Nonasymptotic bounds for suboptimal importance sampling

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Abstract

Importance sampling is a popular variance reduction method for Monte Carlo estimation, where a notorious question is how to design good proposal distributions. While in most cases optimal (zero-variance) estimators are theoretically possible, in practice only suboptimal proposal distributions are available and it can often be observed numerically that those can reduce statistical performance significantly, leading to large relative errors and therefore counteracting the original intention. In this article, we provide nonasymptotic lower and upper bounds on the relative error in importance sampling that depend on the deviation of the actual proposal from optimality, and we thus identify potential robustness issues that importance sampling may have, especially in high dimensions. We focus on path sampling problems for diffusion processes, for which generating good proposals comes with additional technical challenges, and we provide numerous numerical examples that support our findings.

1 Introduction

The numerical approximation of expectations by the Monte Carlo method is ubiquitous in various disciplines such as quantitative finance [25, 26], machine learning [7], computational statistics [23] or statistical physics [52], to name just a few. Depending on the problem at hand, this estimation problem can be more or less difficult, but it turns out that a major challenge are potentially large statistical errors of naive sampling strategies. It is therefore a common goal to build estimators that have a small variance, as compared to the quantity of interest, and thus a small relative error. A typical situation, in which variance reduction is indispensable, is the simulation of rare events with its characteristic exponential divergence of the relative error with the parameter that controls the rarity of the quantity of interest (e.g. a level when computing level-crossing probabilities).

There are multiple strategies for variance reduction in Monte Carlo estimation [3]. In this article, we focus on importance sampling. The idea here is to sample from an alternative probability measure and reweight the resulting random variables with the likelihood ratio in order to produce an unbiased estimator for the quantity of interest. Naturally, the question arises which probability distribution to choose. In theory, under appropriate assumptions, there exists an optimal proposal that yields a zero-variance estimator and therefore removes all the stochasticity from the problem. However this measure depends on the quantity of interest and is therefore practically useless. Coming up with feasible proposals on the other hand is a science in itself, and various numerical experiments demonstrate that it is indeed a crucial one, as making bad choices can even increase the relative error of importance sampling estimators significantly, and therefore counteract the original intention. Loosely speaking, importance sampling gets increasingly difficult and sensitive to small deviations from an optimal proposal distribution if the quantity of interest is mainly supported on small regions which have little overlap with the regions of the proposal measure; such a phenomenon is more likely to appear in high dimensions. Moreover, concentration of measure, that may lead to degeneracies of likelihood ratios when the probability of certain events becomes exponentially small, is more likely to occur in high dimensions [4, 42].

To better understand the robustness (or better: fragility) of the optimal proposal in importance sampling is the main goal of this article. In applications, one often faces situations that the probability measures admit densities on a subset of \mathbb{R}^d or a function space like the space of (semi-)continuous trajectories with values in \mathbb{R}^d (called: path space). In this article, we shall put special emphasis on the latter case, specifically on diffusion processes that are particularly relevant e.g. in molecular dynamics [31], mathematical finance [25], or climate modelling [43]; what the aforementioned examples have in common, is that the quantities of interest are often related to rare events or large

deviations from a mean or an equilibrium state, and, often, the dynamics exhibits metastability, i.e. it features rare transitions between semi-stable equilibria. To simulate these systems, variance reduction techniques like importance sampling are indispensable, and we will provide quantitative bounds on the relative error that explains the fragility of importance sampling in these situations. Some of those bounds are formulated on an abstract measurable space, but they can be readily applied to the density case. For the path space measures, we deduce some additional bounds that, in particular, highlight the challenges due to high dimensionality or long trajectories.

1.1 Literature overview

Importance sampling is a classic variance reduction method in Monte Carlo simulation and introductions can be found in many textbooks, such as in [40, Section 9] or [25, 35], however, mostly for the finite-dimensional case \mathbb{R}^d . The non-robustness of importance sampling in high dimensions is well known and has often been observed in numerical experiments [6, 27, 36, 49]. Recently, the authors of [9] have proved that the sample size required for importance sampling to be accurate scales exponentially in the KL divergence between the proposal and the target measure, when accuracy is understood in the sense of the L^1 error, rather than the commonly used relative error. (Clearly, an unbounded L^1 error implies that the relative error will be unbounded.) Similar results can be found in [1], in which the authors analyze a self-normalized importance sampling estimator, in connection with inverse problems and filtering. Necessary conditions that any importance sampling proposal distribution has to satisfy have been derived in [45], using the more general f-divergences and adopting an information-theoretic perspective.

An important class of techniques for building proposal distributions is known by the name sequential importance sampling, where we recommend [15] for a comprehensive review. Closely related are methods based on interacting particle systems and nonlinear (mean-field) Feynman-Kac semigoups, in which the variance is controlled by adaptively annihilating and generating particles to approximate good proposal distributions [13]. Adaptive importance sampling for rare events simulation has been pioneered in [19, 20]; it is typically based on exponential change of measure techniques and the theory of large deviations, dating back to the seminal work [48]. For diffusion processes, large deviation principles can be used to approximate the optimal change of measure in the small noise regime, where the resulting change of measure turns out to be asymptotically optimal [51, 53]. Pre-asymptotic approximations to the optimal proposal are necessary when studying escape problems, for which the time horizon of the problem is either indefinite or infinitely large, a case that has been analysed in [18]. A non-asymptotic variant of the aforementioned approaches for finite noise diffusions is based on the stochastic control formulation of the optimal change of measure [28, 30]. Furthermore we should note that there have been many attempts to find good (low-dimensional) proposal by taking advantage of specific structures of the problem at hand, using simplified models that approximate a complicated multiscale system [17, 29, 32, 50]. Recently, the scaling properties of certain approximations to control-based importance sampling estimators with the system dimension have been analyzed in [38], suggesting that the empirical loss function that is used to numerically approximate the optimal proposal distribution is essential.

1.2 Outline of the paper

In Section 2 we define importance sampling in an abstract setting and recall the notions of divergences between proposal and target measures, while refining a bound on the relative error and highlighting robustness issues in high dimensions. In Section 3 we move to importance sampling of stochastic processes. We translate the bounds from the previous section to this setting and derive an exact formula for the relative error with which we can state novel bounds that allow for interpretations with respect to robustness in higher dimensions and long time horizons. When focusing on PDE methods in Section 3.2 we can essentially re-derive bounds from the previous section. In Section 3.3 we comment on how our bounds can help to understand potential issues in the small noise regime. Finally, in Section 4 we present a couple of numerical examples with which we illustrate the previously discussed issues. We conclude the article with Section 5 and discuss future perspectives for importance sampling in high dimensions. The article contains an appendix that records some proofs and various technical lemmas.

2 Importance sampling bounds based on divergences

Let us consider the probability space $(\Omega, \mathcal{F}, \nu)$, on which we want to compute expected values^{1,2}

$$\mathcal{Z} = \mathbb{E}\left[e^{-\mathcal{W}(X)}\right],\tag{1}$$

where X is a random variable taking values in Ω that is distributed according to the measure ν , and $\mathcal{W}: \Omega \to \mathbb{R}$ is some functional of X. Later on we will specify Ω to be either \mathbb{R}^d or the path space $C([0,T], \mathbb{R}^d)$.

The idea of importance sampling is to sample instead $\widetilde{X} \in \Omega$ from another distribution $\widetilde{\nu}$ and weight the samples back according to the corresponding likelihood ratio (or Radon-Nikodym derivative), provided that $\nu \ll \widetilde{\nu}$, namely

$$\mathcal{Z} = \mathbb{E}\left[e^{-\mathcal{W}(\tilde{X})}\frac{\mathrm{d}\nu}{\mathrm{d}\tilde{\nu}}(\tilde{X})\right].$$
(2)

One notorious intention of importance sampling is the reduction of the variance of the corresponding Monte Carlo estimator

$$\widehat{\mathcal{Z}}^{K} = \frac{1}{K} \sum_{k=1}^{K} e^{-\mathcal{W}(\widetilde{X}^{k})} \frac{\mathrm{d}\nu}{\mathrm{d}\widetilde{\nu}}(\widetilde{X}^{k}),$$
(3)

where K is the sample size and \widetilde{X}^k are i.i.d. samples from $\widetilde{\nu}$. We therefore study the relative error

$$r(\tilde{\nu}) = \frac{\sqrt{\operatorname{Var}\left(e^{-\mathcal{W}(\tilde{X})}\frac{\mathrm{d}\nu}{\mathrm{d}\tilde{\nu}}(\tilde{X})\right)}}{\mathcal{Z}},\tag{4}$$

noting that the true relative error of the estimator (3) is given by $r(\tilde{\nu})/\sqrt{K}$. It can be readily seen that choosing the optimal proposal measure $\tilde{\nu} = \nu^*$ defined via

$$\frac{\mathrm{d}\nu^*}{\mathrm{d}\nu} = \frac{e^{-\mathcal{W}}}{\mathcal{Z}} \tag{5}$$

yields an unbiased zero-variance estimator. Of course, this estimator is usually infeasible in practice, as Z is just the quantity we are after, and therefore not available. In this article, we study the relative error when using any other absolutely continuous, suboptimal proposal measure $\tilde{\nu} \neq \nu^*$. It turns out that divergences between those measures are helpful in this analysis and we therefore start by noting the equivalence of the squared relative error and the χ^2 divergence between the actual and the optimal proposal measure.

Lemma 2.1 (Equivalence with χ^2 divergence). Let $\tilde{\nu}$ be a measure that is absolutely continuous with respect to ν , let ν^* be the optimal proposal measure as defined in (5) and let $r(\tilde{\nu})$ be the relative error as in (4). Then

$$r^2(\tilde{\nu}) = \chi^2(\nu^*|\tilde{\nu}). \tag{6}$$

Proof. By using the definition of the χ^2 divergence in the first step, we compute

$$\chi^{2}(\nu^{*}|\widetilde{\nu}) = \mathbb{E}_{\widetilde{\nu}}\left[\left(\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right)^{2} - 1\right] = \mathbb{E}_{\widetilde{\nu}}\left[\left(\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right)^{2}\right] - \mathbb{E}_{\widetilde{\nu}}\left[\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right]^{2} = \operatorname{Var}_{\widetilde{\nu}}\left(\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right) = \frac{1}{\mathcal{Z}^{2}}\operatorname{Var}\left(e^{-\mathcal{W}(\widetilde{X})}\frac{\mathrm{d}\nu}{\mathrm{d}\widetilde{\nu}}(\widetilde{X})\right) = r^{2}(\widetilde{\nu}).$$

$$(7)$$

Motivated by known bounds on the χ^2 divergence, we can formulate our first statement, where we quantify the suboptimality by the Kullback-Leibler divergence between the actual and the optimal proposal measure.

¹As a remark on our notation, let us mention that we sometimes endow the expectation operator with a subscript indicating with respect to which measure the expectation is taken, e.g. \mathbb{E}_{ν} indicates that the expectation is considered with respect to the measure ν . When explicitly writing down the corresponding random variable, e.g. $\mathbb{E}[X]$, it is usually clear from the context with respect to which measure the expectation shall be understood, and we omit the subscript.

²The exponential form, e^{-W} , constrains our observable to be positive. We make this choice in order to be able to have a zero variance proposal density without additional tricks, as the optimal proposal measure ν^* defined in (5) has to be non-negative. Assuming strict positivity is convenient in order to get variational dualities that rely on logarithmic transformations, cf. [30]. An extension of importance sampling to observables with negative parts can for instance be found in [39].

Proposition 2.2 (Lower bound on relative error). Let $\mathcal{W} : \Omega \to \mathbb{R}$, let $\tilde{\nu}$ be a measure and let ν^* be the optimal proposal measure as defined in (5), then for the relative error (2) it holds

$$r(\widetilde{\nu}) \ge \sqrt{e^{\mathrm{KL}(\nu^*|\widetilde{\nu})} - 1}.$$
(8)

 \square

Proof. With Jensens's inequality we have

$$\mathrm{KL}(\nu^*|\widetilde{\nu}) = \mathbb{E}_{\nu^*} \left[\log \frac{\mathrm{d}\nu^*}{\mathrm{d}\widetilde{\nu}} \right] \le \log \mathbb{E}_{\nu^*} \left[\frac{\mathrm{d}\nu^*}{\mathrm{d}\widetilde{\nu}} \right].$$
(9)

Combining this with Lemma 2.1 yields

$$r^{2}(\widetilde{\nu}) = \mathbb{E}_{\widetilde{\nu}}\left[\left(\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right)^{2} - 1\right] = \mathbb{E}_{\nu^{*}}\left[\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}} - 1\right] \ge e^{\mathrm{KL}(\nu^{*}|\widetilde{\nu})} - 1$$
(10)

and therefore the desired statement.

Remark 2.3 (Bounds on the χ^2 divergence). In the setting of importance sampling the χ^2 divergence also appears in [10]. A bound of the χ^2 divergence that is sometimes used is $\chi^2(\nu^*|\tilde{\nu}) \ge \text{KL}(\nu^*|\tilde{\nu})$, which is essentially based on $x \le e^{x-1}$ and therefore yields a less tight bound compared to Proposition 2.2. The exponential bound we use instead can for instance be found in [16, Theorem 4] and [46, Proposition 4] in a discrete setting; here, a lower bound in terms of the total variation distance is provided as well. [24] offers a continuous version and some other helpful relations between divergences. An application of the bound to importance sampling relative errors can be found in [1] and more analysis with respect to more general f-divergences has been done in [45]. The statement should also be compared to the results in [9], where the required sample size of importance sampling is proved to be exponentially large in the KL divergence between the proposal and the target measure.

Remark 2.4 (Cross-entropy method). Note that the expression $KL(\nu^*|\tilde{\nu})$ appearing in (8) is exactly the quantity that is minimized in the so-called cross-entropy method [12, 54], which aims at approximating the optimal importance sampling proposal in a family of reference proposals.

Remark 2.5 (Exponential dependence on the dimension). We recall that the KL divergence usually gets larger with increasing state space dimension as can for instance be seen by Lemma A.6 in the appendix, implying that importance sampling is especially difficult in high dimensional settings. Another way of noting bad scaling behavior in high dimensions is motivated by [38, Proposition 5.7]. Assume³

$$\widetilde{\nu} = \bigotimes_{i=1}^{d} \widetilde{\nu}_i, \qquad \nu^* = \bigotimes_{i=1}^{d} \nu_i^*, \tag{11}$$

where each $\tilde{\nu}_i$, and ν_i^* respectively, shall be identical for $i \in \{1, \ldots, d\}$. Then

$$r^{2}(\widetilde{\nu}) = \operatorname{Var}_{\widetilde{\nu}}\left(\frac{\mathrm{d}\nu^{*}}{\mathrm{d}\widetilde{\nu}}\right) = \mathbb{E}_{\widetilde{\nu}_{i}}\left[\left(\frac{\mathrm{d}\nu^{*}_{i}}{\mathrm{d}\widetilde{\nu}_{i}}\right)^{2}\right]^{d} - \mathbb{E}_{\widetilde{\nu}_{i}}\left[\frac{\mathrm{d}\nu^{*}_{i}}{\mathrm{d}\widetilde{\nu}_{i}}\right]^{2d} = \mathbb{E}_{\widetilde{\nu}_{i}}\left[\left(\frac{\mathrm{d}\nu^{*}_{i}}{\mathrm{d}\widetilde{\nu}_{i}}\right)^{2}\right]^{d} - 1 \ge C^{d} - 1, \quad (12)$$

where $C := \mathbb{E}_{\tilde{\nu}_i} \left[\left(\frac{\nu_i^*}{\tilde{\nu}_i} \right)^2 \right] > 1$ if $\tilde{\nu} \neq \nu^*$ due to Jensen's inequality. This can be compared to [45, Section 5.2.1], and, to be fair, we should note that also naive sampling, i.e. choosing $\tilde{\nu} = \nu$, usually leads to an exponential dependency of the relative error on the dimension.

We have so far constructed a lower bound for the relative error. In order to get an upper bound, let us first state the following version of a generalized Jensen inequality, which will turn out to be helpful and is essentially borrowed from [37, Theorem 2].

Proposition 2.6 (Generalized Jensen inequality). Let λ and ν be measures on (Ω, \mathcal{F}) , let

$$J(f,\nu,\varphi) := \mathbb{E}_{\nu} \left[f(\varphi) \right] - f\left(\mathbb{E}_{\nu} \left[\varphi \right] \right)$$
(13)

be the normalized Jensen functional, where $f : \mathbb{R} \to \mathbb{R}$ is convex and $\varphi : \Omega \to \mathbb{R}$ is continuous, and let $m = \inf_{E \in \mathcal{F}} \frac{\nu(E)}{\lambda(E)}$, $M = \sup_{E \in \mathcal{F}} \frac{\nu(E)}{\lambda(E)}$. Then

$$mJ(f,\lambda,\varphi) \le J(f,\nu,\varphi) \le MJ(f,\lambda,\varphi).$$
 (14)

³The factorization of the optimal proposal measure ν^* assumes a factorization of the quantity e^{-g} .

Proof. See Appendix A.1.

We can now derive an upper bound as well as a tighter lower bound for the relative error.

Proposition 2.7 (Refined bounds on relative error). Let $\tilde{\nu}$ be a measure that is absolutely continuous with respect to ν and let ν^* be the optimal proposal measure as in (5). Let m and M be as defined in Proposition 2.6 (with the measures ν and λ being replaced by $\tilde{\nu}$ and ν^* respectively). Then for the relative error (4) it holds

$$\sqrt{e^{m \operatorname{KL}(\widetilde{\nu}|\nu^*) + \operatorname{KL}(\nu^*|\widetilde{\nu})} - 1} \le r(\widetilde{\nu}) \le \sqrt{e^{M \operatorname{KL}(\widetilde{\nu}|\nu^*) + \operatorname{KL}(\nu^*|\widetilde{\nu})} - 1}.$$
(15)

Proof. Inspired by [47] (which focuses on a discrete probability space) we choose $\nu = \nu^*, \lambda = \tilde{\nu}, \varphi = \frac{d\nu^*}{d\tilde{\nu}}$ and $f(x) = -\log(x)$ for the expressions in (14) in order to get

$$J(f,\nu^*,\varphi) = -\mathbb{E}_{\nu^*} \left[\log\left(\frac{\mathrm{d}\nu^*}{\mathrm{d}\widetilde{\nu}}\right) \right] + \log\left(\mathbb{E}_{\nu^*} \left[\frac{\mathrm{d}\nu^*}{\mathrm{d}\widetilde{\nu}}\right]\right) = -\mathrm{KL}(\nu^*|\widetilde{\nu}) + \log\left(\chi^2(\nu^*|\widetilde{\nu}) + 1\right),\tag{16}$$

$$J(f, \tilde{\nu}, \varphi) = -\mathbb{E}_{\tilde{\nu}}\left[\log\left(\frac{\mathrm{d}\nu^*}{\mathrm{d}\tilde{\nu}}\right)\right] + \log\left(\mathbb{E}_{\tilde{\nu}}\left[\frac{\mathrm{d}\nu^*}{\mathrm{d}\tilde{\nu}}\right]\right) = \mathrm{KL}(\tilde{\nu}|\nu^*).$$
(17)

With Proposition 2.6 we then get

$$m \operatorname{KL}(\widetilde{\nu}|\nu^*) + \operatorname{KL}(\nu^*|\widetilde{\nu}) \le \log\left(\chi^2(\nu^*|\widetilde{\nu}) + 1\right) \le M \operatorname{KL}(\widetilde{\nu}|\nu^*) + \operatorname{KL}(\nu^*|\widetilde{\nu})$$
(18)

and with Lemma 2.1 our statement follows.

Remark 2.8. One should note that m and M depend on $\tilde{\nu}$ and ν^* , respectively, and are hard to compute in practice. We have $m \in [0,1]$ and $M \in [1,\infty]$ and indeed it is possible to get m = 0 or $M = \infty$. The former case brings back the ordinary Jensen inequality and the lower bound from Proposition 2.7 is then equivalent to the one from Proposition 2.2. The case $M = \infty$ on the other hand yields a trivial upper bound, for which we provide an illustration in Example 2.9.

Example 2.9 (Upper bound for relative error). In order to illustrate the case where the upper bound in Proposition 2.7 becomes meaningless, consider for instance the measure ν on $[1,\infty) \subset \mathbb{R}$ admitting the one-dimensional density $p(x) = \alpha \frac{1}{x^{\alpha+1}}$ defined for $x \geq 1$.

This density is special since for $\alpha \leq 1$ we have $\mathbb{E}[X] = \infty$, however for $\alpha \in (1,2)$ it holds $\mathbb{E}[X] < \infty$, whereas still $\mathbb{E}[X^2] = \infty$ and therefore $J(x \mapsto x^2, \nu, \varphi) = \infty$ for $\varphi(x) = x$. Now Proposition 2.6 implies that the upper bound also has to be infinity. Let us illustrate this for the particular choice of the measure λ admitting the density $q(x) = 2\alpha \frac{1}{\pi^{2\alpha+1}}$. For this choice we have $J(x \mapsto x^2, \lambda, x \mapsto x) < \infty$ for $\alpha \in (1, 2)$, however we compute

$$M = \sup_{\substack{a,b \in [1,\infty]\\a \neq b}} \frac{\int_a^b p(x) \mathrm{d}x}{\int_a^b q(x) \mathrm{d}x} \ge \sup_{a \in [1,\infty)} \frac{\int_a^\infty p(x) \mathrm{d}x}{\int_a^\infty q(x) \mathrm{d}x} = \sup_{a \in [1,\infty)} \frac{\frac{1}{a^\alpha}}{\frac{1}{a^{2\alpha}}} = \sup_{a \in [1,\infty)} a^\alpha = \infty.$$
(19)

In fact Proposition 2.6 implies that one cannot not find any λ for which both $J(x \mapsto x^2, \lambda, x \mapsto x)$ and M are finite.

To conclude this section, let us illustrate our bounds by looking at a concrete example using Gaussians on $\Omega = \mathbb{R}^d$ (which should be compared to [36, Section 6]).

Example 2.10 (High-dimensional Gaussians). Suppose we want to compute $\mathbb{E}\left[e^{-\alpha \cdot X}\right]$, with a given vector $\alpha \in \mathbb{R}^d$, where $X \sim \mathcal{N}(\mu, \Sigma) =: p$ is distributed according to a multidimensional Gaussian with mean $\mu \in \mathbb{R}^d$ and covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$. Then the optimal importance sampling density is given by

$$p^*(x) = \frac{e^{-\alpha \cdot x}}{\mathcal{Z}} p(x) = \mathcal{N}(\mu - \Sigma \alpha, \Sigma).$$
(20)

If we however sample from a perturbed version

$$\widetilde{p}^{\varepsilon} := \mathcal{N}(\mu - \Sigma(\alpha + \varepsilon), \Sigma)$$
(21)

with a vector $\varepsilon \in \mathbb{R}^d$, we get the relative error

$$r(\tilde{p}^{\varepsilon}) = \frac{1}{\mathcal{Z}} \sqrt{\operatorname{Var}\left(e^{-\alpha \cdot \tilde{X}} \frac{p}{\tilde{p}^{\varepsilon}}(\tilde{X})\right)} = \sqrt{e^{\varepsilon \cdot \Sigma \varepsilon} - 1}.$$
(22)

In this particular case, the computations can be compared to the relative error of a log-normally distributed random variable, see Appendix A.3.1. Taking, for instance, $\varepsilon = (\tilde{\varepsilon}, \dots, \tilde{\varepsilon})^{\top}, \Sigma = \text{diag}(\sigma^2, \dots, \sigma^2)$ yields

$$r(\tilde{p}^{\varepsilon}) = \sqrt{e^{d\sigma^2 \tilde{\varepsilon}^2} - 1},\tag{23}$$

where we see an exponential dependence on the variance σ^2 , the squared suboptimality parameter $\tilde{\varepsilon}$ and the dimension d. This implies that, in order to control the relative error in high dimensions, any suboptimal importance sampling estimator needs about $K = \mathcal{O}(e^{d\sigma^2 \tilde{\varepsilon}^2})$ independent realisations to reach convergence. This observation is in agreement with the seminal result of Bengtsson and Bickel [4] that any importance sampling estimator for Gaussians ceases to be asymptotically efficient when $\log(K)/d \to 0$ as $K, d \to \infty$ (see also [34, Thm. 3.1]).

For this example, we can also apply the bound from Proposition 2.2, by noting that $\mathrm{KL}(p^*|\widetilde{p}^{\varepsilon}) = \frac{1}{2}\varepsilon \cdot \Sigma\varepsilon$, and get

$$r(\tilde{p}^{\varepsilon}) \ge \sqrt{e^{\frac{1}{2}\varepsilon \cdot \Sigma \varepsilon} - 1}.$$
(24)

A comparison to the exact quantity (22) reveals that this lower bound is not tight. For an application of Proposition 2.7 we note that also $\operatorname{KL}(\tilde{p}^{\varepsilon}|p^*) = \frac{1}{2} \varepsilon \cdot \Sigma \varepsilon$, however m and M are intractable. Still, it is intuitively clear that m becomes smaller and M larger, the more the two Gaussians are apart from each other.

We made the particular choice of \tilde{p}^{ε} in (21) in order to have an analogy to the path measure setting, which we will discuss in the next section. In fact, the added term $\Sigma \varepsilon$ in (21) can be compared to a constant control $\sigma \sigma^{\top} \varepsilon$ in a stochastic process as in (25), which, as will be seen in (45), yields a completely analogous expression for the relative error, noting that standard d-dimensional Brownian motion is distributed according to $W_T \sim \mathcal{N}(0, \Sigma)$ with $\Sigma = TI_{d \times d}$.

3 Importance sampling in path space

Up to now we have formulated importance sampling for measures on an abstract probability space and provided some illustrations for densities. Let us now elevate those considerations to solutions of stochastic differential equations (SDEs) of the form

$$dX_s = b(X_s, s) ds + \sigma(X_s, s) dW_s, \qquad X_t = x_{\text{init}},$$
(25)

on the time interval $s \in [t,T]$, $0 \leq t < T < \infty$. Here, $b : \mathbb{R}^d \times [t,T] \to \mathbb{R}^d$ denotes the drift coefficient, $\sigma : \mathbb{R}^d \times [t,T] \to \mathbb{R}^{d \times d}$ the diffusion coefficient, $(W_s)_{t \leq s \leq T}$ standard *d*-dimensional Brownian motion, and $x_{init} \in \mathbb{R}^d$ is the (deterministic) initial condition. Our goal is to compute expectations of the form⁴

$$\mathcal{Z} = \mathbb{E}\left[e^{-\mathcal{W}(X)}\right], \qquad \mathcal{W}(X) = \int_{t}^{T} f(X_s, s) \mathrm{d}s + g(X_T), \tag{26}$$

where $f : \mathbb{R}^d \times [0,T] \to \mathbb{R}, g : \mathbb{R}^d \to \mathbb{R}$ are given functions. We will usually fix the initial time to be t = 0, i.e. consider the SDE (25) on the interval [0,T]. For fixed initial condition $x_{\text{init}} \in \mathbb{R}^d$, let us introduce the path space

$$\mathcal{C} = C_{x_{\text{init}}}([0,T], \mathbb{R}^d) = \left\{ X : [0,T] \to \mathbb{R}^d \mid X \text{ continuous, } X_0 = x_{\text{init}} \right\},$$
(27)

equipped with the supremum norm and the corresponding Borel- σ -algebra, and denote the set of probability measures on \mathcal{C} by $\mathcal{P}(\mathcal{C})$.

As in the previous section, the idea of importance sampling is to not sample from the original path measure $\mathbb{P} \in \mathcal{P}(\mathcal{C})$ that corresponds to paths of SDE (25), but from a different measure $\mathbb{P}^u \in \mathcal{P}(\mathcal{C})$ and weight back accordingly. Just as in (2) one then gets an unbiased estimator via

$$\mathcal{Z} = \mathbb{E}\left[e^{-\mathcal{W}(X^u)}\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{P}^u}(X^u)\right],\tag{28}$$

⁴Whether with X (and r, \mathcal{Z} correspondingly) we refer to random variables in \mathbb{R}^d or solutions to SDEs should usually be clear from the context.

where the Radon-Nikodym derivative is now given by Girsanov's theorem (see Lemma A.2) and it turns out that the SDE corresponding to \mathbb{P}^{u} is just a controlled version of the original one,

$$dX_{s}^{u} = (b(X_{s}^{u}, s) + \sigma(X_{s}^{u}, s)u(X_{s}^{u}, s)) ds + \sigma(X_{s}^{u}, s) dW_{s}, \qquad X_{t}^{u} = x_{\text{init}}.$$
(29)

We think of $u : \mathbb{R}^d \times [t, T] \to \mathbb{R}^d$ as a control term steering the dynamics and note (as already hinted at by the notation) the correspondence between u and \mathbb{P}^u . As before, our quantity of interest is the relative error, which now depends on the control u:

$$r(u) = \frac{\sqrt{\operatorname{Var}\left(e^{-\mathcal{W}(X^u)}\frac{\mathrm{d}\mathbb{P}^u}{\mathrm{d}\mathbb{P}^u}(X^u)\right)}}{\mathcal{Z}}.$$
(30)

Given suitable conditions, there exists $u^* \in \mathcal{U}$ that brings (30), the relative error of the importance sampling estimator, to zero [30]. It turns out that there are multiple equivalent perspectives on the problem of finding such a u^* , for instance by solving either a (high-dimensional) Hamilton-Jacobi-Bellman PDE, a forward-backward SDE, a stochastic optimal control problem, or a conditioning of path measures – the corresponding details regarding those equivalences can for instance be found in [38]. Let us just relate to the last perspective, which claims that \mathcal{W} induces a *reweighted* path measure \mathbb{Q} on \mathcal{C} via

$$\frac{\mathrm{d}\mathbb{Q}}{\mathrm{d}\mathbb{P}} = \frac{e^{-\mathcal{W}}}{\mathcal{Z}},\tag{31}$$

assuming f and g are such that \mathcal{Z} is finite (which we shall tacitly assume from now on). It turns out that $\mathbb{Q} = \mathbb{P}^{u^*}$ and we realize that the above formula is the same as in (5).

Let us now bring an example that shall illustrate why variance reduction methods are indispensable in certain SDE settings.

Example 3.1 (Rare events of SDEs). Monte Carlo estimation gets particularly challenging when considering rare events. As a prominent example, let us consider the one-dimensional Langevin dynamics

$$dX_s = -\nabla \Psi(X_s) \, ds + \sqrt{\eta} \, dW_s, \quad X_0 = x, \tag{32}$$

with double well potential $\Psi(x) = \kappa (x^2 - 1)^2, \kappa > 0$, and noise coefficient $\eta > 0$, as illustrated in Figure 1. We suppose that the dynamics starts in the left well and choose a function g such that e^{-g} is concentrated in the right well, e.g. $g(x) = \rho(x-1)^2, \rho > 0$. We are interested in computing $\mathbb{E}[\exp(-g(X_T))|X_0 = x]$ for, say, x = -1.

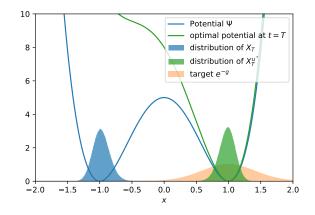


Figure 1: Illustration of rare events in a metastable double well potential. We consider the problem described in Example 3.1 with $\kappa = 5$, $\rho = 3$ on a time horizon T = 10 and display the distributions of X_T as well as $X_T^{u^*}$, which is controlled with the optimal importance sampling control u^* yielding a time-dependent optimal potential.

To understand the difficulties associated with this sampling problem, let p_T be the law of X_T for some T > 0 and recall that the optimal change of measure is given by the (unnormalized) likelihood $dq_T/dp_T \propto \exp(-g)$ that is concentrated in the right well. However, regions where $\exp(-g)$ is strongly supported have probability close to zero under p_T , for p_T drops to zero quickly for x > 0. This can be seen as follows: Let τ be the first exit time of the set $D = \{x : x \leq 0\}$. By Kramer's law [5], the mean first exit time (MFET) satisfies the large deviations asymptotics $\mathbb{E}[\tau] \asymp \exp(2\Delta\Psi/\eta)$ as $\eta \to 0$, where $\Delta\Psi$ is the energy barrier that the dynamics has to overcome to leave the set D, and it turns out that the MFET is independent of the initial condition $x \in D$. Therefore

$$\lim_{\eta \to 0} \eta \log \mathbb{P}(\tau < T) = -2\Delta \Psi, \quad T \ll \mathbb{E}[\tau],$$
(33)

which is is a straight consequence of Kramer's law, combined with the Donsker-Varadhan large deviations principle that, for a system of the form (32) states that $\mathbb{P}(\tau < T) \approx 1 - \exp(\lambda_1 T)$ as $T \to \infty$ and $\eta \to 0$, where $\lambda_1 \approx -1/\mathbb{E}[\tau]$ is the principal eigenvalue of the infinitesimal generator associated with (32); see, e.g. [8].

Now, by (33), we can conclude that $p_T(x) \approx \exp(-2\Delta\Psi/\eta)$ for x > 0. Since p_T is essentially supported on $(-\infty, 1]$, we can approximate $\exp(-g(x))$ by a step function $\mathbb{1}_{\{x\in D^c\}}$ on $x \in (-\infty, 1]$ and it thus follows that (up to an exponentially small error) the relative error for small $\eta > 0$ can be approximated by

$$r(0) = \sqrt{\frac{\mathbb{E}[\exp(-2g(X_T))] - \mathbb{E}[\exp(-g(X_T))]^2}{\mathbb{E}[\exp(-g(X_T))]^2}}$$
(34a)

$$\approx \sqrt{\frac{\exp(-2\Delta\Psi/\eta) - \exp(-4\Delta\Psi/\eta)}{\exp(-4\Delta\Psi/\eta)}} \approx \exp(\Delta\Psi/\eta) \,. \tag{34b}$$

This kind of exponential behavior is typical for rare event simulation and metastable systems like (32). So unless our terminal time T is very large or the energy barrier rather small, X_T is usually mostly supported on the left side of the well and therefore does not overlap very much with e^{-g} , which leads to an extremely large relative error. Note that this problem gets even more severe with growing values of κ and ρ .

3.1 Suboptimal control of stochastic processes and bounds for the relative error

We have stated that, given suitable conditions, there exists $u^* \in \mathcal{U}$ that brings (30), the relative error of the importance sampling estimator, to zero. However, in practice, u^* is usually not available (just as ν^* is not available in the abstract setting). Let us instead consider the setting where we have the control $u \in \mathcal{U}$ at hand. We want to investigate how the relative error (30) behaves depending on how far from optimal u is. For the upcoming analysis, it will turn out that it makes sense to measure the suboptimality and therefore the difference between \mathbb{P}^u and \mathbb{P}^{u^*} in terms of the difference $\delta := u^* - u$. The first statement is an implication of Proposition 2.2.

Corollary 3.2 (Lower bound for relative error on path space). Consider the path measures $\mathbb{P}^{u}, \mathbb{P}^{u^{*}} \in \mathcal{P}(\mathcal{C})$ as previously defined and let $\delta = u^{*} - u$. For the relative error (30) it holds

$$r(u) \ge \left(\exp\left(\mathrm{KL}(\mathbb{P}^{u^*} \mid \mathbb{P}^u)\right) - 1\right)^{\frac{1}{2}}$$
(35)

and therefore

$$r(u) \ge \left(\exp\left(\mathbb{E}\left[\frac{1}{2} \int_{0}^{T} |\delta(X_s^{u^*}, s)|^2 \mathrm{d}s \right] \right) - 1 \right)^{\frac{1}{2}}.$$
(36)

Proof. The first statement is just Proposition 2.2 with the abstract measures replaced by path measures. The second statement then follows from Girsanov's theorem as stated in Lemma A.2. \Box

One can of course also transfer the more general bound from Proposition 2.7 to path measures, however, the computations of the quantities m and M seem even more difficult and impractical than in the density case. In order to still find tighter and more applicable bounds, let us now identify an exact formula for the relative error in the SDE setting.

Proposition 3.3 (Formula for path space relative error). Let X_s^u be the solution to SDE (29) and let $\delta = u^* - u$. Then the relative error (30) is

$$r(u) = \left(\mathbb{E}\left[\exp\left(-\int_{0}^{T} |\delta(X_s^u, s)|^2 \mathrm{d}s + 2\int_{0}^{T} \delta(X_s^u, s) \cdot \mathrm{d}W_s\right) \right] - 1 \right)^{\frac{1}{2}},$$
(37)

or equivalently

$$r(u) = \left(\mathbb{E}\left[\exp\left(\int_{0}^{T} |\delta(X_{s}^{u+2\delta}, s)|^{2} \mathrm{d}s \right) \right] - 1 \right)^{\frac{1}{2}}.$$
(38)

1

Proof. The proof can be found in Appendix A.2. Alternatively, the second statement follows as well from Proposition 3.10.

Remark 3.4. We note that in formula (37) the forward process is controlled by u, whereas in (38) it is controlled by $u + 2\delta = 2u^* - u$, which of course is usually not available in practice. In the upcoming Corollary 3.6 we will see how we can still make use of the formula.

Remark 3.5. Note that Proposition 3.3 entails Corollary 3.2 since

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\right] = \mathbb{E}_{\mathbb{P}^{u^{*}}}\left[\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right] = \mathbb{E}\left[\exp\left(\frac{1}{2}\int_{0}^{T}|\delta(X_{s}^{u^{*}},s)|^{2}\mathrm{d}s + \int_{0}^{T}\delta(X_{s}^{u^{*}},s)\cdot\mathrm{d}W_{s}\right)\right]$$
(39a)

$$\geq \exp\left(\mathbb{E}\left[\frac{1}{2}\int_{0}^{T}|\delta(X_{s}^{u^{*}},s)|^{2}\mathrm{d}s\right]\right).$$
(39b)

Without the change of the measures as in (39a) we obtain

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\right] \geq \exp\left(\mathbb{E}\left[-\int_{0}^{T}|\delta(X_{s}^{u},s)|^{2}\mathrm{d}s\right]\right),\tag{40}$$

where now the process is controlled by u, however this expression has a negative sign in the exponential and is therefore rather useless. The bound

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\right] = \mathbb{E}\left[\exp\left(\int_{0}^{T}|\delta(X_{s}^{u+2\delta},s)|^{2}\mathrm{d}s\right)\right] \ge \exp\left(\mathbb{E}\left[\int_{0}^{T}|\delta(X_{s}^{u+2\delta},s)|^{2}\mathrm{d}s\right]\right)$$
(41)

on the other hand, seems more useful.

The following corollary derives bounds from the previous Proposition 3.3 that might be useful in practice.

Corollary 3.6 (Bounds for path space relative error). Let again $\delta = u^* - u$ and let us assume there exist functions $h_1, h_2: [0,T] \to \mathbb{R}$ such that

$$h_1(t) \le |\delta(x,t)| \le h_2(t) \tag{42}$$

for all $x \in \mathbb{R}^d, t \in [0,T]$, then

$$\left(\exp\left(\int_{0}^{T}h_{1}^{2}(s)\mathrm{d}s\right)-1\right)^{\frac{1}{2}} \leq r(u) \leq \left(\exp\left(\int_{0}^{T}h_{2}^{2}(s)\mathrm{d}s\right)-1\right)^{\frac{1}{2}}.$$
(43)

In particular, if

$$\widetilde{\varepsilon}_1 \le |\delta_i(x,t)| \le \widetilde{\varepsilon}_2$$
(44)

for all components $i \in \{1, \ldots, d\}$ and for all $(x, t) \in \mathbb{R}^d \times [0, T]$ with $\tilde{\varepsilon}_1, \tilde{\varepsilon}_2 \in \mathbb{R}$, then

$$\left(e^{d\tilde{\varepsilon}_1^2 T} - 1\right)^{\frac{1}{2}} \le r(u) \le \left(e^{d\tilde{\varepsilon}_2^2 T} - 1\right)^{\frac{1}{2}}.$$
(45)

Proof. Both statements follow directly from equation (38) in Proposition 3.3 by noting that the dependence on the stochastic process and therefore the expectation disappears if we consider bounds on δ that do not depend on x. Two alternative proofs of the corresponding statements can be found in Appendix A.2.

Remark 3.7. Note that bounding the suboptimality δ for all x can be a strong assumption for practical applications, as often, it might vary substantially in x. Still, even those conservative bounds often yield lower bounds that render importance sampling a very challenging endeavor. On the contrary, it seems to be hard to make x-dependent bounds on δ useful due to potentially very complex stochastic dynamics. Let us further note that the bounds in (43) imply that errors made over different points in time accumulate, i.e. it does not matter if they have been made at the beginning or the end of a trajectory and neither can they be compensated at later stages.

Another upper bound on the relative error can be derived by means of the Hölder inequality.

Proposition 3.8 (Another bound for path space relative error). Let $\delta = u^* - u$. For the relative error (29) it holds

$$r(u) \le \left(\mathbb{E}\left[\exp\left((1 + \sqrt{2})^2 \int_{0}^{T} |\delta(X_s^u, s)|^2 \mathrm{d}s \right) \right]^{\frac{1}{1 + \sqrt{2}}} - 1 \right)^{\frac{1}{2}}$$
(46)

Proof. See Appendix A.2.

Remark 3.9. Some intuition of the quality of this bound can be gained when for instance assuming that $\delta(x,t) = \varepsilon$ with a constant vector $\varepsilon = (\tilde{\varepsilon}, \ldots, \tilde{\varepsilon})^{\top} \in \mathbb{R}^d$. Then this bound yields $r(u) \leq \left(\exp\left((1+\sqrt{2})d\tilde{\varepsilon}^2 T\right)-1\right)^{\frac{1}{2}}$, which is less tight than the bound (45) in Corollary 3.6. Nevertheless the bound is useful in that it only depends on the stochastic process controlled by u, which is a known quantity.

3.2 PDE methods for the study of relative errors

Another means of studying the relativ error r(u) are partial differential equations (PDEs). We will formulate a PDE for the relative error (4), which might be helpful for future analysis and by which we can rederive bounds from the previous section.

By a slight generalization of [51], one can identify a PDE for the *u*-dependent second moment (conditioned on $X_t^u = x$),

$$M_u(x,t) = \mathbb{E}\left[e^{-2\mathcal{W}(X^u)} \left(\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{P}^u}(X^u)\right)^2 \,\middle| X_t^u = x\right],\tag{47}$$

namely

$$(\partial_t + L - \sigma u(x,t) \cdot \nabla - 2f(x,t) + |u(x,t)|^2)M_u(x,t) = 0, \qquad (x,t) \in \mathbb{R}^d \times [0,T), \qquad (48a)$$

$$M_u(x,T) = e^{-2g(x)}, \qquad x \in \mathbb{R}^d, \qquad (48b)$$

where $L = \frac{1}{2}(\sigma\sigma^{\top})(x,t): \nabla^2 + b(x,t) \cdot \nabla$ is the infinitesimal generator associated to the SDE (25).

Defining $\delta = u^* - u$, this then immediately leads to the PDE

$$\begin{aligned} (\partial_t + L + \sigma(\sigma^\top \nabla V(x,t) + \delta(x,t)) \cdot \nabla - 2f(x,t) + |\sigma^\top \nabla V(x,t) + \delta(x,t)|^2) M_u(x,t) &= 0, \\ M_u(x,T) &= e^{-2g(x)}, \end{aligned} \qquad \begin{aligned} (x,t) \in \mathbb{R}^d \times [0,T) \\ (49a) \\ M_u(x,T) &= e^{-2g(x)}, \end{aligned} \qquad \begin{aligned} x \in \mathbb{R}^d \\ (49b) \end{aligned}$$

which describes the second moment of suboptimal importance sampling. It can be shown that for $\delta = 0$, i.e. under the optimal control $u = u^*$, we recover indeed the zero-variance property of the corresponding importance sampling estimator, see Proposition A.5 in the appendix. In the following statement we construct the PDE that is relevant for the relative error r(u) and re-derive a formula that we have already seen before.

Proposition 3.10 (PDE for the relative error). Let $\delta = u^* - u$. We consider the second moment as in (47) and the conditional expectation $\psi(x,t) = \mathbb{E}\left[e^{-W(X^u)} \middle| X_t = x\right]$, then the function $h_u : \mathbb{R}^d \times [0,T] \to \mathbb{R}$ defined by

$$h_u(x,t) = \frac{M_u(x,t)}{\psi^2(x,t)},$$
(50)

solves the PDE

$$\left(\partial_t + L^{u+2\delta} + |\delta(x,t)|^2\right) h_u(x,t) = 0, \qquad (x,t) \in \mathbb{R}^d \times [0,T), \qquad (51a)$$

$$h_u(x,T) = 1, \qquad x \in \mathbb{R}^d, \tag{51b}$$

with $L^{u+2\delta} := L + \sigma(u+2\delta) \cdot \nabla$. This then implies

$$h_u(x,t) = \mathbb{E}\left[\exp\left(\int_t^T |\delta(X_s^{u+2\delta},s)|^2 \mathrm{d}s\right) \left| X_t^{u+2\delta} = x\right].$$
(52)

Proof. We plug the ansatz

$$M_u(x,t) = h_u(x,t)\psi^2(x,t) = h_u(x,t)e^{-2V(x,t)}$$
(53)

into the PDE (49a). Noting that

$$(\sigma\sigma^{\top}): \nabla^{2}(h_{u}e^{-2V}) = (\sigma\sigma^{\top}): \left(\nabla\left(\nabla h_{u}e^{-2V} - 2h_{u}\nabla Ve^{-2V}\right)\right)$$

$$(54a)$$

$$= \frac{-2V}{2}\left(\left(-\frac{1}{2}\right) - \frac{\nabla^{2}}{2}\right) + \frac{1}{2}\left(\left(-\frac{1}{2}\right) -$$

$$= e^{-2V} \left((\sigma \sigma^{\top}) : \nabla^2 h_u - 4 \sigma \sigma^{\top} \nabla V \cdot \nabla h_u + 4 h_u |\sigma^{\top} \nabla V|^2 - 2h_u (\sigma \sigma^{\top}) : \nabla^2 V \right),$$
(54b)

we get the PDE

$$-2h_u\underbrace{\left(\partial_t V + LV - \frac{1}{2}|\sigma^\top \nabla V|^2 + f\right)}_{=0} + \partial_t h_u + Lh_u - \sigma\sigma^\top \nabla V \cdot \nabla h_u + \sigma\delta \cdot \nabla h_u + |\delta|^2 h_u = 0, \tag{55}$$

from which the statement follows from the identity $u^* = -\sigma^\top \nabla V$ and a specific Hamilton-Jacobi-Bellman equation that is for instance stated in [38, Problem 2.2]. The probabilistic representation (52) follows immediately from the Feynman-Kac formula [41, Theorem 1.3.17].

Remark 3.11. First note that h_u from Proposition 3.10 is related to the relative error (30) via $r(u) = \sqrt{h_u(x,0) - 1}$. On the first glance it looks like the PDE (51) does not depend on f and g. This is of course not true and we should note that the PDE depends on u^* , which again depends on f and g. Finally, note that with (52) we recover the result (38) from Proposition 3.3.

3.3 Small noise diffusions

A prominent application of importance sampling in stochastic processes can be found in the context of small noise diffusions and rare event simulations (relating to Example 3.1, see also [17, 50, 51, 53]). We model small noises with the smallness parameter $\eta > 0$ by considering the SDEs⁵

$$dX_s^{\eta} = b(X_s^{\eta}, s) \, ds + \sqrt{\eta} \, \widetilde{\sigma}(X_s^{\eta}, s) \, dW_s, \qquad X_t^{\eta} = x_{\text{init}}, \tag{56}$$

and we want to compute quantities like

$$\psi^{\eta}(x,t) = \mathbb{E}\left[e^{-\frac{1}{\eta}\mathcal{W}(X^{\eta})} \middle| X_t^{\eta} = x\right].$$
(57)

If η gets smaller it becomes harder to estimate $\psi^{\eta}(x,t)$ via Monte Carlo methods as the variance grows exponentially in η . To be more precise, by Varadhan's lemma [14, Theorem 4.3.1], using the quantities

$$\gamma_1 := -\lim_{\eta \to 0} \eta \log \mathbb{E}\left[e^{-\frac{1}{\eta}\mathcal{W}(X^{\eta})}\right] \quad \text{and} \quad \gamma_2 := -\lim_{\eta \to 0} \eta \log \mathbb{E}\left[e^{-\frac{2}{\eta}\mathcal{W}(X^{\eta})}\right], \tag{58}$$

one gets for the relative error of the uncontrolled process

$$r(0) = \sqrt{e^{\frac{2\gamma_1 - \gamma_2 + o(1)}{\eta}} - 1},$$
(59)

⁵To be consistent with the notation from before, we could hide the smallness parameter η in the diffusion coefficient, i.e. $\sigma = \sqrt{\eta}\tilde{\sigma}$. Then the HJB equation that provides the zero variance control is $(\partial_t + \frac{\eta}{2}(\tilde{\sigma}\tilde{\sigma}^{\top}): \nabla^2 + b \cdot \nabla)V - \frac{1}{2}|\sqrt{\eta}\tilde{\sigma}\nabla V|^2 + \frac{1}{\eta}f(x,t) = 0, V(x,T) = \frac{1}{\pi}g(x)$ and the relation $V^{\eta} = \eta V$ yields HJB equation (62).

asymptotically as $\eta \to 0$. By Jensen's inequality we have $2\gamma_1 > \gamma_2$ unless \mathcal{W} is a.s. constant, but we note that even for $2\gamma_1 = \gamma_2$ the relative error explodes in the limit $\eta \to 0$. Let us again consider a controlled process

$$dX_s^{u,\eta} = (b(X_s^{u,\eta}, s) + \widetilde{\sigma}(X_s^{u,\eta}, s)u(X_s^{u,\eta}, s)) ds + \sqrt{\eta}\widetilde{\sigma}(X_s^{u,\eta}, s) dW_s, \qquad X_t^{u,\eta} = x_{\text{init}}, \tag{60}$$

and realize that the optimal importance sampling control that yields zero variance,

$$u^* = -\widetilde{\sigma}^\top \nabla V^\eta = \eta \widetilde{\sigma}^\top \nabla \log \psi^\eta, \tag{61}$$

can be computed via the HJB equation

$$\left(\partial_t + \frac{\eta}{2}(\widetilde{\sigma}\widetilde{\sigma}^{\top})(x,t):\nabla^2 + b(x,t)\cdot\nabla\right)V^{\eta}(x,t) - \frac{1}{2}|(\widetilde{\sigma}^{\top}\nabla V^{\eta})(x,t)|^2 + f(x,t) = 0, \qquad V^{\eta}(x,T) = g(x).$$
(62)

Since solving this PDE is notoriously difficult (especially in high dimensions), various approximations have been suggested that lead to estimators that enjoy log-efficiency or a vanishing relative error in the regime of a vanishing η . However, since log-efficient estimators still often perform badly in practice (as for instances discussed in [2, 27]), in [53] it is suggested to replace u^* by the vanishing viscosity approximation u^0 based on the corresponding HJB equation with $\eta = 0$:

$$u^0 = -\widetilde{\sigma}^\top \nabla V^0, \tag{63}$$

where V^0 is the solution to

$$(\partial_t + b(x,t) \cdot \nabla) V^0(x,t) - \frac{1}{2} |(\tilde{\sigma}^\top \nabla V^0)(x,t)|^2 + f(x,t) = 0, \qquad V^0(x,T) = g(x).$$
(64)

While it can be shown that, given some regularity assumptions on f and g, it holds [53]

$$\lim_{\eta \to 0} r(u^0) = 0, \tag{65}$$

a large relative error for a small, but fixed $\eta > 0$ is still possible. In our notation from before, this situation corresponds to choosing $\delta = u^* - u^0$ and Propositions 3.3 and 3.10 show that

$$r(u^{0}) = \sqrt{\mathbb{E}\left[\exp\left(\int_{0}^{T} |u^{*} - u^{0}|^{2} (X_{s}^{2u^{*} - u^{0}}, s) \mathrm{d}s\right)\right]} - 1.$$
(66)

Even though this expression converges to zero as $\eta \to 0$ provided that $V \to V^0$ and $u^* \to u^0$ [21], we expect an exponential dependence on the time T and the dimension d for any fixed $\eta > 0$ (cf. our numerical experiment in Section 4.4).

In [21] it is proved that

$$\nabla V = \nabla V^0 + \eta \nabla v_1 + o(\eta), \tag{67}$$

uniformly on all compact subsets of $\mathbb{R}^d \times (0, T)$, where v_1 solves the PDE stated in Appendix A.3.2. As a consequence, we can write

$$|\nabla V - \nabla V^0| = |\eta \nabla v_1 + o(\eta)| = \eta |\nabla v_1 + o(1)|$$
(68)

and

$$r(u^{0}) = \mathbb{E}\left[\exp\left(\eta^{2} \int_{0}^{T} |(\sigma^{\top} \nabla v_{1})(X_{s}^{2u^{*}-u_{0}^{*}}, s)|^{2} \mathrm{d}s + o(\eta^{2})\right)\right].$$
(69)

Specifically, if there exist constants $C_1, C_2 > 0$ such that $C_1 < |\nabla v_1(x,t)| < C_2$ for all $(x,t) \in \mathbb{R}^d \times (0,T)$, then the relative error grows exponentially as

$$\sqrt{e^{\eta^2 C_1^2 T + o(\eta^2)} - 1} \le r(u^*) \le \sqrt{e^{\eta^2 C_2^2 T + o(\eta^2)} - 1}$$
(70)

due to Corollary 3.6. We emphasize, however, that it is not clear under which assumptions this uniform bound can be achieved, given that, in practice, v_1 can be strongly x-dependent as is illustrated with a numerical example in Section 4.4.

Remark 3.12. The above considerations show that the relative error is potentially only small if η is (much) smaller than $C_1\sqrt{T}$. This can be compared to equation (5.3) in [51] and in particular to [18], where a concrete example is constructed for which the second moment can be lower bounded by $e^{-\frac{1}{\eta}C_1+(T-K)C_2}$ for $C_1, C_2, K > 0$, i.e. the time T and the smallness parameter η compete. We illustrate the degeneracy with growing T for a toy example in Figure 7.

4 Numerical examples

In this section we provide numerical examples that shall illustrate some of the formulas and bounds derived in the previous sections. We particularly demonstrate that importance sampling can be very sensitive to small perturbations of the optimal proposal measure. Here we focus on path space measures and provide several examples of importance sampling of diffusions. The code can be found at https://github.com/lorenzrichter/suboptimal-importance-sampling.

4.1 Ornstein-Uhlenbeck process

An example where the optimal importance sampling control is analytically computable is the following. Consider the *d*-dimensional Ornstein-Uhlenbeck process

$$\mathrm{d}X_s = AX_s\mathrm{d}s + B\,\mathrm{d}W_s, \quad X_0 = 0,\tag{71}$$

and its controlled version

$$dX_s^u = (AX_s^u + Bu(X_s^u, s)) ds + B dW_s, \quad X_0^u = 0,$$
(72)

where $A, B \in \mathbb{R}^{d \times d}$ are given matrices. In (26) we set f = 0 and $g(x) = \alpha \cdot x$, for a fixed vector $\alpha \in \mathbb{R}^d$, i.e. we want to estimate the quantity

$$\mathcal{Z} = \mathbb{E}\left[e^{-\alpha \cdot X_T}\right].\tag{73}$$

As shown in [38], the zero-variance importance sampling control is given by

$$u^{*}(x,t) = -B^{\top} e^{A^{\top}(T-t)} \alpha.$$
(74)

We choose $A = -3 I_{d \times d} + (\xi_{ij})_{1 \le i,j \le d}$ and $B = I_{d \times d} + (\xi_{ij})_{1 \le i,j \le d}$, where $\xi_{ij} \sim \mathcal{N}(0, \sigma^2)$ are i.i.d. random coefficients that are held fixed throughout the simulation. We set $T = 1, \sigma = 1, \alpha = (1, \ldots, 1)^{\top}$ and first consider the perturbed control

$$u = u^* + (\varepsilon, \dots, \varepsilon)^\top.$$
(75)

In the two left panels of Figure 2 we display a Monte Carlo estimation of the relative error (30) using $K = 10^6$ samples and compare it to the formulas from Corollary 3.6 and the bound from Corollary 3.2, once with varying perturbation strength ε , once with varying dimension d. We see that in both cases the simulations agree with our formula, even though for moderate to large deviations from optimality the estimated values of r are observed to fluctuate.

Ornstein-Uhlenbeck process

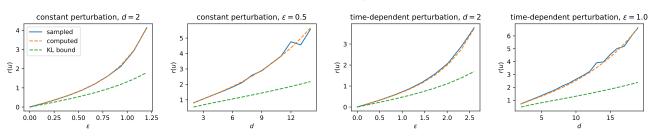


Figure 2: Sampled relative error with varying constant or time-dependent perturbation ε and dimension d compared to the formulas derived in Corollary 3.6 and to the lower bound from Corollary 3.2.

Let us now look at an example with a time-dependent perturbation of the optimal control. More specifically, we consider a perturbation that is active only for a certain amount of time s < T, namely

$$u(x,t) = u^*(x,t) + (\varepsilon,\dots,\varepsilon)^\top \mathbb{1}_{[0,s]}(t),$$
(76)

where in our experiment we choose s = 0.2. In the two right panels of Figure 2 we display the same comparisons as before, however now using formula (43) in order to account for the time-dependent nature of the perturbation.

4.2 Double well potential

For strongly metastable systems, Monte Carlo estimation is notoriously difficult and variance reduction methods are often indispensable. Importance sampling seems like a method of choice, but we want to illustrate that one has to be very careful with the design of the importance sampling control.

As in Example 3.1, let us consider the Langevin SDE

$$dX_s = -\nabla \Psi(X_s) \, ds + B \, dW_s, \quad X_0 = x, \tag{77}$$

in d = 1, where $B \in \mathbb{R}$ is the diffusion coefficient, $\Psi(x) = \kappa (x^2 - 1)^2$ is a double well potential with $\kappa > 0$ and x = -1 is the initial condition. For the observable in (26) we consider f = 0 and $g(x) = \rho(x-1)^2$, where $\rho > 0$; the terminal time is set to T = 1. Note that choosing higher values for ρ and κ accentuates the metastable features, making sample-based estimation of $\mathbb{E} \left[\exp(-g(X_T)) \right]$ more challenging. For an illustration, the two top panels of Figure 3 show the potential Ψ and the weight from (31), $e^{-g(x)}$, for different values of ρ and κ and for B = 1. We also plot the 'optimally tilted potentials' $\Psi^* = \Psi + BB^{\top}V$, noting that $-\nabla\Psi^* = -\nabla\Psi + Bu^*$. In the bottom left panel we show the relative error of the naive estimator depending on different values of ρ and κ .

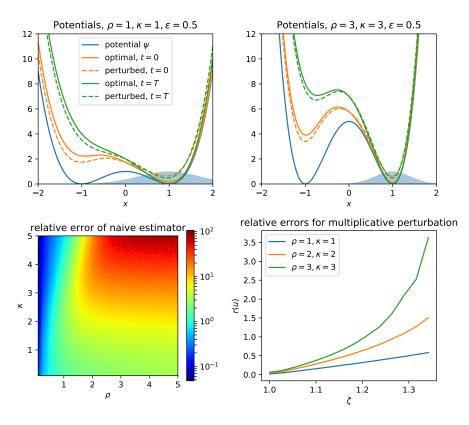


Figure 3: Top panels: Double well potentials and optimal tiltings as well as additive perturbations for different values of ρ and κ . Bottom left: Relative error of the naive Monte Carlo estimator for different values of ρ and κ . Bottom right: Relative error depending on the multiplicative perturbation factor ζ .

As before, let us perturb the optimal control, this time both in an additive and multiplicative way, namely

$$u = u^* + \varepsilon = -B^{\top} \nabla (V - B^{-\top} \varepsilon \cdot x) \quad \text{and} \quad u = \zeta u^*,$$
(78)

where $\varepsilon \in \mathbb{R}^d$, $\zeta \in \mathbb{R}$ specify the perturbation strengths. In the bottom right panel of Figure 3 we show the relative error for the multiplicative perturbation and see that for higher values of ρ and κ the exponential divergence becomes more severe, demonstrating that the robustness issues of importance sampling are particularly present in metastable settings.

Let us now consider perturbations depending either on time or space,

$$u_1(x,t) = u^*(x,t) + \varepsilon \sin(\alpha t)$$
 and $u_2(x,t) = u^*(x,t) + \varepsilon \sin(\alpha x),$ (79)

as illustrated in Figure 4 with $\alpha = 50$.

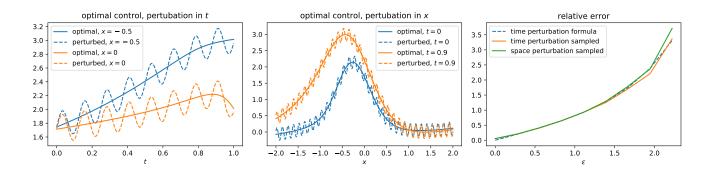


Figure 4: Left: Optimal importance sampling control and time perturbation for two different values of x. Middle: Optimal importance sampling control and space perturbation for two different values of t. Right: Relative error of suboptimal importance sampling estimators depending on the perturbation strength ε ; here, the dashed line refers to the exact formula (80).

In the former case we can analytically compute the relative error due to Corollary 3.6 to be

$$r_1(\varepsilon) = \sqrt{\exp\left(\varepsilon^2 \left(\frac{T}{2} - \frac{\sin(2\alpha T)}{4\alpha}\right)\right) - 1}.$$
(80)

Let us again illustrate how the relative error depends on the perturbation strength ε . In the right panel of Figure 4 we can see the agreement of the sampled version with formula (80) when considering the time-dependent perturbation. We do not have a formula in the case of a space-dependent perturbation, however we can still observe the exponential dependence on the perturbation strength in the estimated relative error, which is expected for instance from formulas (36) and (37).

4.3 Random stopping times

The suboptimal importance sampling bounds from Section 3 can be transferred to problems that involve a random stopping time τ rather than a fixed time horizon T, where mostly $\tau^u = \inf\{t > 0 : X_t^u \notin \mathcal{D}\}$ is defined⁶ as the first exit time of a bounded domain $\mathcal{D} \subset \mathbb{R}^d$. However, one has to be careful with applying our formulas and bounds from above, as τ^u itself depends on the law of the process. For illustration, let us consider a one-dimensional toy example, where the dynamics is a scaled Brownian motion

$$X_t = \sqrt{2}W_t \tag{81}$$

and we choose f = 1, g = 0 in (26), such that

$$\mathcal{Z} = \mathbb{E}\left[e^{-\tau}\right].\tag{82}$$

By noting that $\psi(x) = \mathbb{E}\left[e^{-\tau} | X_0 = x\right]$ fulfills the boundary value problem

$$(\Delta - 1)\psi(x) = 0, \qquad x \in \mathcal{D},\tag{83a}$$

 $\psi(x) = 1, \qquad x \in \partial \mathcal{D},$ (83b)

we can compute the optimal zero-variance importance sampling control to be

$$u^*(x) = \sqrt{2}\nabla \log \psi(x) = \sqrt{2} \frac{1 - e^{-2x}}{e^{-2x} + 1}.$$
(84)

In our experiment, we again perturb the optimal control via

$$u = u^* + \varepsilon. \tag{85}$$

⁶We denote with $\tau = \tau^0$ the hitting time of the uncontrolled process X_t .

Formula (38) provides an expression for the relative error, even if T is replaced by a random time τ (which we leave the reader to check for herself), namely

$$r(u) = \left(\mathbb{E}\left[e^{\varepsilon^{2}\tau^{2u^{*}-u}}\right] - 1\right)^{\frac{1}{2}} \ge \left(e^{\varepsilon^{2}\mathbb{E}\left[\tau^{2u^{*}-u}\right]} - 1\right)^{\frac{1}{2}},\tag{86}$$

where it is essential that τ^{2u^*-u} refers to the hitting time of the process $X_t^{2u^*-u}$. We applied Jensen's inequality in the last expression and note that naively assuming

$$r(u) \approx \left(e^{\varepsilon^2 \mathbb{E}[\tau]} - 1\right)^{\frac{1}{2}} \tag{87}$$

is usually wrong. Figure 5 compares the sampled relative error with the exact formula, the lower bound in (86) and the wrong expression (87).

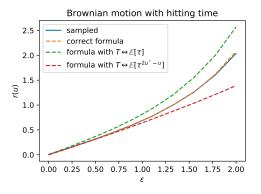


Figure 5: Relative error of a quantity involving a random stopping time compared to the exact formula, a lower bound as well as a naive, but usually wrong approximation.

Remark 4.1. Let us note again that estimating quantities involving hitting times gets particularly challenging in rare event settings, where the expected hitting time might become very large, cf. Example 3.1. The relation (86) for the relative error then indicates that Monte Carlo estimation becomes especially difficult.

4.4 Small noise diffusions

As an example for a small noise diffusion, we consider a modification of a one-dimensional toy example that has been proposed in [53]. We take the scaled Brownian motion

$$X_s^\eta = \sqrt{\eta} W_s, \qquad X_0 = 0.1, \tag{88}$$

and want to compute

$$\mathbb{E}\left[e^{-\frac{1}{\eta}g(X_T^\eta)}\right] \tag{89}$$

with

$$g(x) = \frac{\alpha}{2} \left(1 - \frac{|x|}{\sqrt{\alpha}} \right)^2 \tag{90}$$

for $\alpha > 0$. One readily sees that

$$V^{0}(x,t) = \frac{\alpha \left(1 - \frac{|x|}{\sqrt{\alpha}}\right)^{2}}{2(T - t + 1)}$$
(91)

is the unique viscosity solution to the deterministic problem (64); we refer to [22] for a discussion of the theory of viscosity solutions. Since an explicit solution $V^*(x,t)$ to the second-order HJB equation (62) is not available, we approximate it with finite differences. In Figure 6 we show the corresponding controls $u^0(x,s) = -\sigma^{\top}V^0(x,t)$ and $u^*(x,s) = -\sigma^{\top}V^*(x,t)$ for different values of the noise coefficient η .

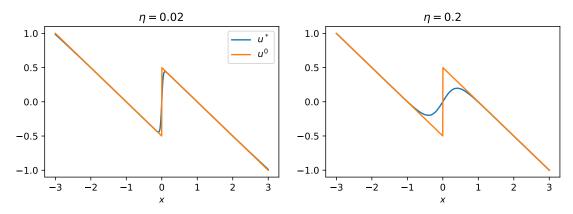


Figure 6: For a small noise diffusion problem we display once the optimal control and once the control resulting from the zero-noise approximation with different noise scalings η .

In the middle panel of Figure 7 we show the relative error depending on the noise parameter η . Unlike one could expect from (70), it seems to not grow exponentially in η , which can be explained by looking at the exponentiated L^2 error, exp $\left(\mathbb{E}\left[\int_0^T |u^* - u^0|^2 (X_s^{u^0}, s) ds\right]\right)$, which we plot in the left panel. The observation that this does not grow exponentially seems to be rooted in the fact that the suboptimality $\delta = u^* - u^0$ is very different for different values of x. If we vary T, however, we can observe an exponential dependency on the time horizon, as displayed in the right panel of Figure 7, again being in accordance with the consideration in Section 3.3.

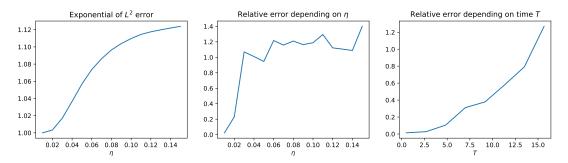


Figure 7: Small noise diffusions with vanishing noise coefficient η . Left: Exponential of L^2 error between u^* and u^0 depending on η for T = 1. Middle: Relative importance sampling error depending on η . Right: Relative importance sampling error depending on T for $\eta = 0.005$.

5 Conclusion and outlook

In this article, we have provided quantitative bounds on the relative error of importance sampling that depend on the divergence between the actual proposal measure and the theoretically optimal one. These bounds indicate that importance sampling is very sensitive with respect to suboptimal choices of the proposals, which has been observed frequently in numerical experiments and is in line with recent theoretical analysis [1, 9, 45]. We showed that the relative error of importance sampling estimators scales exponentially in the KL divergence between the optimal and the proposal measure and argued that this renders importance sampling especially challenging in high dimensions.

We have focused on importance sampling of stochastic processes and derived some novel formulas for the relative error depending on the suboptimality of the function u that controls the drift of the process. These formulas can be used to get practically useful bounds, but they also indicate two potential issues for importance sampling in path space: for systems with large state space and for problems on a long (or infinite) time horizon the relative error becomes exponentially large in the state space dimension d and the time horizon T. We have briefly discussed how this observation can be transferred to random stopping times, such as first hitting times, and have applied our formulas to importance sampling in the small noise regime, offering new perspectives and revealing some potential drawbacks of existing methods.

Even though the key message of the paper regarding the use of path space importance sampling in high dimensions seems to be rather discouraging, let us finally mention that there is hope. In practice, the approximations to optimal proposals use iterative methods to minimize a divergence (or: loss function) between the approximant and the target, using, for instance, stochastic gradient descent. A crucial question then is which divergence to take, and it turns out that different choices lead to proposals with vastly different statistical properties. Let us mention four possible choices for the loss function in the approximation scheme: (a) relative entropy, (b) cross-entropy, (c) χ^2 divergence or relative error, and (d) the recently introduced (see [38]) log-variance divergence $\operatorname{Var}_{\tilde{\nu}}(\log d\nu^*/d\tilde{\nu})$,

where we remark that in all four cases straightforward implementations for both probability densities on finite dimensional spaces and (infinite-dimensional) path measures are available. Since normally we rely on Monte Carlo approximations of the measures and our quantities of interests, it is crucial that the relative error of these divergences and their gradients is as small as possible. While the analysis in this article suggests that the χ^2 divergence cannot be expected to lead to a low-variance gradient estimator in general, the other divergences have been recently analyzed in [38] in the context of path sampling (see [44] for related results on densities), some of which show better scaling properties when going to high dimensions.

We expect that these perspectives can turn out fruitful in the future, in that they can guide the design of stable importance sampling schemes that work even in high dimensions. We therefore conclude that while importance sampling itself is often not robust, there are strategies to approximate the optimal proposal measure in a more robust way that go beyond cross-entropy minimisation and control of the χ^2 divergence.

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A Appendix

A.1 Proofs for Section 2

Proof of Proposition 2.6. We adapt a proof of [37]. Assume first that $m \ge 1$, then for any $E \in \mathcal{F}$

$$\nu(E) - \lambda(E) \ge \nu(E) - m\lambda(E) \ge 0, \tag{92}$$

where the last inequality follows from the definition of m. On the other hand, if $E = \Omega$, then $\nu(E) - \lambda(E) = 0$ and therefore it follows that m = 1, i.e. $\nu = \lambda$.

Let now m < 1. We want to show $mJ(f, \lambda, \varphi) \leq J(f, \nu, \varphi)$, which is equivalent to

$$\mathbb{E}_{\nu}[f(\varphi)] - m \mathbb{E}_{\lambda}[f(\varphi)] + mf\left(\mathbb{E}_{\lambda}[\varphi]\right) \ge f\left(\mathbb{E}_{\nu}[\varphi]\right).$$
(93)

We compute

$$\mathbb{E}_{\nu}[f(\varphi)] - m \mathbb{E}_{\lambda}[f(\varphi)] + mf\left(\mathbb{E}_{\lambda}[f(\varphi)]\right) \ge \left(\mathbb{E}_{\nu}[1] - m \mathbb{E}_{\lambda}[1]\right) f\left(\frac{\mathbb{E}_{\nu}[\varphi] - m \mathbb{E}_{\lambda}[\varphi]}{\mathbb{E}_{\nu}[1] - m \mathbb{E}_{\lambda}[1]}\right) + mf\left(\mathbb{E}_{\lambda}[f(\varphi)]\right)$$
(94a)

$$= (1-m)f\left(\frac{\mathbb{E}_{\nu}[\varphi] - m \mathbb{E}_{\lambda}[\varphi]}{1-m}\right) + mf\left(\mathbb{E}_{\lambda}[f(\varphi)]\right)$$
(94b)

$$\geq f\left(\mathbb{E}_{\nu}[\varphi] - m \,\mathbb{E}_{\lambda}[\varphi] + m \,\mathbb{E}_{\lambda}[\varphi]\right) \tag{94c}$$

$$= f\left(\mathbb{E}_{\nu}[\varphi]\right),\tag{94d}$$

where we used two times the convexity of f. The other inequality follows analogously.

A.2 Proofs for Section 3

Proof of Proposition 3.3. We compute

$$\mathbb{E}\left[e^{-2\mathcal{W}(X^u)}\left(\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{P}^u}(X^u)\right)^2\right] = \mathbb{E}\left[e^{-2\mathcal{W}(X^u)}\left(\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{P}^{u^*}}(X^u)\frac{\mathrm{d}\,\mathbb{P}^{u^*}}{\mathrm{d}\,\mathbb{P}^u}(X^u)\right)^2\right]$$
(95a)

$$= \mathcal{Z}^{2} \mathbb{E}\left[\left(\frac{\mathrm{d} \mathbb{P}^{u^{*}}}{\mathrm{d} \mathbb{P}^{u}} (X^{u}) \right)^{2} \right], \qquad (95b)$$

where we used

$$\frac{\mathrm{d}\,\mathbb{P}}{\mathrm{d}\,\mathbb{P}^{u^*}}(X^u) = e^{\mathcal{W}(X^u)}\,\mathcal{Z}\,.\tag{96}$$

Equation (37) now follows by the Girsanov formula (see Lemma A.2) and the definition of the variance. For equation (38) note that we can write

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\right] = \mathbb{E}_{\mathbb{P}^{u+2\delta}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\frac{\mathrm{d}\,\mathbb{P}^{u}}{\mathrm{d}\,\mathbb{P}^{u+2\delta}}\right].$$
(97)

We compute

$$\frac{\mathrm{d}\mathbb{P}^{u^*}}{\mathrm{d}\mathbb{P}^{u}}(X^{u+2\delta}) = \exp\left(\frac{3}{2}\int_0^T |\delta(X_s^{u+2\delta}, s)|^2 \mathrm{d}s + \int_0^T \delta(X_s^{u+2\delta}, s) \cdot \mathrm{d}W_s\right)$$
(98)

and

$$\frac{\mathrm{d}\,\mathbb{P}^{u}}{\mathrm{d}\,\mathbb{P}^{u+2\delta}}(X^{u+2\delta}) = \exp\left(-2\int_{0}^{T} |\delta(X_{s}^{u+2\delta},s)|^{2}\mathrm{d}s - 2\int_{0}^{T} \delta(X_{s}^{u+2\delta},s) \cdot \mathrm{d}W_{s}\right),\tag{99}$$

from which the desired formula immediately follows.

Alternative proof of Corollary 3.6. We follow the reasoning in [33, Thm. 2.1] and apply Grönwall's inequality to the square integrable exponential martingale Z.⁷ To this end, we define the shorthands $\delta(x,t) := (u^* - u)(x,t)$ and

$$Z_t := \exp\left(-\frac{1}{2}\int\limits_0^t |\delta(X_s,s)|^2 \mathrm{d}s + \int\limits_0^t \delta(X_s,s) \cdot \mathrm{d}W_s\right).$$
(100)

Then, by Itô's formula,

$$Z_t^2 = 1 + 2\int_0^t Z_s dZ_s + \int_0^t Z_s^2 |\delta(X_s, s)|^2 ds$$
(101)

and therefore, after taking expectations,

$$\mathbb{E}\left[Z_t^2\right] = 1 + \mathbb{E}\left[\int_0^t Z_s^2 |\delta(X_s, s)|^2 \mathrm{d}s\right]$$
(102a)

$$\leq 1 + \int_{0}^{t} \mathbb{E}\left[Z_{s}^{2}\right] h_{2}^{2}(s) \mathrm{d}s.$$
(102b)

We can now apply Grönwall's inequality to get

$$\mathbb{E}\left[Z_t^2\right] \le \exp\left(\int_0^t h_2^2(s) \mathrm{d}s\right) \tag{103}$$

and therefore the desired statement after applying Proposition 3.3. The other direction follows analogously by noting that

$$-\mathbb{E}\left[Z_t^2\right] \le -1 - \int_0^t \mathbb{E}\left[Z_s^2\right] h_1^2(s) \mathrm{d}s.$$
(104)

Remark A.1. Yet another alternative to prove Corollary 3.6 is by computing

$$\mathbb{E}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^*}}{\mathrm{d}\,\mathbb{P}^{u}}(X^u)\right)^2\right] = \mathbb{E}\left[\exp\left(-\int_0^T |\delta(X^u_s,s)|^2 \mathrm{d}s + 2\int_0^T \delta(X^u_s,s) \cdot \mathrm{d}W_s\right)\right]$$
(105a)

$$= \mathbb{E}\left[\exp\left(\int_{0}^{T} |\delta(X_{s}^{u},s)|^{2} \mathrm{d}s - 2\int_{0}^{T} |\delta(X_{s}^{u},s)|^{2} \mathrm{d}s + 2\int_{0}^{T} \delta(X_{s}^{u},s) \cdot \mathrm{d}W_{s}\right)\right]$$
(105b)

$$\leq \exp\left(\int_{0}^{T} h_{2}^{2}(s) \mathrm{d}s\right) \mathbb{E}\left[\exp\left(-\frac{1}{2}\int_{0}^{T} |2\delta(X_{s}^{u},s)|^{2} \mathrm{d}s + \int_{0}^{T} 2\delta(X_{s}^{u},s) \cdot \mathrm{d}W_{s}\right)\right]$$
(105c)

$$= \exp\left(\int_{0}^{T} h_2^2(s) \mathrm{d}s\right),\tag{105d}$$

where we used the constant expectation property of the exponential martingale in the last step. The other direction follows analogously.

⁷See also Theorem 2 in http://math.ucsd.edu/~pfitz/downloads/courses/spring05/math280c/expmart.pdf.

Proof of Proposition 3.8. From Lemma A.4 it holds for n, p, q > 1 with $\frac{1}{p} + \frac{1}{q} = 1$ that

$$\mathbb{E}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^*}}{\mathrm{d}\,\mathbb{P}^{u}}(X^u)\right)^n\right] \le \mathbb{E}\left[\exp\left(\frac{nq(np-1)}{2}\int\limits_0^T |u^*-u|^2(X^u_s,s)\mathrm{d}s\right)\right]^{\frac{1}{q}}.$$
(106)

We write $q = \frac{p}{p-1}$ and note that $q(np-1) = \frac{p(np-1)}{p-1}$ is minimized by $p^* = 1 \pm \sqrt{1 - \frac{1}{n}}$, from which we are only allowed to take the positive part due to the constraint $p \ge 1$. For n = 2 this yields $p^* = \frac{\sqrt{2}+1}{\sqrt{2}}$ and $q^* = \sqrt{2} + 1$, and we get the desired statement by recalling

$$r^{2}(u) = \operatorname{Var}_{\mathbb{P}^{u}}\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right) = \mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{2}\right] - 1.$$
(107)

A.3 Auxiliary statements

In this section, we recall some known statements and provide some helpful additional analysis.

First note that the Radon-Nikodym derivative appearing in the importance sampling estimator in path space can be computed explicitly.

Lemma A.2 (Girsanov). For $u \in U$, the measures \mathbb{P} and \mathbb{P}^u , relating to the SDEs (25) and (29), are equivalent. Moreover, the Radon-Nikodym derivative satisfies

$$\frac{\mathrm{d}\,\mathbb{P}^{u}}{\mathrm{d}\,\mathbb{P}}(X) = \exp\left(\int_{0}^{T} \left(u^{\top}\sigma^{-1}\right)(X_{s},s) \cdot \mathrm{d}X_{s} - \int_{0}^{T} (\sigma^{-1}b \cdot u)(X_{s},s) \,\mathrm{d}s - \frac{1}{2}\int_{0}^{T} |u(X_{s},s)|^{2} \,\mathrm{d}s\right).$$
(108)

Proof. See [38, Lemma A.1].

Corollary A.3 (Formula for path space relative error in a special case). If the difference $u^* - u$ does not depend on x, then

$$r(u) = \left(\exp\left(\int_{0}^{T} |u^* - u|^2(s) \mathrm{d}s\right) - 1\right)^{\frac{1}{2}}.$$
(109)

Proof. This is a direct consequence of (38). For the reader's convenience, we provide an alternative proof. If $u^* - u$ does not depend on x, then the random variable

$$Y = -\int_{0}^{T} |u^* - u|^2(s) ds + 2\int_{0}^{T} (u^* - u)(s) \cdot dW_s$$
(110)

is normally distributed, with mean and variance given by

$$\mu = -\int_{0}^{T} |u^* - u|^2(s) \mathrm{d}s, \qquad \sigma^2 = 4 \int_{0}^{T} |u^* - u|^2(s) \mathrm{d}s, \tag{111}$$

where the second expression follows from the Itô isometry. The random variable $\left(\frac{d\mathbb{P}^{u^*}}{d\mathbb{P}^u}(X^u)\right)^2 = e^Y$ is then log-normally distributed and we compute

$$\mathbb{E}\left[e^{Y}\right] = e^{\mu + \frac{\sigma^{2}}{2}} = e^{\frac{\sigma^{2}}{4}},\tag{112}$$

which gives the desired statement.

Lemma A.4. Let n, p, q > 1 with $\frac{1}{p} + \frac{1}{q} = 1$, then it holds that

$$\mathbb{E}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^*}}{\mathrm{d}\,\mathbb{P}^{u}}(X^u)\right)^n\right] \le \mathbb{E}\left[\exp\left(\frac{nq(np-1)}{2}\int\limits_0^T |u^*-u|^2(X^u_s,s)\mathrm{d}s\right)\right]^{\frac{1}{q}}.$$
(113)

Proof. Let us write $\delta(x, s) := (u^* - u)(x, s)$, and let n, p, q > 1, then, using the Hölder inequality with $\frac{1}{p} + \frac{1}{q} = 1$, it holds

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\left(\frac{\mathrm{d}\,\mathbb{P}^{u^{*}}}{\mathrm{d}\,\mathbb{P}^{u}}\right)^{n}\right] = \mathbb{E}_{\mathbb{P}^{u}}\left[\exp\left(n\int_{0}^{T}\delta(X_{s},s)\cdot\mathrm{d}W_{s} - \frac{n^{2}p}{2}\int_{0}^{T}|\delta(X_{s},s)|^{2}\mathrm{d}s + \frac{n(np-1)}{2}\int_{0}^{T}|\delta(X_{s},s)|^{2}\mathrm{d}s\right)\right]$$
(114a)

$$\leq \mathbb{E}_{\mathbb{P}^{u}} \left[\exp\left(\int_{0}^{T} np \, \delta(X_{s}, s) \cdot \mathrm{d}W_{s} - \frac{1}{2} \int_{0}^{T} |np \, \delta(X_{s}, s)|^{2} \mathrm{d}s \right) \right]^{\overline{p}}$$
(114b)

$$\mathbb{E}_{\mathbb{P}^{u}}\left[\exp\left(\frac{nq(np-1)}{2}\int_{0}^{T}|\delta(X_{s},s)|^{2}\mathrm{d}s\right)\right]^{\frac{1}{q}}$$
(114c)

$$= \mathbb{E}_{\mathbb{P}^{u}} \left[\exp\left(\frac{nq(np-1)}{2} \int_{0}^{T} |\delta(X_{s},s)|^{2} \mathrm{d}s\right) \right]^{\frac{1}{q}}.$$
(114d)

Note that, even though Hölder's inequality holds for $p, q \in [1, \infty]$, the inequality becomes useless for q = 1 and $p = \infty$.

Proposition A.5 (Zero-variance property). We get a vanishing relative error r(u) = 0 if and only if $\delta = u^* - u = 0$, *i.e.* when having the optimal control $u = u^* = -\sigma^\top \nabla V$.

Proof. The fact that $\delta = 0$ implies r(u) = 0 follows directly from (38) or (52). For the other direction note that r(u) = 0 implies $M_u(x,t) = \psi^2(x,t)$ (as defined in Proposition 3.10) for all $(x,t) \in \mathbb{R}^d \times [0,T]$ and therefore equation (48a) becomes

$$\partial_t + L - \sigma u(x,t) \cdot \nabla - 2f(x,t) + |u(x,t)|^2)\psi^2(x,t) = 0.$$
(115)

Further note that due to the Kolmogorov backward equation it holds

$$(\partial_t + L - 2f(x,t))\psi^2(x,t) - |(\sigma^\top \nabla \psi)(x,t)|^2 = 0.$$
(116)

Combining these two PDEs brings

$$\psi^{2}(x,t)|u(x,t)|^{2} - 2(\psi\sigma u \cdot \nabla\psi)(x,t) + |(\sigma^{\top}\nabla\psi)(x,t)|^{2} = |(\psi u)(x,t) - (\sigma^{\top}\nabla\psi)(x,t)|^{2} = 0,$$
(117)

which implies that

$$u = \sigma^{\top} \frac{\nabla \psi}{\psi} = \sigma^{\top} \nabla \log \psi = -\sigma^{\top} \nabla V.$$
(118)

The following lemma shows that the KL divergence increases with the number of dimensions. This result follows from the chain-rule of KL divergence, see, e.g., [11].

Lemma A.6 (Dimension dependence of KL divergence). Let $u^{(d)}(z_1, \ldots, z_d)$ and $v^{(d)}(z_1, \ldots, z_d)$ be two arbitrary probability distributions on \mathbb{R}^d . For $j \in \{1, \ldots, d\}$ denote their marginals on the first j coordinates by $u^{(j)}$ and $v^{(j)}$, *i.e.*

$$u^{(j)}(z_1, \dots, z_j) = \int \dots \int u^{(d)}(z_1, \dots, z_d) \, \mathrm{d}z_{j+1} \dots \, \mathrm{d}z_d,$$
(119)

and

$$v^{(j)}(z_1, \dots, z_j) = \int \dots \int v^{(d)}(z_1, \dots, z_d) \, \mathrm{d}z_{j+1} \dots \, \mathrm{d}z_d.$$
(120)

Then

$$\mathrm{KL}(u^{(1)} \mid v^{(1)}) \le \mathrm{KL}(u^{(2)} \mid v^{(2)}) \le \ldots \le \mathrm{KL}(u^{(d)} \mid v^{(d)}), \tag{121}$$

i.e. the function $J \mapsto \mathrm{KL}(u^{(j)} \mid v^{(j)})$ is increasing.

A.3.1 Relative error of log-normal random variables

Let $Y \sim \mathcal{N}(\overline{\mu}, \overline{\Sigma})$ with arbitrary $\overline{\mu} \in \mathbb{R}^d, \overline{\Sigma} \in \mathbb{R}^{d \times d}$ and take $\gamma \in \mathbb{R}^d, c \in \mathbb{R}$, then $e^{\gamma \cdot Y + c}$ is log-normally distributed and its relative error is

$$r(\gamma, \overline{\Sigma}) = \sqrt{\frac{\mathbb{E}\left[e^{2(\gamma \cdot Y + c)}\right]}{\mathbb{E}\left[e^{\gamma \cdot Y + c}\right]^2} - 1}} = \sqrt{\frac{\mathbb{E}\left[e^{2\gamma \cdot Y}\right]}{\mathbb{E}\left[e^{\gamma \cdot Y}\right]^2} - 1}} = \sqrt{e^{\gamma \cdot \overline{\Sigma}\gamma} - 1},$$
(122)

independent of c. With the setting and notation from Example 2.10 we can now for instance compute

$$e^{-g(\widetilde{X})}\frac{p}{\widetilde{p}^{\varepsilon}}(\widetilde{X}) = \exp\left(-\alpha \cdot \widetilde{X} + \log\frac{p}{\widetilde{p}^{\varepsilon}}\right) = \exp\left(\varepsilon \cdot \widetilde{X} - \mu \cdot (\alpha + \varepsilon) + \frac{1}{2}(\alpha + \varepsilon) \cdot \Sigma(\alpha + \varepsilon)\right)$$
(123)

and with $\gamma = \varepsilon, c = -\mu \cdot (\alpha + \varepsilon) + \frac{1}{2}(\alpha + \varepsilon) \cdot \Sigma(\alpha + \varepsilon), \overline{\Sigma} = \Sigma$ one therefore gets the relative error

$$r(\tilde{p}^{\varepsilon}) = \sqrt{e^{\varepsilon \cdot \Sigma \varepsilon} - 1} \tag{124}$$

as stated in (22).

A.3.2 Asymptotic expansion in small noise diffusions

To get further intuition on the small noise diffusions defined in Section 3.3, let us consider the formal expansion of the solution to the HJB equation (62)

$$V = v_0 + \eta v_1 + \eta^2 v_2 + \dots$$
(125)

Inserting into (62) (with $\sigma = I_{d \times d}$) and comparing the powers of η yields the PDEs

$$\partial_t v_0 + b \cdot \nabla v_0 - \frac{1}{2} |\nabla v_0|^2 = 0,$$
(126a)

$$\partial_t v_1 + \frac{1}{2}\Delta v_0 + b \cdot \nabla v_1 - \nabla v_0 \cdot \nabla v_1 = 0, \qquad (126b)$$

$$\partial_t v_2 + \frac{1}{2} \Delta v_1 + b \cdot \nabla v_2 - \nabla v_0 \cdot \nabla v_2 - \frac{1}{2} |\nabla v_1|^2 = 0, \qquad (126c)$$

and so on, where all but the first PDE are transport equations (see [51]). We note that (given some appropriate assumptions) we have $v_0 = V^0$, with V^0 being to solution to (64). In [21] it is proven that

$$\nabla V = \nabla V^0 + \eta \nabla v_1 + o(\eta), \tag{127}$$

where v_1 fulfills the PDE above and V is the solution to the original HJB equation (62).

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