Importance sampling for a multiscale diffusion

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SAMSI

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Problem of interest

Where we want to end up.

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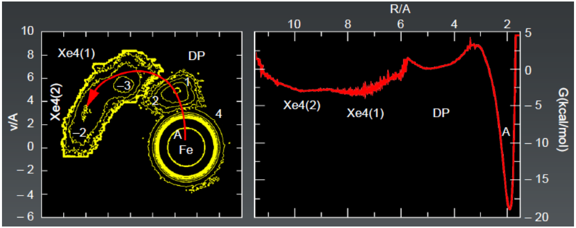
Where we want to end up. Good Monte Carlo estimators to calculate transition probabilities for complex dynamics, e.g., diffusion with drift given by the potential



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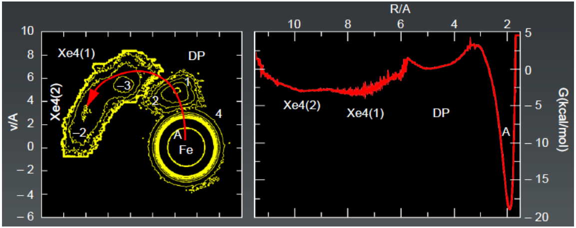

This talk concerns estimators based on change-of-measure, i.e., *importance sampling*.

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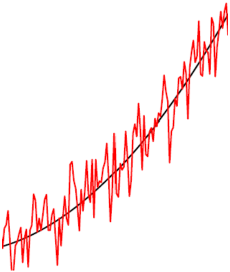

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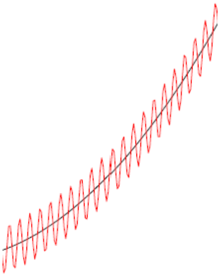
Local model 2: Fast oscillating periodic function, superimposed on slowly varying surface



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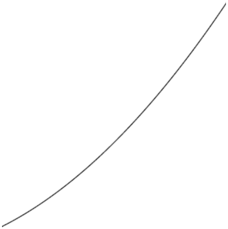
Local model 3: Slowly varying surface



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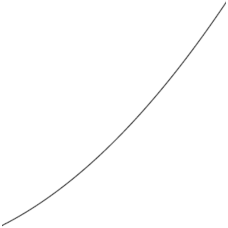

Methodology–there is a PDE/subsolutions approach that can be applied to this model. Can it be adapted to the previous models?

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Answers:

- Yes, numerically and theoretically, to fast oscillating periodic function.

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- Yes, numerically and theoretically, to fast oscillating periodic function.
- Yes numerically, but not yet theoretically, to fast oscillating ergodic random field.
- Nothing attempted yet with original problem

Outline

1. Process model and main assumptions
2. Large deviation theory for periodic model
3. Importance sampling and subsolutions
4. Formal extension to ergodic coefficients

Process model and assumptions

We consider a diffusion with multiple spatial scales:

$$dX^{\varepsilon,\delta} = \left[\frac{\varepsilon}{\delta} b\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right) + c\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right)\right] dt + \sqrt{\varepsilon}\sigma\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right) dW.$$

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Three different limiting behaviors are possible, depending on

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This talk focuses on $\varepsilon/\delta \to \infty$: averaging or homogenization first, then small noise (see reference for other cases).

Process model and assumptions

An important special case:

$$dX^{\varepsilon,\delta} = \left[-\frac{\varepsilon}{\delta}\nabla Q\left(\frac{X^{\varepsilon,\delta}}{\delta}\right) - \nabla S\left(X^{\varepsilon,\delta}\right)\right] dt + \sqrt{2\varepsilon}\, dW,$$

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where S is a slowly varying potential and Q is periodic or ergodic random field. What is a simpler approximating model? Consider 1-D. Since $\varepsilon/\delta \to \infty$ and $\delta \to 0$, by rescaling time the occupation measure

$$\theta^{\varepsilon,\delta}(A) = \frac{1}{\Delta} \int_0^{\Delta} \delta_{X^{\varepsilon,\delta}(s)/\delta}(A) ds$$

is approximately the invariant distribution associated with generator

$$\mathcal{L}f(y) = -\nabla Q(y) \cdot \nabla f(y) + \nabla^2 f(y), \quad y \in [0, \lambda]$$

and periodic b.c.'s, which is

$$\mu(dy) = \frac{1}{L} e^{-Q(y)} dy, \quad L = \int_0^{\lambda} e^{-Q(y)} dy.$$

Process model and assumptions

Let $\xi(y)$ solve

$$\mathcal{L}\xi(y) = -\nabla Q(y), \quad \int_0^\lambda \xi(y)\mu(dy) = 0,$$

which turns out here to be

$$\xi(y) = \frac{1}{\hat{L}} \int_0^y e^{Q(r)} dr \quad \hat{L} = \int_0^\lambda e^{Q(y)} dy.$$

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Recall

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Then by Itô applied to $G(y) = y + \delta\xi(y/\delta)$, we get

$$\begin{aligned} X^{\varepsilon,\delta}(t) - x &= -\int_0^t \left[1 + \xi \left(\frac{X^{\varepsilon,\delta}}{\delta} \right) \right] \nabla S \left(X^{\varepsilon,\delta} \right) dt \\ &\quad + \sqrt{2\varepsilon} \int_0^t \left[1 + \xi \left(\frac{X^{\varepsilon,\delta}}{\delta} \right) \right] dW + \text{small}. \end{aligned}$$

Process model and assumptions

Since

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suggests the approximating process

$$d\bar{X}^{\varepsilon} = r\left(\bar{X}^{\varepsilon}\right) dt + \sqrt{\varepsilon} q\left(\bar{X}^{\varepsilon}\right)^{1/2} dW,$$

with

$$r(x) = -\nabla S(x) \int_0^{\lambda} [1 + \xi(y)]\, \mu(dy), \quad q(x) = \int_0^{\lambda} 2\,[1 + \xi(y)]^2\, \mu(dy).$$

Process model and assumptions

More precisely

$$d\bar{X}^{\varepsilon} = -\frac{\lambda^2}{L\hat{L}}\nabla S\left(\bar{X}^{\varepsilon}\right)dt + \sqrt{\varepsilon}\sqrt{\frac{\lambda^2}{L\hat{L}}2}dW, \quad \hat{L} = \int_0^{\lambda} e^{Q(y)}dy.$$

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By Hölder

$$\lambda^2 = \left(\int_0^{\lambda} dy\right)^2 < L\hat{L},$$

i.e., slower drift and less diffusive.

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3. Let $\mathbb{T}^d$ be the d-dimensional torus and for smooth $f : \mathbb{T}^d \to \mathbb{R}$

$$\mathcal{L}_x f(y) = \langle b(x, y), Df(y)\rangle + \frac{1}{2}\text{tr}\left[\sigma(x, y)\sigma^T(x, y)D^2 f(y)\right]$$

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with periodic boundary conditions. Let $\mu(dy|x)$ be the associated invariant probability. Then the "centering"

$$\int_{\mathbb{T}^d} b(x,y)\mu(dy|x) = 0$$

holds, and a C^2 solution to the "cell problem" exists:

$$\mathcal{L}_x \xi_\ell(x,y) = b(x,y), \quad \int_{\mathbb{T}^d} \xi_\ell(x,y)\mu(dy|x) = 0, \quad \ell = 1,\dots,d.$$

Large deviation theory

The large deviation theory for

$$dX^{\varepsilon,\delta} = \left[\frac{\varepsilon}{\delta} b\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right) + c\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right)\right] dt + \sqrt{\varepsilon}\sigma\left(X^{\varepsilon,\delta}, \frac{X^{\varepsilon,\delta}}{\delta}\right) dW.$$

for all limits

$$\frac{\varepsilon}{\delta} \to \begin{cases} 0 \\ c \in (0,\infty) \\ \infty \end{cases} \quad \text{as } \varepsilon \to 0 \text{ and } \delta \to 0$$

is developed in

- Large deviations for multiscale diffusions via weak convergence methods (D. and K. Spiliopoulos), to appear in *SPA*.

Large deviation theory

While proofs technical, result for $\varepsilon/\delta \to \infty$ motivated by letting $\delta \to 0$ first. Then $X^{\varepsilon,\delta} \to \bar{X}^{\varepsilon}$ in distribution,

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with

$$\begin{aligned} r(x) &= \int_{\mathbb{T}^d} \left(I + \frac{\partial \xi}{\partial y}(x,y) \right) c(x,y)\mu(dy|x) \\ q(x) &= \int_{\mathbb{T}^d} \left(I + \frac{\partial \xi}{\partial y}(x,y) \right) \sigma(x,y)\sigma^T(x,y) \left(I + \frac{\partial \xi}{\partial y}(x,y) \right)^T \mu(dy|x) \end{aligned}$$

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Theorem. The large deviation behaviors of $X^{\varepsilon,\delta}$ and $\bar{X}^{\varepsilon}$ are the same.

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$$\mathbb{P}\left[\frac{X^{\varepsilon,\delta}(\Delta) - X^{\varepsilon,\delta}(0)}{\Delta} \approx \beta \,\middle|\, X^{\varepsilon,\delta}(0) = x \right] \approx \exp -\frac{\Delta}{\varepsilon} L(x,\beta).$$

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Then (Boué-D)

$$L(x,\beta)\approx\inf\left\{E\frac{1}{\Delta}\int_0^\Delta\|v\|^2:\hat{X}^{\varepsilon,\delta}(\Delta)\approx x+\Delta\beta\right\},$$

where $\hat{X}^{\varepsilon,\delta}(0)=x$ and

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$$v(t) = -\sigma\left(x, \frac{\hat{X}^{\varepsilon,\delta}}{\delta} \right)^T \left(I + \frac{\partial \xi}{\partial y}\left(x, \frac{\hat{X}^{\varepsilon,\delta}}{\delta} \right) \right)^T u,$$

with u constant. *Need feedback information on fast variable.*

Importance sampling and subsolutions

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3. not surprisingly, importance sampling based in the homogenized SDE is inadequate for any kind of asymptotic optimality;
4. bring in the solution to the eigenvector/eigenvalue problem used to identify homogenized problem and for large deviation analysis.

Importance sampling and subsolutions

Consider functionals such as

$$J^{\varepsilon,\delta} = \mathbb{E}\left[e^{-\frac{1}{\varepsilon}h(X^{\varepsilon,\delta}(T))}\right], \quad \bar{J}^{\varepsilon} = \mathbb{E}\left[e^{-\frac{1}{\varepsilon}h(\bar{X}^{\varepsilon}(T))}\right]$$

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Subsolutions for the homogenized problem

Associated with $\bar{X}^{\varepsilon}$ is the Hamilton-Jacobi-Bellman equation

$$U_t(x,t) + \langle \nabla U(x,t), r(x)\rangle - \frac{1}{2}\left\|q^{1/2}(x)\nabla U(x,t)\right\|^2 = 0, \quad U(x,T) = h(x),$$

and $-\varepsilon \log \bar{J}^{\varepsilon} \to U(x_0, 0)$.

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and $-\varepsilon \log \bar{J}^{\varepsilon} \to U(x_0,0)$. Let V be a subsolution of the equation, i.e.,

$$V_t(x,t) + \langle \nabla V(x,t), r(x)\rangle - \frac{1}{2}\left\|q^{1/2}(x)\nabla V(x,t)\right\|^2 \geq 0, \quad V(x,T) \leq h(x),$$

Importance sampling and subsolutions

Let $u_2(x,t) = -q^{1/2}(x)\nabla V(x,t)$, simulate

$$d\bar{Y}^{\varepsilon} = r\left(\bar{Y}^{\varepsilon}\right)dt + q\left(\bar{Y}^{\varepsilon}\right)u_2(\bar{Y}^{\varepsilon},t) + \sqrt{\varepsilon}q\left(\bar{Y}^{\varepsilon}\right)dW,$$

and use samples

$$e^{-\frac{1}{\varepsilon}h(\bar{Y}^{\varepsilon}(T))}\frac{dP^x}{dP^y}(\bar{Y}^{\varepsilon}) \quad \text{in place of} \quad e^{-\frac{1}{\varepsilon}h(\bar{X}^{\varepsilon}(T))}.$$

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One has the decay rate

$$\liminf_{\varepsilon\to 0}\varepsilon\log\mathbb{E}^y\left[e^{-\frac{1}{\varepsilon}h(\bar{Y}^{\varepsilon}(T))}\frac{dP^x}{dP^y}(\bar{Y}^{\varepsilon})\right]^2 \geq -U(x_0,0) - V(x_0,0).$$

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$$e^{-\frac{1}{\varepsilon}h(\bar{Y}^{\varepsilon}(T))}\frac{dP^x}{dP^y}(\bar{Y}^{\varepsilon}) \quad \text{in place of} \quad e^{-\frac{1}{\varepsilon}h(\bar{X}^{\varepsilon}(T))}.$$

One has the decay rate

$$\liminf_{\varepsilon\to 0}\varepsilon\log\mathbb{E}^y\left[e^{-\frac{1}{\varepsilon}h(\bar{Y}^{\varepsilon}(T))}\frac{dP^x}{dP^y}(\bar{Y}^{\varepsilon})\right]^2 \geq -U(x_0,0) - V(x_0,0).$$

If $V(x_0,0) = U(x_0,0)$ then one has *logarithmic optimality*. However, analogous change of measure does **not** work for the $X^{\varepsilon,\delta}$ process.

Importance sampling and subsolutions

For $X^{\varepsilon,\delta}$ we should use

$$u_1(x,y,t) = -\sigma^T(x,y)\left(I + \frac{\partial\xi}{\partial y}(x,y)\right)^T \nabla V(x,t),$$

and simulate

$$\begin{aligned} dY^{\varepsilon,\delta} \quad = \quad & \left[\frac{\varepsilon}{\delta} b\left(Y^{\varepsilon,\delta}, \frac{Y^{\varepsilon,\delta}}{\delta}\right) + c\left(Y^{\varepsilon,\delta}, \frac{Y^{\varepsilon,\delta}}{\delta}\right)\right] dt + \sigma\left(Y^{\varepsilon,\delta}, \frac{Y^{\varepsilon,\delta}}{\delta}\right) \\ & \times \left[\sqrt{\varepsilon} dW - \sigma^T\left(Y^{\varepsilon,\delta}, \frac{Y^{\varepsilon,\delta}}{\delta}\right)\left(I + \frac{\partial\xi}{\partial y}\left(Y^{\varepsilon,\delta}, \frac{Y^{\varepsilon,\delta}}{\delta}\right)\right)^T DV(Y^{\varepsilon,\delta}, t)\right]. \end{aligned}$$

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Analogous to the *eigenfunction* appearing in importance sampling for *Markov modulated* processes. With $u_1(x,y,t)$ obtain

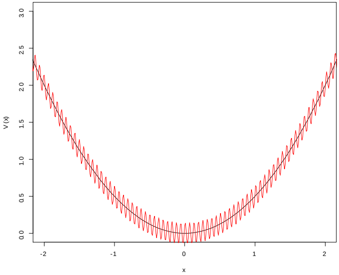
$$\liminf_{\varepsilon\to 0} \varepsilon \log \mathbb{E}^y \left[e^{-\frac{1}{\varepsilon}h(Y^{\epsilon,\delta}(T))}\frac{dP^x}{dP^y}(Y^{\epsilon,\delta}(T))\right]^2 \geq -U(x_0,0) - V(x_0,0).$$

Importance sampling and subsolutions

Numerical example

$$dX^{\varepsilon,\delta} = \left[-\frac{\varepsilon}{\delta}\nabla Q\left(\frac{X^{\varepsilon,\delta}}{\delta}\right) - \nabla S\left(X^{\varepsilon,\delta}\right)\right]dt + \sqrt{\varepsilon}\sqrt{C}dW,$$

$$S(x) = \frac{x^2}{2}, \quad Q(y) = \cos y + \sin y, \quad h(x) = (|x|-1)^2.$$



Importance sampling and subsolutions

No.	ε	δ	ε/δ	$\hat{\theta}_1(\varepsilon,\delta)$	$\hat{\rho}_0(\varepsilon,\delta)$	$\hat{\rho}_1(\varepsilon,\delta)$	$\hat{\rho}_2(\varepsilon,\delta)$
1	0.25	0.1	2.5	$2.25e-01$	1	6	20
2	0.125	0.04	3.125	$3.65e-02$	3	6	5
3	0.0625	0.015625	4	$8.75e-04$	34	4	13
4	0.03125	0.007	4.46	$6.87e-07$	141	3	105
5	0.025	0.004	6.25	$1.61e-08$	217	2	97
6	0.02	0.002	10	$1.99e-10$	1294	1	157
7	0.015	0.0013	11.54	$1.37e-13$	800	1	588

where

$$\hat{\rho}_i(\varepsilon,\delta) \approx \frac{\text{Estimated standard deviation of one sample}}{\theta(\varepsilon,\delta)},$$

and $i=0$ means ordinary Monte Carlo, $i=1$ subsolution with correction, $i=2$ subsolution and no correction.

Formal extension to ergodic coefficients

Consider model

$$dX^{\varepsilon,\delta} = \left[-\frac{\varepsilon}{\delta} \nabla Q \left(\frac{X^{\varepsilon,\delta}}{\delta} \right) - \nabla S \left(X^{\varepsilon,\delta} \right) \right] dt + \sqrt{\varepsilon} \sqrt{C} dW,$$

assume Q is stationary, ergodic, and a.s. C^2 and bounded.

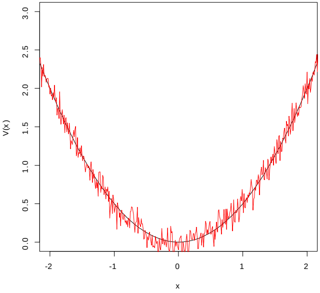
Formal extension to ergodic coefficients

Consider model

$$dX^{\varepsilon,\delta} = \left[-\frac{\varepsilon}{\delta} \nabla Q \left(\frac{X^{\varepsilon,\delta}}{\delta} \right) - \nabla S \left(X^{\varepsilon,\delta} \right) \right] dt + \sqrt{\varepsilon}\sqrt{C} dW,$$

assume Q is stationary, ergodic, and a.s. C^2 and bounded. E.g., $S(x) = x^2/2$ and $Q(y)$ zero mean Gaussian with

$$\mathbb{E}\left[Q(y_1)Q(y_2)\right] = e^{-|y_1 - y_2|^2}.$$



Formal extension to ergodic coefficients

Then save that

$$\int_{\mathbb{T}} e^{-\frac{Q(y)}{C}} dy, \int_{\mathbb{T}} e^{\frac{Q(y)}{C}} dy \quad \text{replaced by} \quad \mathbb{E}\left[e^{-\frac{Q(y)}{C}}\right], \mathbb{E}\left[e^{\frac{Q(y)}{C}}\right],$$

one expects it to go through as before, with

$$u_1(y) = \sqrt{2} e^{\frac{Q(y)}{C}} \Big/ \sqrt{C} \mathbb{E}\left[e^{\frac{Q(y)}{C}}\right], \quad u_2 = \sqrt{2} \Big/ \sqrt{C \mathbb{E}\left[e^{-\frac{Q(y)}{C}}\right] \mathbb{E}\left[e^{\frac{Q(y)}{C}}\right]}.$$

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We look at estimating $\mathbb{P}\left\{X^{\varepsilon,\delta} \text{ hits } 0.8 \text{ before } 0.0 | X^{\varepsilon,\delta}(0) = 0.1\right\}$.

No.	ε	δ	ε/δ	$\hat{\theta}_1(\varepsilon,\delta)$	$\hat{\rho}_0(\varepsilon,\delta)$	$\hat{\rho}_1(\varepsilon,\delta)$	$\hat{\rho}_2(\varepsilon,\delta)$
1	0.25	0.1	2.5	$1.38e-1$	3	0.5	3
2	0.125	0.04	3.125	$1.31e-2$	7	16	8
3	0.0625	0.018	3.472	$6.13e-4$	36	18	42
4	0.05	0.01	5	$2.30e-5$	212	28	316
5	0.04	0.007	5.72	$5.93e-6$	396	75	332
6	0.025	0.004	6.25	$7.82e-10$	–	22	1856

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