

Variance reduction for irreversible Langevin samplers and diffusion on graphs*

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Abstract

In recent papers it has been demonstrated that sampling a Gibbs distribution from an appropriate time-irreversible Langevin process is, from several points of view, advantageous when compared to sampling from a time-reversible one. Adding an appropriate irreversible drift to the overdamped Langevin equation results in a larger large deviations rate function for the empirical measure of the process, a smaller variance for the long time average of observables of the process, as well as a larger spectral gap. In this work, we concentrate on irreversible Langevin samplers with a drift of increasing intensity. The asymptotic variance is monotonically decreasing with respect to the growth of the drift and we characterize its limiting behavior. For a Gibbs measure whose potential has one or more critical points, adding a large irreversible drift results in a decomposition of the process in a slow and fast component with fast motion along the level sets of the potential and slow motion in the orthogonal direction. This result helps understanding the variance reduction, which can be explained at the process level by the induced fast motion of the process along the level sets of the potential. The limit of the asymptotic variance as the magnitude of the irreversible perturbation grows is the asymptotic variance associated to the limiting slow motion. The latter is a diffusion process on a graph.

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1 Introduction

It is often the case that one is given a high dimensional distribution $\pi(dx)$, which is known only up to normalizing constants, a state space E and an observable f and the goal is to compute an integral of the form $f = \int_E f(x)\pi(dx)$. Typically, such integrals cannot be computed in closed forms, so one has to resort to approximations. What is typically done is to construct a Markov process X_t , which has π as its invariant distribution. Then under the assumption of positive recurrence, the ergodic theorem guarantees that for any $f \in L^1(\pi)$,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(X_s) ds = \int_E f(x) \pi(dx), \quad \text{a.s.}$$

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Then, the estimator $\frac{1}{t} \int_0^t f(X_s) ds$ is used to approximate the integral of interest. However, the degree of accuracy of such an approximation depends on both the choice of the Markov process X_t and on the criterion used for comparison.

Let us assume that $\pi(dx)$ is of Gibbs type on the state space E and in particular that

$$\pi(dx) = Z^{-1} e^{-\frac{U(x)}{\beta}} dx, \quad \text{where } Z = \int_E e^{-\frac{U(x)}{\beta}} dx. \quad (1.1)$$

A Markov process that has π as its invariant distribution is the time-reversible Langevin diffusion

$$dX_t = -\nabla U(X_t) dt + \sqrt{2\beta} dW_t. \quad (1.2)$$

However, as it has been argued in the literature [11, 13], it is advantageous to use appropriate irreversible diffusions of the form

$$dX_t = [-\nabla U(X_t) + C(X_t)] dt + \sqrt{2\beta} dW_t$$

and if the vector fields C satisfy $\text{div}(C e^{-U/\beta}) = 0$ or equivalently

$$\text{div} C = \beta^{-1} C \nabla U,$$

then the measure π is still invariant.

The main result of [11] is that under certain conditions the absolute value of the second largest eigenvalue of the Markov semigroup in $L^2(\pi)$ decreases when $C \neq 0$, which naturally implies faster convergence to equilibrium. In [5], the Donsker-Varadhan large deviations rate function [4] has been proposed as a natural tool to compare the convergence to equilibrium for ergodic averages and it was used to analyze parallel tempering type algorithms. In [13], this criterion is used as a guide to design and analyze non-reversible Markov processes and compare them with reversible ones. It is proven that the large deviations rate function monotonically increases under the addition of an irreversible drift. Moreover upon connecting the large deviations rate function with the asymptotic variance of the estimator, it is proven in [13], that adding a drift C also decreases the asymptotic variance of the estimator, in the sense that

$$\sigma_{f,C}^2 = \lim_{t \rightarrow \infty} t \text{Var} \left(\frac{1}{t} \int_0^t f(X_s) ds \right),$$

is smaller than the asymptotic variance with $C = 0$, i.e, smaller than $\sigma_{f,0}^2$.

The goal of the current work is to study the situation when the additional drift has the form $\frac{1}{\epsilon} C(x)$ and to consider what happens when $\epsilon \rightarrow 0$. A similar question, but from a different perspective, has been studied in [3, 6]. There, the authors studied the behavior of the spectral gap for diffusions on compact manifolds with $U = 0$ and a one-parameter families of perturbations $\frac{1}{\epsilon} C$ for some divergence free vector field C . In those papers the behavior of the spectral gap is related to the ergodic properties of the flow generated by C (for example if the flow is weak-mixing then the second largest eigenvalue tends to 0 as $\epsilon \rightarrow 0$). In the present paper we want to understand the effect that increasing $1/\epsilon$ has on the asymptotic variance and on the paths of X_t .

We find that the asymptotic variance of the estimator is monotonically decreasing in $\delta = 1/\epsilon$. Using an averaging argument, we characterize the limiting asymptotic variance as $\epsilon \downarrow 0$. Focusing on the case where the potential $U(x)$ has one or more critical points, the irreversible perturbations with a small ϵ induce a fast motion on the constant potential surface and slow motion in the orthogonal direction. Using the theory of diffusions on graphs and the related averaging principle as developed in a series of works [2, 7, 8, 9], we identify the limiting motion of the slow component. The fast motion

on constant potential surfaces decreases the variance as the phase space is explored faster. The limit of the asymptotic variance as $\epsilon \rightarrow 0$ is the asymptotic variance of a one-dimensional estimation problem on a graph, which is where the slow component of the process lives in the limit as $\epsilon \downarrow 0$.

Upon completion of this work, we became aware of the recent paper [12] where an alternative expression of the limiting asymptotic variance is provided, see also Remark 2.4. The methods of [12] are analytical and the characterization of the limiting variance is expressed as the projection to a kernel of a certain operator. Our approach provides complementary information and is dynamical since we are using an averaging principle which allows us to make direct connections with the limiting behavior of the underlying process itself, relating the limiting variance with an estimation problem on an one-dimensional graph.

The rest of the paper is organized as follows. In Section 2 we formulate the problem precisely and present our main results. The averaging problem treating the limit of the slow component of the process is discussed in Section 3. Due to the special structure of the model, one can perform explicit computations and thus derive precise results. The formula for the limit of the asymptotic variance as the perturbation grows is in Section 4. Numerical simulations illustrating the theoretical findings are in Section 5.

2 Statement of the problem and main results

The papers [3, 6, 11, 13] motivate to look at a one parameter family of irreversible drifts $\frac{1}{\epsilon}C(x)$. For this purpose, we consider the model

$$dX_t^\epsilon = \left[-\nabla U(X_t^\epsilon) + \frac{1}{\epsilon}C(X_t^\epsilon) \right] dt + \sqrt{2\beta}dW_t, \quad (2.1)$$

where $\frac{1}{\epsilon}C$ is a one-parameter family of vector fields, $\epsilon \in \mathbb{R}$ and the vector field C satisfies $\text{div}(Ce^{-U/\beta}) = 0$. As mentioned in the introduction, the invariant measure is maintained if the vector fields C satisfies $\text{div}(Ce^{-U/\beta}) = 0$, or equivalently

$$\text{div}C = \beta^{-1}C\nabla U.$$

A convenient choice, which we assume henceforth, is to pick C such that

$$\text{div}C = 0, \quad \text{and} \quad C\nabla U = 0.$$

This is not the most general choice for C , but it has the advantage that allows to choose C independently of β . A standard choice of $C(x)$ is $C(x) = S\nabla U(x)$, where S is any antisymmetric matrix. A more elaborate discussion on other possible choices of $C(x)$ can be found in [13]. The meaning of these conditions is straightforward: the flow generated by C must preserve Lebesgue measure since it is divergence-free but since U is a constant of the motion, the micro-canonical measure on the surfaces $\{U = z\}$ are preserved as well.

We assume here that the diffusion process X_t^ϵ is on a d -dimensional compact smooth manifold without boundary and that U and C are sufficiently smooth. The ergodicity of X_t^ϵ implies that the empirical measure

$$\pi_t^\epsilon \equiv \frac{1}{t} \int_0^t \delta_{X_s^\epsilon} ds,$$

converges to π almost surely as $t \rightarrow \infty$. Under our assumptions we have a large deviation principle (uniformly in the initial condition) for the family of measures π_t^ϵ , which we write, symbolically, as

$$\mathbb{P} \{ \pi_t^\epsilon \approx \mu \} \asymp \exp(-tI_{1/\epsilon}(\mu)),$$

where \asymp denotes logarithmic equivalence. (Since C is fixed we have suppressed the dependence of $I_{1/\epsilon}$ on C .) The rate function $I_{1/\epsilon}(\mu)$ quantifies the exponential rate at which the (random) measure π_t^ϵ converges to π as $t \rightarrow \infty$. It is proven in [13] (see Theorem 2.1 below) that the rate function $I_{1/\epsilon}(\mu)$ is quadratic in ϵ .

The information in $I_{1/\epsilon}(\mu)$ can be used to study the rate of convergence of observables. If $f \in \mathcal{C}(E; \mathbb{R})$ then we have the large deviation principle

$$\mathbb{P} \left\{ \frac{1}{t} \int_0^t f(X_s^\epsilon) ds \approx \ell \right\} \asymp \exp \left(-t \tilde{I}_{f,1/\epsilon}(\ell) \right),$$

where, by the contraction principle, we have

$$\tilde{I}_{f,1/\epsilon}(\ell) = \inf_{\mu \in \mathcal{P}(E)} \left\{ I_{1/\epsilon}(\mu); \int f d\mu = \ell \right\}.$$

An alternative formula for $\tilde{I}_{f,1/\epsilon}(\ell)$ is in terms of the Legendre transform of the maximal eigenvalue $\lambda(\gamma)$ of the Feynmann-Kac semigroup $T_\gamma^t h(x) = \mathbf{E}_x \left[e^{\gamma \int_0^t f(X_s^\epsilon) ds} h(X_t^\epsilon) \right]$ acting on $\mathcal{C}(E; \mathbb{R})$. For ℓ in the range of f we have

$$\tilde{I}_{f,1/\epsilon}(\ell) = \sup_{\gamma} [\gamma \ell - \lambda(\gamma)] = \hat{\gamma}(\ell) \ell - \lambda(\hat{\gamma}(\ell)) \quad \text{where} \quad \lambda'(\hat{\gamma}) = \ell. \quad (2.2)$$

For $f \in L^2(\pi)$ with $\bar{f} = \int f d\pi$ the asymptotic variance is given by, see e.g. Proposition I.V.1.3 in [1],

$$\sigma_{f,1/\epsilon}^2 = \lim_{t \rightarrow \infty} t \text{Var} \left(\frac{1}{t} \int_0^t f(X_s^\epsilon) ds \right) = 2 \int_0^\infty \mathbb{E}_\pi \left[(f(X_0^\epsilon) - \bar{f})(f(X_t^\epsilon) - \bar{f}) \right] dt$$

and, if $f \in \mathcal{C}(E; \mathbb{R})$, it is related to the rate function $\tilde{I}_{f,1/\epsilon}(\ell)$ by

$$\tilde{I}_{f,1/\epsilon}''(\bar{f}) = \frac{1}{2\sigma_{f,1/\epsilon}^2}.$$

We have the following theorem from [13].

Theorem 2.1 (Theorems 2.3, 2.4, and 2.6 of [13]). *Assume that E is a smooth connected manifold without boundary and assume that for some $\alpha > 0$, $U \in \mathcal{C}^{(2+\alpha)}(E)$ and $C \in \mathcal{C}^{(1+\alpha)}(E)$ are such that $\text{div}(Ce^{-U/\beta}) = 0$. Then π is the invariant measure of the process X_t^ϵ and the following hold.*

i. *Let $\mu(dx) = p(x)dx$ be a measure with positive density $p \in \mathcal{C}^{(2+\alpha)}(E)$. Then we have*

$$I_{1/\epsilon}(\mu) = I_0(\mu) + \frac{1}{\epsilon^2} K(\mu),$$

where the functional $K(\mu)$ is positive and strictly positive if and only if $\text{div}(p(x)C(x)) \neq 0$. It takes the explicit form

$$K(\mu) = \frac{1}{2} \int_E |\nabla \xi(x)|^2 d\mu(x),$$

where ξ is the unique solution (up to a constant) of the equation $\text{div}[p(C + \nabla \xi)] = 0$.

ii. *We have $\tilde{I}_{f, \frac{1}{\epsilon} C}(\ell) \geq \tilde{I}_{f,0}(\ell)$ and generically the inequality is strict: for $f \in \mathcal{C}^{(\alpha)}(E)$ we have $\tilde{I}_{f, \frac{1}{\epsilon} C}(\ell) = \tilde{I}_{f,0}(\ell)$ if and only if there exists G invariant under the vector field C such that*

$$\hat{\gamma}(\ell) f = \mathcal{H}(G + U),$$

where $\mathcal{H}(G + U) = e^{-(G+U)} \mathcal{L}_0 e^{G+U}$ with $\mathcal{L}_0 = \beta \Delta - \nabla U \nabla$.

iii. For the asymptotic variance we have

$$\sigma_{f,1/\epsilon}^2 \leq \sigma_{f,0}^2,$$

with strict inequality if $\tilde{I}_{f, \frac{1}{\epsilon}C}(\ell) > \tilde{I}_{f,0}(\ell)$ in a neighborhood of $\bar{f} = \int_E f(x)\pi(dx)$, but excluding \bar{f} . More generally the map $|\epsilon| \mapsto \sigma_{f, \frac{1}{\epsilon}}^2$ is a monotone increasing function and thus its limit as $\epsilon \rightarrow 0$ exists.

For notational convenience we shall write, from now on,

$$\sigma_f^2(\epsilon) = \sigma_{f, \frac{1}{\epsilon}}^2,$$

and, without loss of generality, we may and will assume that $\bar{f} = 0$. We want to characterize the behavior of the asymptotic variance as $\epsilon \downarrow 0$, namely to find $\lim_{\epsilon \downarrow 0} \sigma_f^2(\epsilon)$, and to connect it with the limiting behavior of the trajectories X_t^ϵ as $\epsilon \downarrow 0$.

Notice that we can write

$$\sigma_f^2(\epsilon) = 2 \int_0^\infty \mathbb{E}_\pi [f(X_0^\epsilon)f(X_t^\epsilon)] dt = 2 \int_E \Phi^\epsilon(x)f(x)\pi(dx),$$

where $\Phi^\epsilon(x)$ is the unique solution (up to constants) of the Poisson equation

$$-\mathcal{L}_\epsilon \Phi^\epsilon(x) = f(x), \tag{2.3}$$

with $\int_E \Phi^\epsilon(x)\pi(dx) = 0$. Here \mathcal{L}_ϵ is the infinitesimal generator of the process X_t^ϵ given by (2.1). Dissipativity of the operator \mathcal{L}_ϵ implies that

$$\sigma_f^2(\epsilon) = 2 \int_E \Phi^\epsilon(x)f(x)\pi(dx) = 2 \int_E \Phi^\epsilon(x)(-\mathcal{L}_\epsilon \Phi^\epsilon(x))\pi(dx) \geq 0.$$

It is easy to see that as $\epsilon \rightarrow 0$, the solution to (2.3) becomes constant on the stream lines of $C(x)$. In particular, if we multiply (2.3) by ϵ and then take $\epsilon \rightarrow 0$, we formally obtain that $C(x) \cdot \nabla \Phi(x) = 0$. Making this rigorous is the purpose of Sections 3 and 4. Note that this heuristic argument makes it immediately clear that for $f \in \mathcal{L}^2(\pi)$

$$\text{if } [\text{Ker}(C \cdot \nabla) = \{0\}] \implies [\sigma_f^2(0) = 0].$$

Hence, we next investigate what happens in the non-trivial case, i.e., when $\text{Ker}(C \cdot \nabla) \neq \{0\}$. Our goal is to relate the behavior of the variance as $\epsilon \rightarrow 0$ with that of the process X_t^ϵ . It turns out that as $\epsilon \rightarrow 0$, the behavior of the process X_t^ϵ can be decomposed into fast motion on the constant potential surface and slow motion in the orthogonal direction. Using averaging principle, see for example [2, 7, 8, 9], we can identify the limiting behavior of the slow component and then compute $\sigma_f^2(0) = \lim_{\epsilon \rightarrow 0} \sigma_f^2(\epsilon)$. To be more precise, the slow component of the motion can be characterized in the limit as $\epsilon \rightarrow 0$ as an one-dimensional Markov process on a graph and $\sigma_f^2(0)$ turns out to be associated with the asymptotic variance of an estimation problem on the graph itself.

The precise behavior of the process X_t^ϵ as $\epsilon \rightarrow 0$ has been investigated in [7, 9]. We will state the precise assumptions and results in Section 3. However, let us briefly review the result here. Following [9], we consider a finite graph Γ , which represents the structure of the level sets of the potential function U on E . To construct the graph we identify the points that belong to the connected components of each of the level sets of U . We assume that U has finitely many non-degenerate critical points and that each connected level set component of U contains at most one critical point. In that way, each of the domains that is bounded by the separatrices gets mapped into an edge of the graph. At the same time the separatrices gets mapped to the vertexes of Γ . In particular,

exterior vertexes correspond to minima of U , whereas interior vertexes correspond to saddle points of U . Edges of Γ are indexed by I_1, \dots, I_m . Each point on Γ is indexed by a pair $y = (z, i)$ where z is the value of U on the level set corresponding to y and i is the edge number containing y . Clearly the pair $y = (z, i)$ forms a global coordinate on Γ . Let $Q : E \mapsto \Gamma$ with $Q(x) = (U(x), i(x))$ be the corresponding projection on the graph.

Consider the process X_t^ϵ on E to be the solution to (3.3). As we describe in Section 3, the additional noise that appears in (3.3) is added for regularization reasons and the limit does not depend on it. Moreover, the additional regularizing noise is not needed if $C(x)$ generates an ergodic dynamical system with a unique invariant measure within each connected component of the level sets of U . It is proven in Theorem 2.1 of [7] and in Theorem 2.2 of [9] (if C is an Hamiltonian vector field) that the process $Q(X_t^\epsilon)$ converges to a certain Markov process on Γ with continuous trajectories, which is exponentially mixing. The precise result will be stated in Section 3, but roughly speaking it goes as follows.

Theorem 2.2 ([7, 9]). *Let us assume that Conditions 3.1, 3.2 and 3.3 hold. Then, for any $0 < T < \infty$, the process $Y_t^\epsilon = Q(X_t^\epsilon)$, where X_t^ϵ satisfies (3.3), converges weakly in $\mathcal{C}([0, T], \Gamma)$ to a Markov process, denoted by Y_t , on Γ with continuous trajectories, which is exponentially mixing.*

We remark here that the classical Freidlin-Wentzell theory, see [9], assumes that the diffusion is on \mathbb{R}^d with $\lim_{|x| \rightarrow \infty} U(x) = \infty$. But the results apply in the compact case as well.

Based on Theorem 2.2, we can then establish the limiting behavior of the asymptotic variance as $\epsilon \downarrow 0$ and then make connections to estimation problems on the graph. In particular we have the following result which is discussed and proven in Section 4.

Theorem 2.3. *Let us assume that Conditions 3.1, 3.2 and 3.3 hold and let Y_t be the continuous Markov process on the graph Γ indicated in Theorem 3.5. Let $f \in \mathcal{C}^{2+\alpha}(E)$ such that $\bar{f} = 0$. For $(z, i) \in \Gamma$, define $\hat{f}(z, i)$ to be the average of f on the graph Γ over the corresponding connected component of the level set U (see equation (3.6) for precise definition). Then, we have that $\sigma_f^2(0) = \lim_{\epsilon \rightarrow 0} \sigma_f^2(\epsilon)$, where*

$$\sigma_f^2(0) = 2 \int_0^\infty \mathbb{E}_\mu \left[\hat{f}(Y_0) \hat{f}(Y_t) \right] dt \tag{2.4}$$

and $\mu = \pi \circ \Gamma^{-1}$ is the invariant measure of the process Y on Γ .

Theorem 2.3 is proven in Section 4. It is straightforward to see that this is the asymptotic variance of an ergodic average on the graph. In particular, we have

$$\sigma_f^2(0) = \lim_{t \rightarrow \infty} t \text{Var} \left(\frac{1}{t} \int_0^t \hat{f}(Y_s) ds \right). \tag{2.5}$$

Remark 2.4. For completeness purposes, we briefly recall here the result of [12] that is related to the present situation. When the irreversible perturbation is of the form $\frac{1}{\epsilon}C$ with C chosen such that $\text{div}(Ce^{-U/\beta}) = 0$, Theorem 4.3 of [12] states that $\sigma_f^2(0) = 2P\mathcal{L}_0^{-1/2}f$. Here \mathcal{L}_0 is the infinitesimal generator of the process X_t in (1.2) and P is the projection on $\text{Ker} \left(i\mathcal{L}_0^{-1/2} (C \cdot \nabla) \mathcal{L}_0^{-1/2} \right)$.

The methods of [12] are analytical based on an analysis of the spectrum of the operator and of the related spectral measure. The methods of our paper are dynamic, formula (2.4) is derived using an averaging principle and it is valid under the constraint $\text{div}C = C\nabla U = 0$. Since the methodologies for deriving the two results are very different, one naturally obtains different equivalent expressions for the limiting asymptotic variance. It is of great interest to understand how one can go from one formulation to

the other, at least in the case $\operatorname{div}C = C\nabla U = 0$. Doing so, would then also allow one to connect the projection operators that appear in [12] with objects such as diffusions processes on graphs.

3 The averaging problem

In this section we discuss the behavior of the process X_t^ϵ as $\epsilon \downarrow 0$. Such problems have been studied in [2, 8, 7, 9] and we recall here the results which are relevant to us. It turns out that as $\epsilon \rightarrow 0$, the behavior of the process X_t^ϵ can be decomposed into fast motion on the constant potential surface and slow motion in the orthogonal direction.

Let us consider the level set

$$d(z) = \{x \in E : U(x) = z\} \tag{3.1}$$

and denote by $d_i(z)$ the connected components of $d(z)$, i.e.,

$$d(z) = \bigcup_i d_i(z). \tag{3.2}$$

Then, we let Γ be the graph which is homeomorphic to the set of connected components $d_i(z)$ of the level sets $d(z)$. Exterior vertexes correspond to minima of U , whereas interior vertexes correspond to saddle points of U . The edges of Γ are indexed by I_1, \dots, I_m . Each point on Γ is indexed by a pair $y = (z, i)$ where z is the value of U on the level set corresponding to y and i is the edge number containing y . Clearly the pair $y = (z, i)$ forms a global coordinate on Γ . Let $Q : E \mapsto \Gamma$ with $Q(x) = (U(x), i(x))$ be the corresponding projection on the graph. For an edge I_k and a vertex O_j we write $I_k \sim O_j$ if O_j lies at the boundary of the edge I_k . We endow the tree Γ with the natural topology. It is known that Γ forms a graph with interior vertexes of order two or three, see for example [9].

Let us next consider X_t^ϵ with an additional artificial noise component in the fast dynamics, i.e.,

$$dX_t^\epsilon = \left[-\nabla U(X_t^\epsilon)dt + \sqrt{2\beta}dW_t \right] + \left[\frac{1}{\epsilon}\tilde{C}(X_t^\epsilon)dt + \sqrt{\frac{\kappa}{\epsilon}}\sigma(X_t^\epsilon)dW_t^o \right], \tag{3.3}$$

where W and W^o are independent standard Wiener processes, and we have defined

$$\tilde{C}(x) = C(x) + \frac{\kappa}{2} \sum_{j=1}^d \frac{\partial [\sigma\sigma^T(x)]_{j,i}}{\partial x_j}.$$

If $\kappa = 0$ then we get the process X_t^ϵ that we have been considering until now.

We make several technical assumptions on $C(x)$, $U(x)$ and $\sigma(x)$ in order to guarantee that the averaging principle applies. We make these assumptions in order to guarantee that the fast process has a unique invariant measure and will have U as a smooth first integral. If $\kappa = 0$ then the fast motion is the deterministic dynamical system $\dot{x}_t = C(x_t)$ and X_t^ϵ is a random perturbation of this dynamical system. For example, if d is even we can take C to be the Hamiltonian vector field $C(x) = \bar{\nabla}U(x)$. If $\kappa > 0$ we have random perturbations of diffusion processes with a conservation law. In order to guarantee the existence of a unique invariant measure for the fast dynamics we assume:

Condition 3.1. *In dimension $d = 2$, we take $\kappa \geq 0$. In dimension $d > 2$, we either assume that the dynamical system $\dot{x}_t = C(x_t)$ has a unique invariant measure on each connected component $d_i(z)$, in which case $\kappa \geq 0$, or otherwise we assume that $\kappa > 0$.*

As far as the potential function $U(x)$ and the perturbation $C(x)$ are concerned, we shall assume:

Condition 3.2. *i. There exists $a > 0$ such that $U \in \mathcal{C}^{(2+a)}(E)$ and $C \in \mathcal{C}^{(1+a)}(E)$.*

ii. $\operatorname{div}C(x) = 0$ and $C(x) \cdot \nabla U(x) = 0$.

iii. U has a finite number of critical points x_1, \dots, x_m and at these points the Hessian matrix is non-degenerate.

iv. There is at most one critical point for each connected level set component of U .

v. If x_k is a critical point of U , then there exists $d_k > 0$ such that $C(x) \leq d_k|x - x_k|$.

vi. If $d = 2$ and $\kappa = 0$, then $C(x) = 0$ implies $\nabla U(x) = 0$ and for any saddle point x_k of $U(x)$, there exists a constant $c_k > 0$ such that $|C(x)| \geq c_k|x - x_k|$.

In regards to the additional artificial perturbation by the noise W_t^σ , i.e., when $\kappa > 0$, we assume:

Condition 3.3. *i. The matrix $\sigma(x)\sigma^T(x)$ is non-negative definite, symmetric with smooth entries.*

ii. $\sigma(x)\sigma^T(x)\nabla U(x) = 0$ for all $x \in E$.

iii. For any $x \in E$ such that $\xi \cdot \nabla U(x) = 0$ we have that $\lambda_1(x)|\xi|^2 \leq \xi^T \sigma(x)\sigma^T(x)\xi \leq \lambda_2(x)|\xi|^2$ where $\lambda_1(x) > 0$ if $\nabla U(x) \neq 0$ and there exists a constant K such that $\lambda_2(x) < K$ for all $x \in E$. Moreover if x_k is a critical point for U , then there are positive constants k_1, k_2 such that for all x in a neighborhood of x_k

$$\lambda_1(x) \geq k_1|x - x_k|^2, \text{ and } \lambda_2(x) \leq k_2|x - x_k|^2.$$

iv. Let $\lambda_{i,k}$ be the eigenvalues of the Hessian of $U(x)$ at the critical points x_k where $k = 1, \dots, m$ and $i = 1, \dots, d$. Then we assume that $\kappa < (K \max_{i,k} \lambda_{i,k})^{-1}$.

Obviously Condition 3.3 is relevant in the case $d > 2$ and if $C(x)$ does not generate an ergodic dynamical system (since otherwise we can just take $\kappa = 0$). In the case $\kappa > 0$, the procedure of incorporating an appropriate artificial noise in the system, allows to single out the correct averaging that should be done in the system. We remark here that the end result does not depend on the additional regularizing noise, since $\sigma(x)$ does not appear in the limiting dynamics.

It is clear that the dynamics can be decomposed in a fast component and a slow component. The fast motion corresponds to the infinitesimal generator

$$\hat{\mathcal{L}}g(x) = \tilde{C}(x)\nabla g(x) + \frac{\kappa}{2} \operatorname{tr} [\sigma\sigma^T(x)\nabla^2 g(x)] .$$

Let us write \hat{X}_t for the diffusion process that has infinitesimal generator $\hat{\mathcal{L}}$. Conditions 3.2 and 3.3 guarantee that with probability one, if the initial point of \hat{X} is in a connected component $d_i(z)$, then $\hat{X}_t \in d_i(z)$ for all $t \geq 0$. Indeed, by Itô formula we have

$$U(\hat{X}_t) = U(\hat{X}_0) + \int_0^t \hat{\mathcal{L}}U(\hat{X}_s)ds + \int_0^t \nabla U(\hat{X}_s)\sigma(\hat{X}_s)dW_s.$$

Since $C(x)\nabla U(x) = 0$ and $\sigma(x)\sigma^T(x)\nabla U(x) = 0$ we obtain with probability one $\int_0^t \hat{\mathcal{L}}(\hat{X}_s)ds = 0$. The quadratic variation of the stochastic integral is also zero, due to $\sigma(x)\sigma^T(x)\nabla U(x) = 0$, which implies that with probability one $\int_0^t \nabla U(\hat{X}_s)\sigma(\hat{X}_s)dW_s = 0$. Thus, we indeed get that for all $t \geq 0$ $\hat{X}_t \in d_i(z)$ given that the initial point belongs to the particular connected component $d_i(z)$.

Let us turn now our attention to invariant measures. Let $m(x)$ be a smooth invariant density with respect to Lebesgue measure for the process \hat{X}_t . Then, the proof of Lemma 2.3 of [7] and the fact that $t \geq 0$ $\hat{X}_t \in d_i(z)$ if $\hat{X}_0 \in d_i(z)$ imply that if $(z, i) \in \Gamma$ is not

a vertex, there exists a unique invariant measure $\mu_{z,i}$ concentrated on the connected component $d_i(z)$ of $d(z)$ which takes the form

$$\mu_{z,i}(A) = \frac{1}{T_i(z)} \oint_A \frac{m(x)}{|\nabla U(x)|} \ell(dx), \tag{3.4}$$

where $T_i(z) = \oint_{d_i(z)} \frac{m(x)}{|\nabla U(x)|} \ell(dx)$. Notice that if $(z, i) \in \Gamma$ is not a vertex, then the invariant density on $d_i(z)$ is

$$m_{z,i}(x) = \frac{m(x)}{T_i(z) |\nabla U(x)|}, \quad x \in d_i(z). \tag{3.5}$$

We remark here that in the case $\kappa > 0$, it is relatively easy to see that independently of the form of the matrix $\sigma(x)\sigma^T(x)$, the fact that $\text{div}(C) = 0$ implies that the Lebesgue measure is invariant for the diffusion process corresponding to the operator $\hat{\mathcal{L}}$. Hence, in that case any constant function is an invariant density. Also, in the case $d = 2$ and $\kappa = 0$, one immediately obtains from Condition 3.2 that $m(x) = \frac{|\nabla U(x)|}{|C(x)|}$, see Proposition 2.1 in [7].

Given a sufficiently smooth function $f(x)$, define its average over the related connected component of the level set of $U(x)$ by

$$\hat{f}(z, i) = \oint_{d_i(z)} f(x) m_{z,i}(x) \ell(dx) = \frac{1}{T_i(z)} \oint_{d_i(z)} \frac{f(x)}{|\nabla U(x)|} m(x) \ell(dx) \tag{3.6}$$

Let us consider the process $Q(X_t^\epsilon) = (U(X_t^\epsilon), i(X_t^\epsilon))$ and consider its limiting behavior. We write \mathcal{L}_0 for the infinitesimal generator of the process X_t given by (1.2). Let us set

$$\begin{aligned} \widehat{\mathcal{L}_0 U}(z, i) &= \oint_{d_i(z)} \mathcal{L}_0 U(x) m_{z,i}(x) \ell(dx) = \frac{1}{T_i(z)} \oint_{d_i(z)} \frac{\mathcal{L}_0 U(x)}{|\nabla U(x)|} m(x) \ell(dx), \\ \hat{A}(z, i) &= \oint_{d_i(z)} 2\beta |\nabla U(x)|^2 T_i(z) m_{z,i}(x) \ell(dx) = \oint_{d_i(z)} \frac{2\beta \nabla U(x) \cdot \nabla U(x)}{|\nabla U(x)|} m(x) \ell(dx) \end{aligned}$$

and then consider the one-dimensional process Y_t which within the branch I_i is governed by the infinitesimal generator

$$\mathcal{L}_i^Y g(z) = \widehat{\mathcal{L}_0 U}(z, i) g'(z) + \frac{1}{2} \frac{\hat{A}(z, i)}{T_i(z)} g''(z)$$

Within each edge I_i of Γ , $Q(X_t^\epsilon)$ converges as $\epsilon \downarrow 0$ to a process with infinitesimal generator \mathcal{L}_i^Y . In order to uniquely define the limiting process, we need to specify the behavior at the vertexes of the tree, which amounts to imposing restrictions on the domain of definition of the generator, say \mathcal{L}^Y , of the Markov process.

Definition 3.4. We say that g belongs in the domain of definition of \mathcal{L}^Y , denoted by \mathcal{D} , of the diffusion Y , if

- i. The function $g(z)$ is twice continuously differentiable in the interior of an edge I_i .
- ii. The function $z \mapsto \mathcal{L}_i^Y g(z)$ is continuous on Γ .
- iii. At each interior vertex O_j with edges I_k that meet at O_j , the following gluing condition holds

$$\sum_{k: I_k \sim O_j} \pm b_{jk} D_k g(O_j) = 0$$

where, if γ_{jk} is the separatrixes curves that meet at O_j , we have set

$$b_{jk} = \oint_{\gamma_{jk}} \frac{2\beta |\nabla U(x)|^2}{|\nabla U(x)|} m(x) \ell(dx) = 2\beta \oint_{\gamma_{jk}} |\nabla U(x)| m(x) \ell(dx).$$

Here one chooses $+$ or $-$ depending on whether the value of U increases or decreases respectively along the edge I_k as we approach O_j . Moreover D_k represents the derivative in the direction of the edge I_k .

Moreover, within each edge I_i the process Y_t is a diffusion process with infinitesimal generator \mathcal{L}_i^Y .

Consider now the process Y_t that has the aforementioned \mathcal{L}^Y as its infinitesimal generator with domain of definition \mathcal{D} , as defined in Definition 3.4. Such a process is a continuous strong Markov process, e.g., Chapter 8 of [9].

Then, for any $T > 0$, $Q(X_t^\epsilon)$ converges weakly in $\mathcal{C}([0, T]; \Gamma)$ to the process Y_t as $\epsilon \downarrow 0$. In particular, we have the following theorem.

Theorem 3.5 (Theorem 2.1 of [7]). *Let X_t^ϵ be the process that satisfies (3.3). Assume Conditions 3.1, 3.2 and 3.3. Let $T > 0$ and consider the Markov process $\{Y_t, t \in [0, T]\}$ as defined in Definition 3.4. We have*

$$Q(X^\epsilon) \rightarrow Y, \text{ weakly in } \mathcal{C}([0, T]; \Gamma), \text{ as } \epsilon \downarrow 0. \tag{3.7}$$

It is important to note that the limiting process Y_t does not depend on $\sigma(x)$. Next, we show that in our case of interest and for every $i = 1, \dots, m$, the operator \mathcal{L}_i^Y which governs the motion of the limiting process within the I_i branch of the graph takes a more explicit form. Let us denote $G_i(z) = \text{int}(d_i(z))$. Notice that by Gauss theorem we have

$$\begin{aligned} \widehat{\mathcal{L}_0 U}(z, i) &= \frac{1}{T_i(z)} \oint_{d_i(z)} \frac{\mathcal{L}_0 U(x)}{|\nabla U(x)|} m(x) \ell(dx) = \frac{1}{T_i(z)} \oint_{d_i(z)} \frac{-|\nabla U(x)|^2 + \beta \Delta U(x)}{|\nabla U(x)|} m(x) \ell(dx) \\ &= \frac{1}{T_i(z)} \left[- \int_{G_i(z)} \text{div}(m(x) \nabla U(x)) dx + \beta \oint_{d_i(z)} \frac{\Delta U(x)}{|\nabla U(x)|} m(x) \ell(dx) \right], \end{aligned}$$

and similarly

$$\widehat{A}_i(z) = \oint_{d_i(z)} \frac{2\beta \nabla U(x) \cdot \nabla U(x)}{|\nabla U(x)|} m(x) \ell(dx) = 2\beta \int_{G_i(z)} \text{div}(m(x) \nabla U(x)) dx.$$

Next, we notice that

$$\frac{d}{dz} \int_{G_i(z)} \Delta U(x) m(x) dx = \oint_{d_i(z)} \frac{\Delta U(x)}{|\nabla U(x)|} m(x) \ell(dx).$$

Hence, we can write

$$\widehat{\mathcal{L}_0 U}(z) = \frac{1}{T_i(z)} \left[- \int_{G_i(z)} \mathcal{L}_0^* m(x) dx + \frac{1}{2} \widehat{A}_i(z) \right],$$

where \mathcal{L}_0^* is the formal adjoint operator to \mathcal{L}_0 . Thus, the infinitesimal generator \mathcal{L}_i^Y , can be written equivalently as

$$\mathcal{L}_i^Y g(z) = \frac{1}{T_i(z)} \left[- \int_{G_i(z)} \mathcal{L}_0^* m(x) dx \right] g'(z) + \frac{1}{2T_i(z)} \frac{d}{dz} \left\{ \widehat{A}_i(z) g'(z) \right\}.$$

In particular, if the Lebesgue measure is the invariant measure (e.g., in the case $\kappa > 0$), then $m(x)$ is a constant. By denoting $M_i(z) = \int_{G_i(z)} \Delta U(x) dx > 0$, we can then rewrite \mathcal{L}_i^Y in the more explicit form

$$\begin{aligned} \mathcal{L}_i^Y g(z) &= - \frac{1}{T_i(z)} M_i(z) g'(z) + \frac{\beta}{T_i(z)} \frac{d}{dz} \{ M_i(z) g'(z) \} \\ &= \frac{-M_i(z) + \beta M_i'(z)}{T_i(z)} g'(z) + \beta \frac{M_i(z)}{T_i(z)} g''(z). \end{aligned}$$

4 Limiting behavior of the asymptotic variance

In this section we identify $\sigma_f^2(0) = \lim_{\epsilon \downarrow 0} \sigma_f^2(\epsilon)$ using the averaging results of Section 3. In particular, we prove the representation of Theorem 2.3.

Recall that without loss of generality we assume $\bar{f} = 0$. Our starting point is the formula

$$\sigma_f^2(\epsilon) = 2 \int_0^\infty \mathbb{E}_\pi [f(X_0^\epsilon) f(X_s^\epsilon)] ds,$$

where the process X_t^ϵ is the unique strong solution of (3.3). Standard PDE arguments, e.g., Section 3.2 of [7], show that for any point $(z, i) \in I_i$ that is not a vertex, the PDE

$$-\hat{\mathcal{L}}u(x) = f(x) - \hat{f}(U(x), i(x)), \quad \text{for } x \in d_i(z) \tag{4.1}$$

has a unique solution (up to constants) $\mathcal{C}^{2+\alpha'}$ solution with $\alpha' \in (0, \alpha)$. We fix the free constant by setting $\hat{u}(z, i) = 0$. Then, the solution $u(x)$ can be written as

$$u(x) = \int_0^\infty \mathbb{E}_x [f(\hat{X}_s) - \hat{f}(U(\hat{X}_s), i(\hat{X}_s))] ds.$$

Moreover, there exist constants $\lambda = \lambda(z, i) > 0$ such that for $x \in d_i(z)$,

$$|u(x)| \leq \frac{2}{\lambda} \sup_{x \in d_i(z)} |f(x) - \hat{f}(U(x), i(x))|. \tag{4.2}$$

Let us consider $\theta > 0$ small and for an edge I_i of the graph set

$$I_i^\theta = \{(z, i) \in I_i : \text{dist}((z, i), \partial I_i) > \theta\}$$

and define

$$\tau_i = \min\{t > 0 : Q(X_t^\epsilon) \notin I_i^\theta\}.$$

Then, by applying Itô formula to the solution of (4.1) with stochastic process X_t^ϵ one immediately gets that for any $T < \infty$, for any initial point x that does not belong to any of the separatrices of U and for every I_i

$$\lim_{\epsilon \downarrow 0} \sup_{t \in [0, T]} \mathbb{E}_x \left[\int_0^{t \wedge \tau_i} \left(f(X_s^\epsilon) - \hat{f}(U(X_s^\epsilon), i(X_s^\epsilon)) \right) ds \right] = 0, \tag{4.3}$$

uniformly in $x \in D_i(z) = \{x \in \mathbb{R}^d : Q(x) \subset \text{int}(I_i)\}$. Indeed, applying Itô formula to $u(x)$ with $x = X_s^\epsilon$, we have

$$\begin{aligned} u(X_t^\epsilon) &= u(x_0) + \int_0^t \left[-\nabla U(X_s^\epsilon) \nabla u(X_s^\epsilon) + \frac{1}{\epsilon} \hat{\mathcal{L}}u(X_s^\epsilon) + \beta \Delta u(X_s^\epsilon) \right] ds \\ &\quad + \int_0^t \sqrt{2\beta} \nabla u(X_s^\epsilon) dW_s + \sqrt{\frac{\kappa}{\epsilon}} \int_0^t \nabla u(X_s^\epsilon) \sigma(X_s^\epsilon) dW_s^o \end{aligned}$$

and recalling that $u(x)$ is solution to (4.1) we get

$$\begin{aligned} \int_0^{t \wedge \tau_i} \left(f(X_s^\epsilon) - \hat{f}(U(X_s^\epsilon), i(X_s^\epsilon)) \right) ds &= \epsilon [u(x_0) - u(X_{t \wedge \tau_i}^\epsilon)] + \epsilon \int_0^{t \wedge \tau_i} [-\nabla U \nabla u + \beta \Delta u](X_s^\epsilon) ds \\ &\quad + \epsilon \int_0^{t \wedge \tau_i} \sqrt{2\beta} \nabla u(X_s^\epsilon) dW_s + \sqrt{\kappa \epsilon} \int_0^{t \wedge \tau_i} \nabla u(X_s^\epsilon) \sigma(X_s^\epsilon) dW_s^o. \end{aligned}$$

Taking expected value, the right hand side of this inequality goes to zero as $\epsilon \downarrow 0$, by (4.2) and because continuity of the integrands implies that Riemann integrals are bounded. Hence, the averaging result (4.3) follows immediately.

At the same time, by the results of [7, 9] the limiting process Y_t spends time of Lebesgue measure zero at the interior and exterior vertexes. For $\zeta > 0$ and for a vertex of the graph O_j , let us define

$$D_j(\pm\zeta) = \{x \in \mathbb{R}^d : U(O_j) - \zeta < U(x) < U(O_j) + \zeta\} .$$

If O_j is an exterior vertex of Γ , then for every $\eta > 0$, there exists $\zeta > 0$ such that for sufficiently small ϵ and for all $x \in D_j(\pm\zeta)$ we have that (Lemma 3.6 in [7])

$$\mathbb{E}_x \tau_j^\epsilon(\pm\zeta) < \eta ,$$

where $\tau_j^\epsilon(\pm\zeta)$ is the first exit time of X_t^ϵ from $D_j(\pm\zeta)$. The behavior for an interior vertex is similar. Lemma 3.7 of [7] implies that if O_j is an interior vertex, then for every $\eta > 0$, and for all sufficiently small $\zeta > 0$

$$\mathbb{E}_x \tau_j^\epsilon(\pm\zeta) < \eta\zeta$$

for sufficiently small ϵ and for all $x \in D_j(\pm\zeta)$. Recall now that $Q(x) = (U(x), i(x))$. Then, (4.3) and the fact that the process Y_t spends time of Lebesgue measure zero at all vertexes, imply that for any $t < \infty$

$$\begin{aligned} \lim_{\epsilon \downarrow 0} \int_0^t \mathbb{E}_\pi [f(X_0^\epsilon) f(X_s^\epsilon)] ds &= \lim_{\epsilon \downarrow 0} \int_0^t \mathbb{E}_\pi \left[f(X_0^\epsilon) \widehat{f}(U(X_s^\epsilon), i(X_s^\epsilon)) \right] ds \\ &= \lim_{\epsilon \downarrow 0} \int_0^t \mathbb{E}_\pi \left[\widehat{f}(Q(X_0^\epsilon)) \widehat{f}(Q(X_s^\epsilon)) \right] ds . \end{aligned} \tag{4.4}$$

Since, the invariant measure of X_t^ϵ is the Gibbs measure π , we have that the invariant measure of $Y_t^\epsilon = Q(X_t^\epsilon)$ and of Y_t on the graph is the projection of the Gibbs measure π on Γ . Denoting this invariant measure by μ , we have that for any Borel set $\gamma \subset \Gamma$, $\mu(\gamma) = \pi(\Gamma^{-1}(\gamma))$. Thus, by the weak convergence of Theorem 3.5 we have that for any $t < \infty$

$$\lim_{\epsilon \downarrow 0} \int_0^t \mathbb{E}_\pi [f(X_0^\epsilon) f(X_s^\epsilon)] ds = \int_0^t \mathbb{E}_\mu \left[\widehat{f}(Y_0) \widehat{f}(Y_s) \right] ds . \tag{4.5}$$

The strong Markov processes X_t^ϵ and Y_t , on E and Γ respectively, are uniform mixing. This implies that, by selecting $t > 0$ to be large enough, we can make the integrals

$$\int_t^\infty \mathbb{E}_\pi [f(X_0^\epsilon) f(X_s^\epsilon)] ds \quad \text{and} \quad \int_t^\infty \mathbb{E}_\mu \left[\widehat{f}(Y_0) \widehat{f}(Y_s) \right] ds$$

arbitrarily small. Therefore, we indeed obtain that

$$\lim_{\epsilon \rightarrow 0} \sigma_f^2(\epsilon) = \sigma_f^2(0) = 2 \int_0^\infty \mathbb{E}_\mu \left[\widehat{f}(Y_0) \widehat{f}(Y_s) \right] ds ,$$

concluding the proof of Theorem 2.3.

5 Numerical Simulations

In this section, we explore numerically the behavior of the process under growing perturbations of the drift. In the examples below we fix $\beta = 0.1$.

The first example that we study is a simple 2-dimensional example where the potential U has a single critical point. In particular, we define $U(x, y) = \frac{1}{2}x^2 + \frac{1}{2}y^2$. Let $C(x, y) = S\nabla U(x, y)$, where S is the standard 2×2 antisymmetric matrix, i.e., $S_{12} = 1$ and $S_{21} = -1$. In Figure 1, we see that the more irreversibility one adds (in the sense of increasing

the $\delta = 1/\epsilon$ parameter in the perturbation $\delta C(x, y)$, the faster the process explores the phase space. Since, it is perhaps convenient to think in terms of $1/\epsilon$ and not ϵ , we set $\delta = 1/\epsilon$.

Furthermore, notice that what the theory predicts is also shown in the numerical simulations. Namely, we observe fast motion long the level sets of the potential and slow motion in the orthogonal direction.

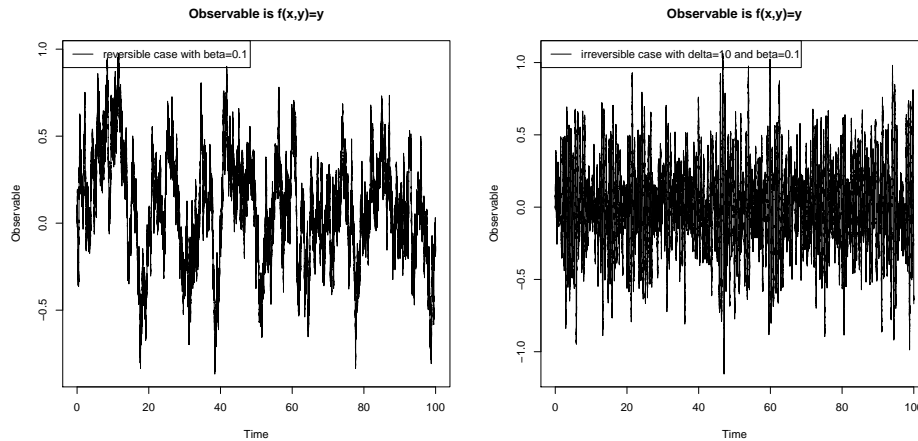


Figure 1: On the left: reversible case, i.e. $\delta = 0$. On the right: irreversible case with $\delta = 10$. In both cases $\beta = 0.1$.

Next, we consider a two-dimensional SDE with two asymptotically stable points. In particular, we define the potential $U(x, y) = \frac{1}{4}(x^2 - 1)^2 + \frac{1}{2}y^2$ and we consider growing perturbation $\delta C(x, y)$ with $C(x, y) = S\nabla U(x, y)$. Here, $\delta \in \mathbb{R}$ and S is the standard 2×2 antisymmetric matrix.

Notice that the potential function $U(x, y)$ has two local minima in $(-1, 0)$ and $(1, 0)$ and a local maximum at $(0, 0)$. In Figures 2 and 3, we plot the x -component of the (x, y) trajectory versus time. We see that the more irreversibility one adds (in the sense of increasing the δ parameter in the perturbation $\delta C(x, y)$), the faster the process moves along the level sets of the potential. As Figures 2 and 3 show, in the present case, this means faster switches between the two metastable states.

Lastly, to get a sense of the magnitude of the variance reduction, we take the observable $f(x, y) = x^2 + y^2$ (still $U(x, y) = \frac{1}{4}(x^2 - 1)^2 + \frac{1}{2}y^2$) and we use the standard batch means method, see [1], to estimate the asymptotic variance of $t^{-1} \int_0^t f(X_s) ds$, see Figure 4.

We present in Table 1, variance estimates for different values of $\delta = 1/\epsilon$ and time horizon t . These numerical values are part of the values that were used to plot Figure 4. It is clear that the variance reduction for this particular example is at the order of at least 2 magnitudes. Moreover, by Theorem 2.3, it is clear that for small $\epsilon > 0$, the variance estimate can be also considered as an approximation to the asymptotic variance of the corresponding estimation problem on the graph, see (2.5).

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Variance reduction for irreversible Langevin samplers

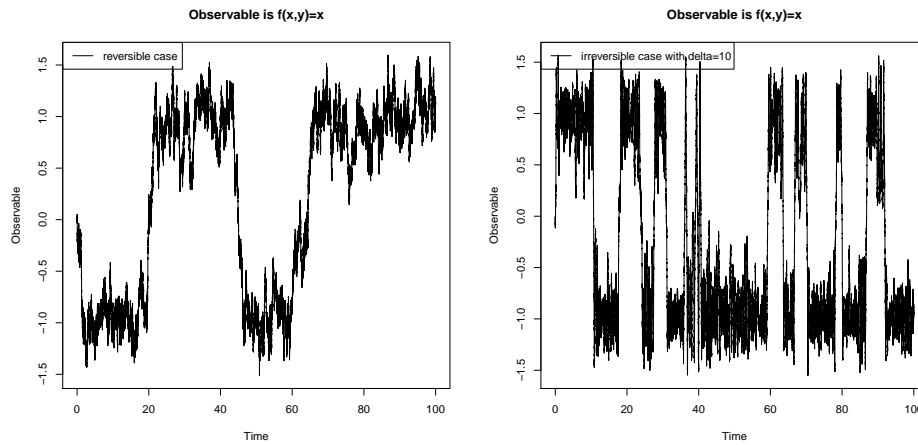


Figure 2: On the left: reversible case, i.e. $\delta = 0$. On the right: irreversible case with $\delta = 10$.

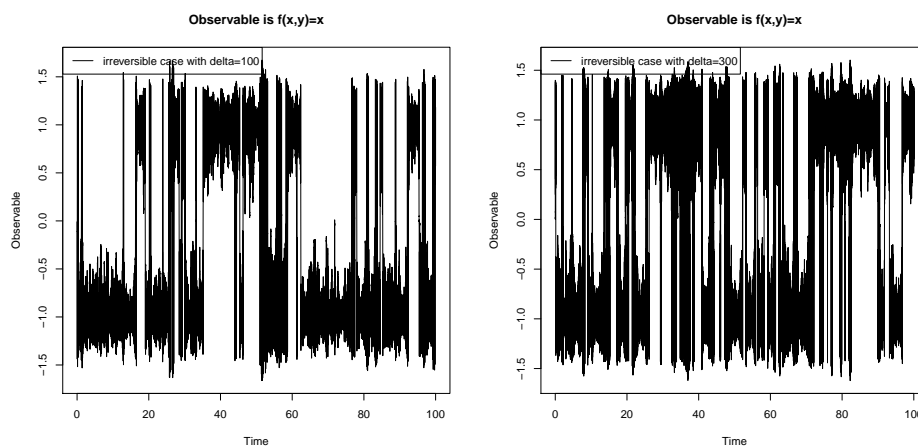


Figure 3: On the left: irreversible case with $\delta = 100$. On the right: irreversible case with $\delta = 300$.

Variance reduction for irreversible Langevin samplers

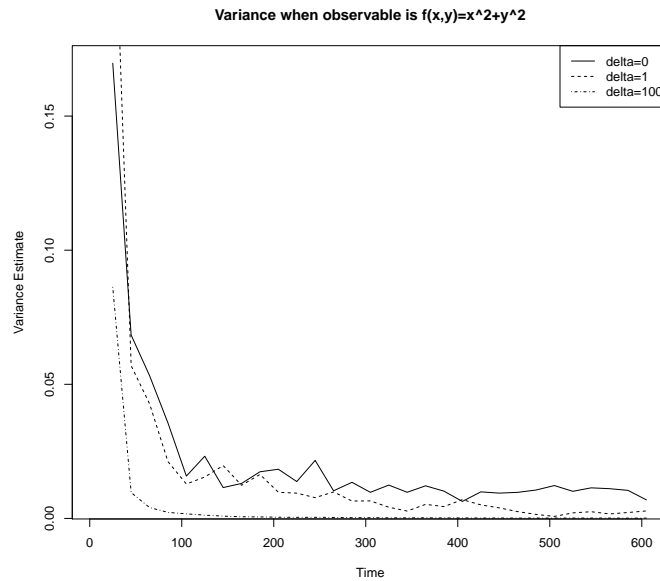


Figure 4: Variance estimator for $f(x, y) = x^2 + y^2$

$\delta \mid t$	25	100	200	300	400	500	600
0	0.16	0.015	0.018	0.010	0.006	0.012	0.007
1	0.25	0.012	0.009	0.006	0.005	0.001	0.002
100	0.09	0.002	$4e - 04$	$2e - 04$	$2e - 04$	$1e - 04$	$1e - 04$

Table 1: Estimated variance values for different pairs (δ, t) .

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