) - \tilde{V}(x_0) \right) \right]
\]

See Figure 1.

In Theorem 4.3 below is shown that if the well has a flat boundary, then an asymptotically optimal scheme is obtained by inverting the potential well inside \( D \); see Figure 2.

Theorem 4.3. Assume \( V \in C^2_b(\mathbb{R}^d) \) and that \( \nabla V(x) \equiv 0 \) on \( \partial D \). Then WLOG we may take \( V(x) \equiv 0 \) on \( \partial D \). Define
\[
\tilde{V}(x) = \begin{cases} 
-V(x) & \text{if } x \in D \\
V(x) & \text{if } x \notin D
\end{cases}
\]
Figure 1. Using the sampling potential $\tilde{V}$ to estimate the rare observable $P(X_\epsilon \notin D)$, for $D = (a, b)$. The logarithm of the reduction of variance compared to standard Monte Carlo is closely related to the length of the vertical line.

and assume $\tilde{V} \in C^2(\mathbb{R}^d)$. Define

$$K \equiv \sup_{x \in D} |\Delta \tilde{V}| = \sup_{x \in D} |\Delta V|$$

Let $\tilde{\mathbb{P}}$ be the reference measure under which $X_\epsilon^t$ satisfies (29), and define $\mathbb{P}$ as in (5), so that under $\mathbb{P}$, $X_\epsilon^t$ satisfies (30). (The dependence of $\mathbb{P}$ and $\tilde{\mathbb{P}}$ on $\epsilon$ is suppressed.) Furthermore assume the solution $y = y(t)$ to the IVP

$$\frac{dy}{dt} = -\nabla \tilde{V}(y), \quad y(0) = x_0$$

satisfies $y(T) \notin D$. Then

$$\lim_{\epsilon \to 0} \epsilon \log \Lambda_\epsilon = 0$$

Proof. From the proof of Theorem 4.2

$$\lim_{\epsilon \to 0} \epsilon \log \Lambda_\epsilon \leq 2V(x_0) + I_V(x_0)$$

$$= 2V(x_0) - \lim_{\epsilon \to 0} \epsilon \log \mathbb{P}(A_\epsilon)$$

Now Theorem 2.1 gives

$$\mathbb{P}(A_\epsilon) \geq e^{2V(x_0) - TK \tilde{\mathbb{P}}(A_\epsilon)}$$
From Definition 4.1 and continuity of $\nabla \tilde{V}$ it follows that $A_\epsilon$ is a continuity set with respect to the rate function
\[
\phi \mapsto \begin{cases} 
\frac{1}{2} \int_0^T \left| \dot{\phi}(t) + \nabla \tilde{V}(\phi(t)) \right|^2 dt, & \phi \in H^1_{x_0,T} \\
\infty, & \phi \notin H^1_{x_0,T}
\end{cases}
\]
Therefore by assumption (36),
\[
\lim_{\epsilon \to 0} \epsilon \log \bar{P}(A_\epsilon) = -I_{\tilde{V}}(x_0) = 0
\]
From (39) it follows that
\[
\lim_{\epsilon \to 0} \epsilon \log \mathbb{P}(A_\epsilon) \geq 2V(x_0) \tag{40}
\]
By comparing (40) with (37)-(38),
\[
\lim_{\epsilon \to 0} \epsilon \log \Lambda_\epsilon \leq 0
\]
From Jensen’s inequality $\Lambda_\epsilon \geq 1$ and the result follows. \qed

Although the assumptions of Theorem 4.3 are very restrictive, the result suggests what changes in potential should be most effective more generally. In particular, by inspecting (5) and the proof of Theorem 4.2, one sees that in choosing an optimal $\tilde{V}$, there is a competition between maximizing $\tilde{V}(x_0)$ while also minimizing $|\nabla \tilde{V}(x)|$ and maximizing $\Delta \tilde{V}(x)$ for $x \in D$, in the sense that when any two of these three is fixed, optimizing
the third reduces the variance. Here it is assumed that $\tilde{V}$ agrees with $V$ outside $D$. Theorem 4.2 shows that in the small noise limit, maximizing $\Delta\tilde{V}(x)$ becomes irrelevant; Theorem 4.3 suggests that it may be near optimal to choose a $\tilde{V}$ which maximizes $\tilde{V}(x_0)$ while also minimizing $||\nabla\tilde{V}(x) - |\nabla V(x)|||$ for $x \in D$.

5. Example

Consider the one-dimensional overdamped Langevin SDE

$$dX_t = -\frac{d}{dx}V(X_t)\, dt + dW_t, \quad X_0 = 0, \quad 0 \leq t \leq T \tag{41}$$

where $V(x) = -\cos x - 1$ and $W_t$ is a Wiener process. Let $T = 1$, define

$$\mathcal{A} = \{X : X_T \notin (-\pi, \pi)\} \tag{42}$$

and suppose the probability of interest is $P(\mathcal{A})$ where $P$ is the probability of the process (41). Consider the importance sampling scheme of Section 4, with sampling potentials

$$\tilde{V}^A(x) = \begin{cases} 0, & \text{if } x \in (-\pi, \pi) \\ V(x), & \text{otherwise} \end{cases}$$

$$\tilde{V}^B(x) = \begin{cases} -V(x), & \text{if } x \in (-\pi, \pi) \\ V(x), & \text{otherwise} \end{cases}$$

Let $\tilde{P}^A$ be the reference measure under which $X_t$ satisfies

$$dX_t = -\frac{d}{dx}\tilde{V}^A(X_t)\, dt + d\tilde{W}^A_t, \quad X_0 = x_0, \quad 0 \leq t \leq T \tag{43}$$

and let $\tilde{P}^B$ be the reference measure under which $X_t$ satisfies

$$dX_t = -\frac{d}{dx}\tilde{V}^B(X_t)\, dt + d\tilde{W}^B_t, \quad X_0 = x_0, \quad 0 \leq t \leq T \tag{44}$$

where $d\tilde{W}^A_t$ and $d\tilde{W}^B_t$ are $\tilde{P}^A$- and $\tilde{P}^B$-Wiener processes, respectively. Then under $P$ defined by (5), $X_t$ satisfies (41). The following table compares standard Monte Carlo estimates of $P(\mathcal{A})$, using $\Theta$ defined in (22), to estimates from the scheme outlined in Section 4. The importance sampling estimators $\tilde{\Theta}^A$ and $\tilde{\Theta}^B$ corresponding to $\tilde{P}^A$ and $\tilde{P}^B$ are defined as in (24). Samples are obtained using Euler approximations of (41) and (43)-(44) with step size $h = 10^{-5}$ and Riemann approximations of (5) with mesh size $\tau$.

| estimator | potential | $N$ (# of samples) | $\tau$ | sample average | sample variance |
|-----------|-----------|---------------------|--------|----------------|-----------------|
| $\Theta$  | $V$       | $10^5$              | N/A    | 0.000192       | 0.000192        |
| $\tilde{\Theta}^A$ | $\tilde{V}^A$ | $10^7$              | $10^{-1}$ | 0.000195       | 0.000022        |
| $\tilde{\Theta}^A$ | $\tilde{V}^A$ | $10^7$              | $10^{-2}$ | 0.000193       | 0.000022        |
| $\tilde{\Theta}^A$ | $\tilde{V}^A$ | $10^7$              | $10^{-3}$ | 0.000193       | 0.000022        |
| $\tilde{\Theta}^B$ | $\tilde{V}^B$ | $10^7$              | $10^{-1}$ | 0.000204       | 0.0000039       |
| $\tilde{\Theta}^B$ | $\tilde{V}^B$ | $10^7$              | $10^{-2}$ | 0.000196       | 0.0000039       |
| $\tilde{\Theta}^B$ | $\tilde{V}^B$ | $10^7$              | $10^{-3}$ | 0.000197       | 0.0000039       |
Note that sampling with either $\tilde{V}^A$ or $\tilde{V}^B$ reduces the variance significantly. The greater reduction in variance is obtained by sampling with $\tilde{V}^B$. This is consistent with Theorem 4.3 which suggests $\tilde{V}^B$ is asymptotically optimal. Note that $\tilde{V}^A$ and $\tilde{V}^B$ do not quite satisfy the conditions of the theorem since

$$\frac{\partial^2}{\partial x^2} \tilde{V}^A(\pm \pi), \frac{\partial^2}{\partial x^2} \tilde{V}^B(\pm \pi)$$

do not exist, yet the scheme is nonetheless accurate and effective. One suspects the assumption $\tilde{V} \in C^2_b(\mathbb{R}^d)$ in Theorem 4.2 and Theorem 4.3 can be relaxed to $\tilde{V} \in C^0_b(\mathbb{R}^d)$ on $\partial D$; this generalization is not pursued here. Though $\epsilon = 1$ here is “far” from zero, one expects that $P(A)$ being small means exactly that one is effectively in the small noise regime.

6. Conclusion

The problem of estimating small probabilities of the overdamped Langevin process, a well-known and important model of physical systems, is explored. Since standard Monte Carlo techniques are often impractical in this setting, it is useful to have alternative means of estimating averages of observables, in particular of transition probabilities. This paper explores small transition probabilities of Langevin processes in two asymptotic regimes: $t \approx 0$ and $\beta = 2\epsilon^{-1} \approx \infty$. A first-order accurate asymptotic correction to transition probability densities as $t \to 0$ is proved in Theorem 3.1, and an importance sampling technique for estimating escape probabilities as $\beta \to \infty$ is shown in Theorem 4.2 to perform exponentially better than standard Monte Carlo. It is shown that this technique is asymptotically optimal in some cases (Theorem 4.3). The importance sampling scheme has the virtue of requiring nearly negligible added computation (compared with standard Monte Carlo) during simulations, and it is shown to be effective in a simple numerical example.

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