Variance Reduction for Diffusions

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Outline

Try to understand the Monte Carlo method from a mathematical viewpoint.

U is a given energy function and π the probability with density proportional to $e^{-U(x)}$. To sample from π a usually used diffusion is the time reversible Langevin equation with π as equilibrium measure

$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}W_t - \nabla U(X_t)\,\mathrm{d}t, \quad (1)$$

where (W_t) is a Brownian motion.

Markov processes (chains), regarded as 'conceptual algorithms', are used to approximate/ sample from π.

How to evaluate the approximation?
Define comparison criteria depending on various purposes.

Asymptotic variance, spectral gap, variational norm, the second-largest eigenvalue in absolute value (spectral radius)(*).

Worst-case analysis, average-case analysis, uniform analysis.

Perturbing the reversible diffusion by adding an antisymmetric drift term results in

$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}W_t - \nabla U(X_t)\,\mathrm{d}t + C(X_t)\,\mathrm{d}t, \tag{2}$$

where the vector field C is weighted divergence-free with respect to π, i.e., $\mathrm{div}(Ce^{-U}) = 0$. This ensures that the non-reversible diffusion also has equilibrium π. That there are many ways to choose such a perturbation C, such as taking $C = Q\nabla U$ for an antisymmetric matrix Q. Note that, in any case, it is unnecessary to know the normalization constant for π.

Let $-L$ (we use the sign convention to make L positive) denote the infinitesimal generator of (1). Formally

$$L = -\Delta + \nabla U \cdot \nabla$$

This process is reversible, which amounts to saying that L is symmetric in $\mathcal{L}^2(\pi)$, the space of square-integrable complex functions with respect to π.

On the other hand, the generator of the modified equation is given by $-L_C$, where

$$L_C = L - C \cdot \nabla.$$

It has the adjoint $L_C^* f = L^* f + \mathrm{div}(fC)$. Hence, to ensure that the diffusion (2) also has π as its invariant measure, it is necessary to assume that $L_C^* \pi = 0$, i.e., $\mathrm{div}(Ce^{-U}) = 0$. In [H., Hwang-Ma, Sheu 2005] it is shown therein that L_C has a larger spectral gap than L, which is just a way to say that the irreversible algorithm performs better than the reversible one.

The spectral gap measures the exponential rate in the convergence of the distribution of (X_t) to π. The comparison of these algorithms in terms of asymptotic variance rather measures the speed of convergence of the *average* of $f(X_t)$ to the mean $\int f \, \mathrm{d}\pi$.

Let us explain our motivation and results. Assume that $(X_t)_{t \geq 0}$ is an ergodic Markov process with equilibrium measure π. Let $\mathcal{L}^2(\pi)$ be the space of functions which are square-integrable with respect to π, with inner product $\langle \cdot, \cdot \rangle_\pi$. Denote by $-G$ the generator of (X_t) in $\mathcal{L}^2(\pi)$, with domain $\mathcal{D}$. Take $f \in \mathcal{L}^2(\pi)$ and assume that there is a solution $h \in \mathcal{D}$ to the Poisson equation

$$Gh = f. \tag{3}$$

Then a central limit theorem holds:

$$\sqrt{t}\left(\frac{1}{t}\int_0^t f(X_s)\,\mathrm{d}s - \int f\,\mathrm{d}\pi\right) \overset{(d)}{\to} \mathcal{N}(0, \sigma^2(f)),$$

where

$$\sigma^2(f) = 2\langle f, h\rangle_\pi \tag{4}$$

is called the asymptotic variance (associated with f),Chapter 2 of [Komorowski, Landim, Olla 2012]. This explains why the asymptotic variance is a natural gauge of the efficiency of the Monte-Carlo algorithm. Finite state case was studied in [Frigessi, H, Younes 1992], [Chen, Chen, H, Pai 2012], [Chen, H 2013].

We prove that, in the sense of asymptotic variance, the irreversible diffusion (2) converges to equilibrium faster than (1). More precisely, if $\sigma_C^2(f)$ and $\sigma_0^2(f)$ denote the corresponding asymptotic variances, then under mild conditions,

$$\sigma_C^2(f) \le \sigma_0^2(f). \tag{5}$$

This amounts to proving that

$$\langle L_C^{-1} f, f \rangle_\pi \le \langle L^{-1} f, f \rangle_\pi, \tag{6}$$

and that is merely a result on operators.

First we provide conditions on operators for (6) to hold. Under mild conditions the diffusions (1) and (2) are well-behaved, that the CLT holds, and that their generators enjoy properties that ensure (6).

We characterize the cases of equality in (5), study the worst-case analysis, and finally the behavior of $\sigma_C^2(f)$ when the amplitude of the drift grows, as was done in [Franke, Hwang, Pai, Sheu 2010] for the spectral gap.

Consider a *complex* Hilbert space $\mathcal{H}$ with an inner product $\langle \cdot, \cdot \rangle$, and a self-adjoint operator T with domain $\mathcal{D}$. Let $\sigma(T) \subset \mathbb{R}$ be its spectrum.

1. For any bounded Borel function $\phi : \sigma(T) \to \mathbb{C}$, one can define the bounded operator $\phi(T)$, and $\phi \mapsto \phi(T)$ is an algebra homomorphism.
2. For any $v \in \mathcal{H}$, there exists a Borel measure μ_v, called the spectral measure associated with v, such that for any bounded Borel function $\phi : \sigma(T) \to \mathbb{C}$,

$$\langle v, \phi(T)(v) \rangle = \int_{\sigma(T)} \phi(s)\, \mu_v(\mathrm{d}s).$$

In particular $\mu_v(\sigma(T)) = \langle v, v \rangle$.

We want to establish inequality (6) under the general assumptions **(G1)**, **(G2)** and **(G3)** below. This result says that, formally, adding an antisymmetric perturbation to a reversible Markov process decreases the asymptotic variance. It however relies on fine properties of the generators, which are usually hard to check.

We obviously want to consider real functions. Hence, we fix a *real* Hilbert space $\mathcal{H}$ with an inner product $\langle \cdot, \cdot \rangle$. Take S to be an (unbounded) operator on $\mathcal{H}$ with domain $\mathcal{D}$, A be another operator whose domain contains $\mathcal{D}$, and let $S_A = S + A$ (with domain $\mathcal{D}$).

(G1) S is symmetric and positive, and A is antisymmetric;

(G2) S is a bijection from $\mathcal{D}$ onto $\mathcal{H}$ with a bounded inverse;

(G3) S_A and S_{-A} are bijections from $\mathcal{D}$ onto $\mathcal{H}$.

Theorem (2.1)

*Assume **(G1)**, **(G2)** and **(G3)**. Then, for any $f \in \mathcal{H}$,*

$$\langle S_A^{-1} f, f \rangle \le \langle S^{-1} f, f \rangle.$$

The proof of this result is essentially computation. The goal of our assumptions, however, is to obtain nice properties for some operators which allow to rigorously justify that computation.

Although we work with real functions, however, the spectrum of our operators lies in the complex plane. Consider $\mathcal{H}_{\mathbb{C}}$ the complexification of $\mathcal{H}$, with inner product still written $\langle \cdot, \cdot \rangle$. The inner product is taken to be sesquilinear on the left to have the same convention as in Volume I of [Reed, Simon]. The domain and range of the operators are complexified accordingly with the same notations for both spaces.

- S is a symmetric bijection from $\mathcal{D}$ onto $\mathcal{H}_{\mathbb{C}}$;
- S^{-1} is a bounded self-adjoint bijection from $\mathcal{H}_{\mathbb{C}}$ onto $\mathcal{D}$;
- $V = S^{-1/2}$ is a bounded self-adjoint bijection from $\mathcal{H}_{\mathbb{C}}$ onto $\mathcal{R} = V(\mathcal{H}_{\mathbb{C}})$;
- the restriction of V to $\mathcal{R}$ is a bijection onto $\mathcal{D}$.

Define

$$B = iVAV$$

with domain $\mathcal{R}$. Since V is symmetric and A antisymmetric,

$$B^* \supset -i(V)^* A^* (V)^* \supset -iV(-A)V = B,$$

so that B is symmetric. The main reason for **(G3)** is that it allows to prove the much stronger following result.

Lemma (2.1)

The operator B is essentially self-adjoint.

Informally a formula for $S_A^{-1} = (S+A)^{-1}$ is

$$
\begin{aligned}
(S+A)^{-1} &= \left(S^{1/2}(I + S^{-1/2}AS^{-1/2})S^{1/2}\right)^{-1} \\
&= S^{-1/2}(I + VAV)^{-1}S^{-1/2} \\
&= V(I - iB)^{-1}V.
\end{aligned}
$$

Lemma (2.2)

We have the equality

$$S_A^{-1} = V(I - iB)^{-1}V.$$

The essential point for the proof of Theorem (2.1) is the following computation.

Let $f \in \mathcal{H}$ (not $\mathcal{H}_{\mathbb{C}}$) and $g = Vf$. Let μ_g be the spectral measure of B associated with g. By Lemma (2.2)

$$\begin{aligned}
\langle S_A^{-1} f, f \rangle &= \langle V(I - iB)^{-1} Vf, f \rangle \\
&= \langle (I - iB)^{-1} g, g \rangle \\
&= \int_{\sigma(B)} \frac{1}{1 - iy} \mu_g(\mathrm{d}y) \\
&= \int_{\sigma(B)} \frac{1 + iy}{1 + y^2} \mu_g(\mathrm{d}y) \\
&= \int_{\sigma(B)} \frac{1}{1 + y^2} \mu_g(\mathrm{d}y),
\end{aligned}$$

where the last inequality is justified by the fact that we consider real quantities, or alternatively that μ_g is symmetric. Finally,

$$\int_{\sigma(B)} \frac{1}{1+y^2} \mu_g(\mathrm{d}y) \leq \int_{\sigma(B)} 1 \ \mu_g(\mathrm{d}y)$$
$$= \mu_g(\sigma(B)) = \langle g, g \rangle = \langle Vf, Vf \rangle = \langle S^{-1} f, f \rangle.$$

Theorem (2.1) follows.

We now apply the results in the previous section to the generators of the diffusions (1) and (2) on a space M: either $M = \mathbb{R}^d$, or M is a smooth compact connected d-dimensional Riemannian manifold with the following assumptions.

(A1) $U : M \to \mathbb{R}$ is C^2 and $C : M \to M$ is C^1;

(A2) $\int_M e^{-U(x)}\,\mathrm{d}x < \infty$;

(A3) $\mathrm{div}(Ce^{-U}) = 0$.

To simplify, in the manifold case, we will even assume

(A1') $U : M \to \mathbb{R}$ and $C : M \to M$ are smooth.

In the compact manifold case, there is no issue with explosion of the diffusion, or boundedness of the functions considered, and that is all we shall assume. On $\mathbb{R}^d$, we will need certain growth conditions on U and C.

The norm of $\mathcal{L}^2(\pi)$ is denoted by $\|\cdot\|_\pi$ and the inner product by

$$\langle f, g\rangle_\pi = \int_M \bar{f} g \,\mathrm{d}\pi.$$

For $m \geq 0$, $\mathcal{H}^m(\pi)$ is the completion of C_c^∞ with respect to

$$\langle f, g\rangle_{\mathcal{H}^m(\pi)} = \sum_{|a| \leq m} \langle \partial_a f, \partial_a g\rangle_\pi.$$

For any subspace $\mathcal{X}$ of $\mathcal{L}^2(\pi)$, we set

$$\mathcal{X}_0 = \left\{ f \in \mathcal{X}, \int f \,\mathrm{d}\pi = 0 \right\}.$$

Let us define

$$L = -\Delta + \nabla U \cdot \nabla \tag{7}$$

and

$$L_C = L - C \cdot \nabla. \tag{8}$$

With well-chosen domains they are operators on $\mathcal{L}^2(\pi)$. In any case for $f, g \in C_c^\infty$,

$$\langle Lf, g\rangle_\pi = \langle \nabla f, \nabla g\rangle_\pi = \langle f, Lg\rangle_\pi \tag{9}$$

and

$$\langle C \cdot \nabla f, g\rangle_\pi = -\langle f, C \cdot \nabla g\rangle_\pi. \tag{10}$$

On $\mathbb{R}^d$ we make the following extra growth assumptions on U and C:

(A4) for all $\varepsilon > 0$, there is a $c_\varepsilon > 0$ such that

$$|C \cdot \nabla U| + |D^2 U| \leq \varepsilon |\nabla U|^2 + c_\varepsilon,$$

where $D^2 U$ is the Hessian matrix of U and $|\cdot|$ is any norm;

(A5) there is a constant K such that

$$|C| \leq K(|\nabla U| + 1);$$

(A6) as $x \to \infty$,

$$|\nabla U(x)| \to \infty.$$

The assumptions are similar to those in [Lunadi 1997], [Metafune, Prüss, Rhandi, Schnaubelt 2005].

Theorem (3.1)

*Assume **(A1)**, **(A2)**, **(A3)** , **(A4)**, **(A5)**. Then the following hold.*

1. *Equation (2) has a unique strong solution, and this solution is not explosive.*
2. *The measure π is its unique invariant distribution.*
3. *The generator of (2) on $\mathcal{L}^2(\pi)$ is $-L_C$, with domain $\mathcal{H}^2(\pi)$.*

Theorem (3.2)

*Assume **(A1)**, **(A2)**, **(A3)**, **(A4)**, **(A5)**, **(A6)**. Then L_C is onto $\mathcal{L}^2(\pi)_0$, and for $f \in \mathcal{L}^2(\pi)_0$ and $h \in \mathcal{H}^2(\pi)$ such that $L_C h = f$:*

$$t^{-1/2} \int_0^t f(X_s)\,\mathrm{d}s$$

converges weakly to a normal variable $r.v.$ with mean zero, variance

$$\sigma_C^2(f) = 2\langle f, h\rangle_\pi.$$

And adding an antisymmetric drift reduces the asymptotic variance, that is for all $f \in \mathcal{L}^2(\pi)_0$,

$$\sigma_C^2(f) \le \sigma_0^2(f).$$

For simplicity assume that U and C are smooth. Let

$$\mathcal{W}^2(\pi) = \left\{ f \in \mathcal{H}^1(\pi),\ Lf \in \mathcal{L}^2(\pi) \right\}.$$

Operators L, $C \cdot \nabla$ and L_C make sense as unbounded operators on $\mathcal{L}^2(\pi)$, with domain $\mathcal{W}^2(\pi)$.

Theorem (3.3)

*Assume **(A1')**, **(A2)**, **(A3)**. Then the following hold.*

1. *Equation (2) has a unique strong solution.*
2. *The measure π is its unique invariant distribution.*
3. *The generator of (1) on $\mathcal{L}^2(\pi)$ is given by $-L$, with domain $\mathcal{W}^2(\pi)$.*
4. *The generator of (2) on $\mathcal{L}^2(\pi)$ has a domain containing $\mathcal{W}^2(\pi)$, and is equal to $-L_C$ on $\mathcal{W}^2(\pi)$.*

Theorem (3.4)

*Assume **(A1')**, **(A2)**, **(A3)**. Then L_C is onto $\mathcal{L}^2(\pi)_0$, and for $f \in \mathcal{L}^2(\pi)_0$ and $h \in \mathcal{H}^2(\pi)$ such that $L_C h = f$,*

$$t^{-1/2} \int_0^t f(X_s)\,\mathrm{d}s$$

converges weakly to a normal $r.v.$ with mean zero, variance

$$\sigma_C^2(f) = 2\langle f, h\rangle_\pi.$$

And adding an antisymmetric drift reduces the asymptotic variance, that is for all $f \in \mathcal{L}^2(\pi)_0$,

$$\sigma_C^2(f) \le \sigma_0^2(f).$$

We have shown that for any $f \in \mathcal{L}^2(\pi)_0$,

$$\begin{aligned} \sigma_C^2(f) &= 2\int_{\sigma(B)} \frac{1}{1+y^2}\,\mu_g(dy) \\ &\le 2\int_{\sigma(B)} 1\,\mu_g(dy) = 2\|g\|_\pi^2 = 2\|L^{-1/2}f\|_\pi^2 = \sigma^2(f), \end{aligned} \tag{11}$$

where $B = iL^{-1/2}(C\cdot\nabla)L^{-1/2}$, $g = L^{-1/2}f$, and μ_g is the spectral measure of B associated with the vector g. We will derive more detailed results concerning the variance reduction.

Let us first give a condition for equality in (11).

Corollary (4.1)

Under the assumptions of Theorem 3.2 (resp. Theorem 3.4), we have $\sigma_C^2(f) = \sigma^2(f)$ *if and only if* $f \in L(\mathrm{Ker}(C \cdot \nabla))$. *In particular,* $\sigma_c^2(f) < \sigma_0^2(f)$ *for all nonzero* $f \in \mathcal{L}^2(\pi)_0$ *when* $C \cdot \nabla$ *is injective on* $\mathcal{H}^2(\pi)_0$ *(resp.* $\mathcal{W}^2(\pi)_0$*).*

Proof.

From (11) $\sigma_C^2(f) = \sigma^2(f)$ if and only if μ_g puts all its mass at zero, which means that $g \in \mathrm{Ker}(B)$, i.e. $C \cdot \nabla L^{-1} f = 0$, whence the first part follows. The second part only uses that L^{-1} has range $\mathcal{H}^2(\pi)_0$ (resp. $\mathcal{W}^2(\pi)_0$). □

Therefore, one would prefer a C such that $\mathrm{Ker}(C \cdot \nabla) = \{0\}$, even more considering the following results. However, we do not know how to find such a C, or even if one necessarily exists.

consider the worst-case analysis comparison

$$\sup_{\|f\|_\pi = 1} \sigma_C^2(f) \leq \sup_{\|f\|_\pi = 1} \sigma_0^2(f), \tag{12}$$

where the sup is over the real $f \in \mathcal{L}^2(\pi)_0$. The following result provides a condition such that the irreversible algorithm performs strictly better than the reversible algorithm in the worst possible situation. It is worth mentioning that this result is similar to Theorem 1 in [H, Hwang-Ma, Sheu 2005]. Let λ denote the spectral gap of L.

Theorem (4.1)

Under the assumptions of Theorem 3.2 or 3.4, if

$$\mathrm{Ker}(L-\lambda)\cap\mathrm{Ker}(C\cdot\nabla)=\{0\},$$

then

$$\sup_{\|f\|_\pi=1}\sigma_C^2(f)<\sup_{\|f\|_\pi=1}\sigma_0^2(f)=\frac{2}{\lambda}. \tag{13}$$

Theorem (4.2)

For any $f \in \mathcal{L}^2(\pi)$, $\sigma^2_{kC}(f)$ *is decreasing in* k *and* P *is the projection on* Ker B,

$$\lim_{k\to\infty} \sigma^2_{kC}(f) = 2\|PL^{-1/2}f\|^2_\pi.$$

If $\mathrm{Ker}(C \cdot \nabla) = \{0\}$, *then*

$$\lim_{k\to\infty} \sigma^2_{kC}(f) = 0.$$

If B *has a spectral gap, then*

$$\lim_{k\to\infty} \sup_{\|f\|_\pi = 1} \sigma^2_{kC}(f) = 0.$$

In [H, Hwang-Ma, Sheu 1993], for Ornstein-Uhlenbeck processes it is shown that the spectral gap needs not be increasing in k, and that the smallest spectral gap can be attained for some finite k. In [Pai, H 2013], antisymmetric perturbations of the Laplace-Beltrami operator on the torus are considered, and the authors prove that the spectral gap as a finite limit as $k \to +\infty$, but can be made arbitrarily close to 0 for well-chosen C. In [Franke, H, Pai, Sheu 2005], the limit of the spectral gap as $k \to +\infty$ is investigated, and shown to be infinite, except if a very strict condition is verified. We ignore whether the condition that B has a spectral gap in our result is restrictive.

Our results mainly provide qualitative information on the asymptotic variance, with less quantitative information due to the difficulty encountered in the manipulation of spectral measures. Of course, within the family of all possible choices of C (with unit norm, say), one would like the one that gives the smaller asymptotic variance, and maybe even the value of this lower bound. The theoretical existence and practical construction of such a perturbation C would of course be of great interest. In a similar direction, the results of Section (Extensions) show that a C with Ker$(C \cdot \nabla) = \{0\}$ is preferable. As mentioned, we do not know if such a C always exists, and, even more to the point, if it can be constructed. The same goes for finding a B with a spectral gap as in Theorem 4.2.

In the case of an Ornstein-Uhlenbeck process, where U is quadratic, it is reasonable to only consider C of the form $Q\nabla U$, for an antisymmetric matrix Q. The existence of a best C of this type is then obvious, and it would be interesting to get a closed form for it. However, one cannot have $\mathrm{Ker}(C \cdot \nabla) = \{0\}$, so that $\sigma^2_{kC}(f)$ has a positive limit as $k \to +\infty$. A closed form for this limit might shed some light on the open questions considered above.

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