Toward practical rare event simulation for small noise diffusions

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Goals

1. Generate samples of the rare event
2. Accurately estimate their probability

Applications

- Device reliability
- Options pricing
- Chemical reactions
- Data assimilation?
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Example: the Kuroshio current

Figure: Top: Mean flow paths in the large meander state. Bottom: Mean flow paths in the small meander state.
Figure: Projected view of transitions.
Rare event simulation for diffusions

$X^\epsilon$ is the solution of the stochastic differential equation

$$dX^\epsilon(t) = b(X^\epsilon(t)) \, dt + \sqrt{\epsilon} \sigma(X^\epsilon(t)) \, dW(t), \quad X^\epsilon(0) = x_0$$

How should we approximate

$$E \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]$$

where $g$ is a functional of the path of $X^\epsilon$?

Or the special case

$$P \left( X^\epsilon \in A \right)$$
If we use the standard Monte Carlo estimator,

\[
\delta^\epsilon = \frac{1}{M} \sum_{j=1}^{M} e^{-\frac{1}{\epsilon} g(X_j^\epsilon)} \quad X_j^\epsilon \text{ i.i.d.,}
\]

the variance is

\[
\text{Var}(\delta^\epsilon) = \frac{1}{\sqrt{M}} \left( \mathbb{E} \left[ e^{-\frac{1}{\epsilon} 2g(X^\epsilon)} \right] - \mathbb{E} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]^2 \right)
\]

and the relative error is

\[
\frac{\sqrt{\text{Var}(\delta^\epsilon)}}{\mathbb{E} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]} = \frac{1}{\sqrt{M}} \frac{1}{\sqrt{R^\epsilon - 1}}
\]

where

\[
R^\epsilon = \frac{\mathbb{E} \left[ e^{-\frac{2}{\epsilon} g(X^\epsilon)} \right]}{\mathbb{E} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]^2}
\]
We’ll focus on

\[ R^\varepsilon = \frac{E \left[ e^{-2\varepsilon g(X^\varepsilon)} \right]}{E \left[ e^{-1\varepsilon g(X^\varepsilon)} \right]^2} \]

First Notice that \( R^\varepsilon \geq 1 \) from Jensen’s inequality.

The Laplace Principle for \( X^\varepsilon \) gives us constants \( \gamma_1 \) and \( \gamma_2 \) such that

\[ E \left[ e^{-\frac{1}{\varepsilon} g(X^\varepsilon)} \right] = e^{-\frac{\gamma_1 + o(1)}{\varepsilon}} \text{ and } E \left[ e^{-\frac{1}{\varepsilon} 2g(X^\varepsilon)} \right] = e^{-\frac{\gamma_2 + o(1)}{\varepsilon}} \]

Therefore

\[ R^\varepsilon = \exp \left( \frac{2\gamma_1 - \gamma_2 + o(1)}{\varepsilon} \right) \]

Since \( \gamma_2 \leq 2\gamma_1 \) this is very bad news. We’ll need exponentially many samples.
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Therefore

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Since \( \gamma_2 \leq 2\gamma_1 \) this is very bad news. We’ll need exponentially many samples.
More precisely

\[ R^\varepsilon = \exp\left( \frac{2\gamma_1 - \gamma_2 + o(1)}{\varepsilon} \right) \]

where

\[ \gamma_1 = \inf_{\varphi \in AC([0, T]), \varphi(0)=x_0} \left\{ \int_0^T \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 ds + g(\varphi) \right\}, \quad (1) \]

and

\[ \gamma_2 = \inf_{\varphi \in AC([0, T]), \varphi(0)=x_0} \left\{ \int_0^T \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 ds + 2g(\varphi) \right\}, \quad (2) \]
Data assimilation picture:

Suppose for example that the observation model is of the form

\[ Y_n = r(X_{tn}) + \sqrt{\epsilon} \xi_n, \]

where the \( \xi_n \) are i.i.d. Gaussian.

For a particle filter the weights for each particle will look like:

\[ w(x) = e^{-\frac{1}{\epsilon}(y - r(x))^2} = e^{-\frac{1}{\epsilon}g_y(x)} \]

The effective sample size of the ensemble is related to the quantity

\[
\frac{\mathbb{E} \left[ e^{-\frac{1}{\epsilon}g_y(X^\epsilon)} \right]^2}{\mathbb{E} \left[ e^{-\frac{2}{\epsilon}g_y(X^\epsilon)} \right]} = \frac{1}{R^\epsilon}
\]

Other methods suffer related problems.
Importance sampling.

What’s the problem? We generate a huge number of samples that result in near zero values of $e^{-\frac{1}{\epsilon}g(X_j^\epsilon)}$ and if we’re lucky we get one sample with a relatively large value of $e^{-\frac{1}{\epsilon}g(X_j^\epsilon)}$.

Solution: Try to “pull” the process toward the region where $e^{-\frac{1}{\epsilon}g(X_j^\epsilon)}$ is relatively large.

Instead of sampling the solution, $X^\epsilon$, of

$$dX^\epsilon(t) = b(X^\epsilon(t)) \, dt + \sqrt{\epsilon} \sigma(X^\epsilon(t)) \, dW(t)$$

sample the solution, $\hat{X}^\epsilon$, of

$$d\hat{X}^\epsilon(t) = \left( b(\hat{X}^\epsilon(t)) + \sigma(\hat{X}^\epsilon(t)) v(t, \hat{X}^\epsilon(t)) \right) \, dt + \sqrt{\epsilon} \sigma(\hat{X}^\epsilon(t)) \, dW(t).$$

and assign a weight $Z^\epsilon$ to each sample so that

$$\mathbb{E} \left[ e^{-\frac{1}{\epsilon}g(\hat{X}^\epsilon)} Z^\epsilon \right] = \mathbb{E} \left[ e^{-\frac{1}{\epsilon}g(X^\epsilon)} \right].$$
The importance sampling estimator is:

\[
\delta^\epsilon = \frac{1}{M} \sum_{j=1}^{M} e^{-\frac{1}{\epsilon} g(\hat{X}_j^\epsilon)} Z_j^\epsilon
\]

where \((\hat{X}_j^\epsilon, W_j)\) are independent samples of \((\hat{X}^\epsilon, W)\) and, from Girsanov’s formula,

\[
Z_j^\epsilon = \exp \left( -\frac{1}{\sqrt{\epsilon}} \int_0^T \nu(t, \hat{X}_j^\epsilon(t)) \, dW_j(t) - \frac{1}{2\epsilon} \int_0^T \nu(t, \hat{X}_j^\epsilon(t))^2 \, dt \right).
\]

Now we have

\[
\text{rel err} = \frac{1}{\sqrt{M}} \sqrt{R^\epsilon - 1} \quad \text{and} \quad R^\epsilon = \frac{\mathbb{E} \left[ e^{-\frac{2}{\epsilon} g(\hat{X}^\epsilon)} (Z^\epsilon)^2 \right]}{\mathbb{E} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]^2}
\]

We want to choose the function \(\nu\) to make \(R^\epsilon \approx 1\).
The importance sampling estimator is:

\[ \delta^\epsilon = \frac{1}{M} \sum_{j=1}^{M} e^{-\frac{1}{\epsilon} g(\hat{X}^\epsilon_j)} Z^\epsilon_j \]

where \((\hat{X}^\epsilon_j, W_j)\) are independent samples of \((\hat{X}^\epsilon, W)\) and, from Girsanov's formula,

\[ Z^\epsilon_j = \exp \left( -\frac{1}{\sqrt{\epsilon}} \int_0^T v(t, \hat{X}^\epsilon_j(t)) \ dW_j(t) - \frac{1}{2\epsilon} \int_0^T v(t, \hat{X}^\epsilon_j(t))^2 \ dt \right). \]

Now we have

\[ \text{rel err} = \frac{1}{\sqrt{M}} \sqrt{R^\epsilon} - 1 \quad \text{and} \quad R^\epsilon = \frac{\mathbb{E} \left[ e^{-\frac{2}{\epsilon} g(\hat{X}^\epsilon) (Z^\epsilon)^2} \right]}{\mathbb{E} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon)} \right]^2} \]

We want to choose the function \(v\) to make \(R^\epsilon \approx 1\).
Now
\[ R^\epsilon \sim \exp \left( \frac{2\gamma_1 - \gamma_2 + o(1)}{\epsilon} \right) \]

where, as before
\[ \gamma_1 = \inf_{\varphi \in AC([0, T]), \varphi(0) = x_0} \left\{ \int_0^T \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 \, ds + g(\varphi) \right\}, \]

and \( \gamma_2 \) is now given by (at least when \( v \) is smooth),
\[ \gamma_2 = \inf_{\varphi \in AC([0, T]), \varphi(0) = x_0} \left\{ \int_0^T L(s, \varphi(s), \dot{\varphi}(s)) \, ds + 2g(\varphi) \right\} \]

where
\[ L(t, x, \beta) = \| \sigma^{-1}(x)(\beta - b(x)) \|^2 \]
\[ - \frac{1}{2} \| \sigma^{-1}(x)(\beta - b(x) - \sigma(x) v(t, x)) \|^2 \]

We want to choose the \( v \) that makes \( \gamma_2 \) as large as possible.
If we want \( R^{\epsilon} \approx 1 \) we had better have that \( \gamma_2 = 2\gamma_1 \). Such an estimator is called \textbf{log-efficient}.

Note: log-efficiency only implies that \( R^{\epsilon} \sim e^{o(1)/\epsilon} \).

We’ll see that it is possible to do much better.
The common “optimal twist” method corresponds to the choice

\[ v(t, x) = \sigma(x)^{-1}(\dot{\varphi}_{0,x_0}(t) - b(x)) \]

where

\[ \hat{\varphi}_{0,x_0} \in \arg \min_{\varphi \in AC([0,T])} \left\{ \int_0^T \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 \, ds + g(\varphi) \right\} . \]

In this case

\[ \hat{X}^\epsilon(t) = \hat{\varphi}_{0,x_0}(t) + \sqrt{\epsilon} \int_0^t \sigma(X^\epsilon(s)) \, dW(s), \]

One can think of \( \hat{\varphi}_{0,x_0} \) as the most likely path of \( X^\epsilon \) (in the small \( \epsilon \) limit) when all possible trajectories are reweighted by \( e^{-\frac{1}{\epsilon}g(\cdot)} \).

Unfortunately this method is typically not even log-efficient.
The common “optimal twist” method corresponds to the choice

\[ \nu(t, x) = \sigma(x)^{-1}(\dot{\phi}_0, x_0(t) - b(x)) \]

where

\[ \hat{\phi}_0, x_0 \in \arg \min_{\varphi \in AC([0, T]), \varphi(0)=x_0} \left\{ \int_0^T \frac{1}{2} \|\sigma^{-1}(\dot{\varphi} - b)\|^2 \, ds + g(\varphi) \right\} . \]

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Unfortunately this method is typically not even log-efficient.
Focusing on the case that $g(\varphi) = g(\varphi(T))$, consider the function
\[ \Phi^\epsilon(t, x) = \mathbb{E}_{t,x} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(T))} \right]. \]

It’s easy to see that the importance sampling estimator of $\mathbb{E}_{0,x_0} \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(T))} \right] = \Phi^\epsilon(0, x_0)$ with
\[ \nu^\epsilon = -\epsilon \frac{\sigma^T \Phi^\epsilon_x}{\Phi^\epsilon} \]
has zero variance, i.e. $R^\epsilon = 1$.

$\Phi^\epsilon$ solve a linear second order parabolic PDE with terminal condition $\Phi^\epsilon(T, x) = e^{-\frac{1}{\epsilon} g(x)}$.

Of course there’s no hope of finding a global solution of the PDE in more than a few dimensions.
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Of course there’s no hope of finding a global solution of the PDE in more than a few dimensions.
Instead we’ll consider the $\epsilon \to 0$ limit of the log transform of $\Phi^\epsilon$,

$$G^\epsilon = -\epsilon \log \Phi^\epsilon$$

which solves the second order Hamilton-Jacobi Equation

$$-G_t^\epsilon - bG_x^\epsilon + \frac{1}{2} \left( \sigma^T G_x^\epsilon \right)^2 - \frac{\epsilon}{2} \sigma^T G_x^\epsilon G_{xx}^\epsilon = 0, \quad G^\epsilon(T,x) = g(x)$$

In terms of $G^\epsilon$

$$v^\epsilon = -\sigma^T G_x^\epsilon.$$ 

So we can set

$$v^0 = -\sigma^T G_x$$

where $G$ is the viscosity solution of

$$-G_t - bG_x + \frac{1}{2} \left( \sigma^T G_x \right)^2 = 0, \quad G(T,x) = g(x)$$

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$$v^\epsilon = -\sigma^T G^\epsilon_x.$$ 

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$$-G_t - bG_x + \frac{1}{2} \left( \sigma^T G_x \right)^2 = 0, \quad G(T, x) = g(x)$$

and hope for the best.
$G$ has the control representation

$$G(t, x) = \inf_{\varphi \in AC([t, T]), \varphi(t) = x} \left\{ \int_{t}^{T} \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 ds + g(\varphi(T)) \right\}.$$  

Notice that $\gamma_1 = G(0, x_0)$.

$G$ is the rate appearing in the Laplace Principle.

Furthermore, where $G$ is differentiable,

$$b(t, x) + \sigma(t, x) V^0(t, x) = \dot{\hat{\varphi}}_{t, x}(t)$$

where

$$\hat{\varphi}_{t, x} = \arg \min_{\varphi \in AC([t, T]), \varphi(t) = x} \left\{ \int_{t}^{T} \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b) \|^2 ds + g(\varphi(T)) \right\}.$$
For $\nu^0$ we have that

$$d\hat{X}^\epsilon(t) = \hat{\phi}_{t,\hat{X}^\epsilon(t)} dt + \sqrt{\epsilon} \sigma(\hat{X}^\epsilon(t)) dW(t).$$

An analogue of this estimator, in a discrete time setup, first appears in


for problems in which one can compute $G$ by hand.

**Our approach:** Solve the optimization problem for $\hat{\phi}_{t,\hat{X}^\epsilon(t)}$ on-the-fly at each point along the trajectory of $\hat{X}^\epsilon$.

This procedure can be carried out at reasonable cost and, as we prove, the estimator has very favorable error properties.
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This procedure can be carried out at reasonable cost and, as we prove, the estimator has very favorable error properties.
Illustration of vanishing error:

\[ X^\epsilon = \sqrt{\epsilon} \, W, \quad x_0 = 0.1 \]

Estimate \( E \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(1))} \right] \) where \( g(x) = \begin{cases} \frac{1}{2} (1-x)^2, & x \geq 0, \\ \frac{1}{2} (1+x)^2, & x < 0. \end{cases} \)

<table>
<thead>
<tr>
<th>( \epsilon )</th>
<th>standard MC ( R^\epsilon )</th>
<th>optimal twist ( R^\epsilon )</th>
<th>new ( R^\epsilon )</th>
<th>our estimate</th>
<th>( E \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(1))} \right] )</th>
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<td>( 0.1666 \times 10^{-5} )</td>
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\( M = 10^9 \)
What happens at the discontinuities of $\nu^0$?

$$X^\epsilon = \sqrt{\epsilon} \ W, \quad x_0 = 0$$

Estimate $E \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(1))} \right]$ where $g(x) = \begin{cases} \frac{1}{2} (1 - x)^2, & x \geq 0, \\ \frac{1}{2} (1 + x)^2, & x < 0. \end{cases}$

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<th>new $R^\epsilon$</th>
<th>our estimate</th>
<th>$E \left[ e^{-\frac{1}{\epsilon} g(X^\epsilon(1))} \right]$</th>
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</table>

$M = 10^9$
Theoretical Issues:

For any chosen discretization scheme

\[ \text{relative error} \approx \sqrt{\text{statistical error} + \text{relative bias}} \]

For the Euler discretization we prove

**Theorem**

*If G is smooth on \([0, T]\), then*

\[ \text{statistical error} \sim O \left( \frac{\Delta}{\epsilon} \right) + O \left( \epsilon \right) \quad \text{and} \quad \text{relative bias} \sim O \left( \frac{\Delta}{\epsilon} \right) \]

*If G is smooth on \([0, T)\), then*

\[ \text{statistical error} \sim C + O \left( \frac{\Delta}{\epsilon} \right) + O \left( \epsilon \right) \quad \text{and} \quad \text{relative bias} \sim O \left( \frac{\Delta}{\epsilon} \right) \]

One can decrease the step size \(\Delta\) algebraically with \(\epsilon\) instead of exponentially.
A nontrivial test problem:

\[ u_t^\varepsilon = \nu u_{xx}^\varepsilon - \frac{1}{\nu} V'(u^\varepsilon) + \sqrt{\varepsilon} \eta \]

where \( \eta \) is a space-time white noise, \( \nu > 0 \) is a small parameter, and

\[ V(u) = (1 - u^2)^2. \]

The deterministic equation has two steady states:

\[ u_- \approx -1 \quad \text{and} \quad u_+ \approx +1 \]
We’ll try to approximate

\[ p^\varepsilon = P \left( \int_0^1 u^\varepsilon(T, x) \, dx \geq 0 \right) \]

A classic paper by Faris and Jona-Lasinio shows that the Large Deviations action functional for \( u^\varepsilon \) is

\[ I(u) = \int_0^T \int_0^1 \left( u_t - \nu u_{xx} + \frac{1}{\nu} V'(u) \right)^2 \, dx \, dt, \]

i.e. that

\[ -\varepsilon \log p^\varepsilon \longrightarrow \inf_{u: u(0, \cdot) = u_-} \inf_{\int_0^1 u(T, x) \, dx \geq 0} I(u). \]
Outline of a continuation strategy:

1. Compute the first few local minimizers of $I(u)$ for the initial state $\hat{X}^\varepsilon(0) = u_-$ with time horizon $T$.
2. Compute $v^0(0, \hat{X}^\varepsilon(0))$ using the local minimizer with lowest value of $I(u)$.
3. Compute $\hat{X}^\varepsilon(\triangle)$.
4. Using the local minimizers computed in step 1 as initial conditions find new local minimizers given the state $\hat{X}^\varepsilon(\triangle)$ and a time horizon of $T - \triangle$.
5. ...
We track each local min by continuation and assume that the global minimizer is one of these local min.

<table>
<thead>
<tr>
<th>number of local min tracked</th>
<th>relative error</th>
<th>our estimate</th>
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<td>2</td>
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<tr>
<td>3</td>
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</tr>
<tr>
<td>4</td>
<td>0.28</td>
<td>$9.462 \times 10^{-9}$</td>
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</tbody>
</table>

$M = 100$, $\nu = 0.05$, and $\epsilon = 0.1$
Revisiting the optimal twist

If we assume that the initial condition is $N\left(a, \frac{1}{\epsilon} \Gamma \Gamma^T\right)$, the Large Deviations rate functional becomes

$$F(\varphi) = \frac{1}{2} \| \Gamma^{-1}(\varphi(0) - a) \|^2 + \int_0^T \frac{1}{2} \| \sigma^{-1}(\dot{\varphi} - b(\varphi)) \|^2 \, ds + g(\varphi)$$

If $F$ is convex then the optimal twist is log-efficient.

Is this convexity reasonable for weather/climate data assimilation problems?

Note that this doesn’t require that the predictive distribution is log-convex.
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If $\mathcal{F}$ is convex then the optimal twist is log-efficient.

Is this convexity reasonable for weather/climate data assimilation problems?

Note that this doesn’t require that the predictive distribution is log-convex.
Incorporating optimal twist in ensemble schemes

For example we could

1. Approximate the current posterior distribution by an $N(a, \Gamma \Gamma^T)$.
2. Minimize $\mathcal{F}$.
3. Generate samples using the control found in step 2 and calculate the first few moments of the next posterior.
4. Weight and resample (as in a particle filter) or transform the samples (as in an ensemble Kalman filter).
5. Set $a$ to be the new posterior mean and $\Gamma \Gamma^T$ to be the new covariance matrix... repeat.