HAL open science

Optimal importance sampling for overdamped Langevin dynamics

Martin Chak, Tony Lelièvre, Gabriel Stoltz, Urbain Vaes

▶ **To cite this version:**

Martin Chak, Tony Lelièvre, Gabriel Stoltz, Urbain Vaes. Optimal importance sampling for overdamped Langevin dynamics. 2023. hal-04169540

HAL Id: hal-04169540

https://hal.science/hal-04169540v1

Preprint submitted on 24 Jul 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Optimal importance sampling for overdamped Langevin dynamics

M. Chak* T. Lelièvre† G. Stoltz‡ U. Vaes§

July 24, 2023

Abstract

Calculating averages with respect to multimodal probability distributions is often necessary in applications. Markov chain Monte Carlo (MCMC) methods to this end, which are based on time averages along a realization of a Markov process ergodic with respect to the target probability distribution, are usually plagued by a large variance due to the metastability of the process. In this work, we mathematically analyze an importance sampling approach for MCMC methods that rely on the overdamped Langevin dynamics. Specifically, we study an estimator based on an ergodic average along a realization of an overdamped Langevin process for a modified potential. The estimator we consider incorporates a reweighting term in order to rectify the bias that would otherwise be introduced by this modification of the potential. We obtain an explicit expression in dimension 1 for the biasing potential that minimizes the asymptotic variance of the estimator for a given observable, and propose a general numerical approach for approximating the optimal potential in the multi-dimensional setting. We also investigate an alternative approach where, instead of the asymptotic variance for a given observable, a weighted average of the asymptotic variances corresponding to a class of observables is minimized. Finally, we demonstrate the capabilities of the proposed method by means of numerical experiments.

1 Introduction

1.1 Context

In many applications ranging from Bayesian inference to statistical physics and computational biology, it is often necessary to calculate expectations with respect to high-dimensional probability distributions of the form

$$\mu = \frac{\mathrm{e}^{-V}}{Z}, \qquad Z = \int_{\mathbb{D}^d} \mathrm{e}^{-V}, \tag{1}$$

where $\mathbb{D} \in \{\mathbb{R}, \mathbb{T}\}$, with $\mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ the one-dimensional torus, and $V \colon \mathbb{D}^d \to \mathbb{R}$ is a potential energy function (confining if $\mathbb{D} = \mathbb{R}$ and periodic if $\mathbb{D} = \mathbb{T}$) such that e^{-V} is Lebesgue integrable. In the context of Bayesian inference, the distribution μ usually describes likelihoods of the possible values of an unknown parameter given some observed data [27, 50], while in statistical physics, the distribution μ assigns probabilities to the possible configurations of a molecular system. In the latter setting, averages with respect to μ give access to macroscopic properties of the system, such as the heat capacity or equations of state relating pressure, density and temperature [17, 33, 30, 29, 4].

*LJLL, Sorbonne Université (martin.chak@sorbonne-universite.fr)

†CERMICS, École des Ponts, France & MATHERIALS project-team, Inria Paris (tony.lelievre@enpc.fr)

‡CERMICS, École des Ponts, France & MATHERIALS project-team, Inria Paris (gabriel.stoltz@enpc.fr)

§MATHERIALS project-team, Inria Paris & CERMICS, École des Ponts (urbain.vaes@inria.fr)

The first systematic approach to sampling probability distributions originates from the 1950s with the seminal work of Metropolis et al. [38]. In 1970, Hastings generalized this approach and proposed a sampling method [21] which was later recognized as a particular case of what is now known as a Markov chain Monte Carlo (MCMC) method. The MCMC approach to sampling is based on the use of a Markov process that admits the target probability distribution as unique invariant measure. A simple yet widely used Markov process that is ergodic with respect to μ under appropriate conditions on the potential V is the overdamped Langevin dynamics,

$$\mathrm{d}Y_t = -\nabla V(Y_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t, \tag{2}$$

where W_t denotes a standard d-dimensional Wiener process. Under appropriate assumptions on the potential V, the average with respect to μ of an observable $f \in L^1(\mu)$ can be approximated by a time average along a realization of the solution to this equation:

$$\mu^T(f) := \frac{1}{T}\int_0^T f(Y_t)\,\mathrm{d}t \xrightarrow[T\to\infty]{\text{a.s.}} \int_{\mathbb{D}^d} f\,\mathrm{d}\mu =: \mu(f) =: I, \tag{3}$$

see e.g. [35, Theorem 5.1], [26], [43] and references therein, [32, Chapter 9 and proof of Theorem 1.6.2] and [19, Proposition 2]. In practice, it is necessary to discretize the dynamics (2), and the resulting discrete-time Markov process is generally ergodic with respect to not μ but a probability measure $\mu_{\Delta t}$ differing from μ at order Δt^α, for some exponent α larger than or equal to the weak order of convergence of the scheme. The bias introduced by the discretization can usually be bounded from above as a function of the time step; such estimates were first obtained by Talay and Tubaro [51] for general SDEs. They were later made precise for implicit schemes for Langevin and overdamped Langevin dynamics in [36], and then refined in works such as [37, 15, 1, 28]. Alternatively, it may be possible to consider the numerical scheme as a proposal to be accepted or rejected in a Metropolis–Hastings scheme, so that the resulting discrete-time process is also ergodic with respect to μ. This is the Metropolis-adjusted Langevin algorithm (MALA) [46, 45, 44].

In this paper, we focus on the continuous-time dynamics (2) and show that modifying the potential V, in combination with importance sampling, can be used for variance reduction. Importance sampling is widely used to make the sampling of high dimensional probability measures easier; see for instance [3] for a review. The idea of using importance sampling in the context of MCMC methods was already suggested in Hastings' 1970 paper, see [21, Section 5]. If $(X_t)_{t\geqslant 0}$ is a Markov process that is ergodic with respect to a probability measure

$$\mu_U = \frac{\mathrm{e}^{-V-U}}{Z[U]}, \qquad Z[U] = \int_{\mathbb{D}^d} \mathrm{e}^{-V-U}, \tag{4}$$

where $U\colon \mathbb{D}^d \to \mathbb{R}$ is a smooth function such that e^{-V-U} is Lebesgue integrable over $\mathbb{D}^d$, then $\mu(f)$ may be approximated by

$$\mu_U^T(f) = \frac{\displaystyle\int_0^T (f\mathrm{e}^U)(X_t)\,\mathrm{d}t}{\displaystyle\int_0^T (\mathrm{e}^U)(X_t)\,\mathrm{d}t}. \tag{5}$$

Like $\mu^T(f)$, this estimator converges to I almost surely in the limit as $T \to \infty$, and it does not require the knowledge of the normalization constants Z and $Z[U]$. The main objective of this work is to study the properties of $\mu_U^T(f)$ when $(X_t)_{t\geqslant 0}$ is the solution to the overdamped Langevin dynamics with the potential $V + U$:

$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t - \nabla U(X_t)\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t. \tag{6}$$

In particular, we study whether it is possible to find a biasing potential U such that the asymptotic variance of $\mu_T^U(f)$, which we define more precisely in Lemma 11, is minimized for either a single observable (Section 3) or a class of observables (Section 4). Let us also mention here the recent work [11] where optimal importance sampling is performed over a class of distributions.

Before considering the MCMC estimator (5), it is instructive to present background material on importance sampling in the independent and identically distributed (i.i.d.) setting. This is the aim of Section 2. In all the theoretical results presented in this work, we assume that the following assumptions on V and f are satisfied, even when this is not explicitly mentioned.

Assumption 1.

- *The potential V is smooth over $\mathbb{D}^d$ (in particular $\mathrm{supp}(\mathrm{e}^{-V}) = \mathbb{D}^d$).*
- *The function e^{-V} is Lebesgue integrable over $\mathbb{D}^d$.*
- *Any observable f considered (just one in Sections 2 and 3 and set of them in Section 4) is smooth, integrable with respect to the probability measure $\mu \propto \mathrm{e}^{-V}$, and not μ-almost everywhere constant.*

1.2 Our contributions

The contributions of this paper are the following:

- In the one-dimensional setting ($d = 1$) either with $\mathbb{D} = \mathbb{T}$ or $\mathbb{D} = \mathbb{R}$, and for a given observable f, we obtain an explicit expression for the biasing potential U in (5)–(6) that is optimal in terms of asymptotic variance. We also prove that when $\mathbb{D} = \mathbb{R}$, the asymptotic variance $\sigma_f^2[U]$ of $\mu_U^T(f)$, viewed as a functional of U, is convex.
- In the general multi-dimensional setting, we obtain an expression for the $L^2(\mu)$ functional derivative of $\sigma_f^2[U]$ with respect to U, and we propose a gradient descent approach for finding a minimizer of $\sigma_f^2[U]$. We also prove that any minimizer of $\sigma_f^2[U]$ is necessarily singular when $\mathbb{D} = \mathbb{T}$.
- We propose a method for minimizing the asymptotic variance over a class of observables. More precisely, we present an approach for minimizing the average asymptotic variance when a simple Gaussian probability distribution is placed on the observable. We demonstrate through theoretical results and numerical experiments that this approach usually leads to a smooth optimizer, and may thus be more suitable for applications.
- We present examples and numerical experiments illustrating the properties of the optimal biasing potential and the performance of the method, both in the one-dimensional case and the multi-dimensional setting.

Plan of the paper. The remainder of the paper is organized as follows. We begin in Section 2 by presenting background material on importance sampling in the i.i.d. setting. In Section 3, we investigate the problem of minimizing the asymptotic variance for a given observable, first in the one-dimensional case and then in the multi-dimensional setting. In Section 4, we generalize the approach to the problem of minimizing the asymptotic variance over a class of observables. Examples and numerical experiments are presented in Section 5. Section 6 is reserved for conclusions and perspectives for future works. This section is followed by four appendices: Appendices A and B contain proofs of auxiliary results, Appendix C presents a derivation of the second variation of the asymptotic variance, and Appendix D provides a detailed analysis of the numerical scheme employed for approximating the functional derivative of the asymptotic variance.

2 Background: the i.i.d. setting

We recall in this section the expression of the optimal importance distribution μ_U in the setting where I is estimated from i.i.d. samples from μ_U, as opposed to the ergodic approach in (5). Specifically, we consider the estimator

$$\mu_U^N(f) := \frac{\sum_{n=1}^N (f\mathrm{e}^U)(X^n)}{\sum_{n=1}^N (\mathrm{e}^U)(X^n)} = I + \frac{\sum_{n=1}^N \left((f-I)\mathrm{e}^U\right)(X^n)}{\sum_{n=1}^N (\mathrm{e}^U)(X^n)}, \tag{7}$$

where $(X^n)_{n\in\mathbb{N}}$ are i.i.d. samples from μ_U. The right-most expression is not useful in practice because the value of I is unknown, but this expression is convenient for the theoretical analysis. We first comment briefly on the connection between this estimator and the estimator (5) in Subsection 2.1, then obtain an expression for the asymptotic variance of the estimator (7) in Subsection 2.2. and finally prove bounds on the asymptotic variance in Subsection 2.3.

2.1 Connection between the estimators (5) and (7)

The estimators (5) and (7) can be viewed as two limiting cases, corresponding to the limits $\tau \to 0$ and $\tau \to \infty$ respectively, of the estimator given in the second row and right-most column of Table 1. The latter estimator is based not on the full solution to (6) but on discrete periodic evaluations of it with a period τ.

The analysis presented in this paper can be repeated for the estimators in the middle column of Table 1, which can be employed when the normalization constants Z and $Z[U]$ are known. In this case, different optimal potentials are obtained. However, since the normalization constants are usually unknown in high-dimensional settings, we focus in most of this paper on the self-normalized estimators in the right-most column of Table 1.

	Z and $Z[U]$ are **known**	Z and $Z[U]$ are **unknown**
Continuous ($\tau = 0$)	$\frac{1}{T}\left(\frac{Z[U]}{Z}\right)\int_0^T \left(f\mathrm{e}^U\right)(X_t)\,\mathrm{d}t$	$\frac{\int_0^T \left(f\mathrm{e}^U\right)(X_t)\,\mathrm{d}t}{\int_0^T (\mathrm{e}^U)(X_t)\,\mathrm{d}t}$
$0 < \tau < \infty$	$\frac{1}{N}\left(\frac{Z[U]}{Z}\right)\sum_{n=0}^{N-1} \left(f\mathrm{e}^U\right)(X_{n\tau})$	$\frac{\sum_{n=0}^{N-1} \left(f\mathrm{e}^U\right)(X_{n\tau})}{\sum_{n=0}^{N-1} (\mathrm{e}^U)(X_{n\tau})}$
i.i.d ($\tau = \infty$)	$\frac{1}{N}\left(\frac{Z[U]}{Z}\right)\sum_{n=1}^{N} \left(f\mathrm{e}^U\right)(X^n)$	$\frac{\sum_{n=1}^{N} \left(f\mathrm{e}^U\right)(X^n)}{\sum_{n=1}^{N} (\mathrm{e}^U)(X^n)}$

Table 1: Classification of importance sampling estimators according to two criteria: the correlation between samples, and use of the normalization constants Z and $Z[U]$. Here $(X_t)_{t\in\mathbb{R}_{\geqslant 0}}$ is a solution to (6) and $(X^n)_{n\in\mathbb{N}}$ are i.i.d. samples from μ_U.

2.2 Asymptotic variance

In the whole Section 2, we suppose that Assumption 1 holds, in particular that the potential V is smooth, but we do not assume that the function U is smooth; we assume only that $U\colon \mathbb{D}^d \to \mathbb{R}\cup\{\infty\}$ is measurable and such that the following minimal requirements are satisfied:

- the function e^{-V-U} is Lebesgue integrable with $Z[U] > 0$;

- the estimator (7) converges to I almost surely, i.e. it holds that

$$\int_{\mathbb{D}^d} (f-I)\mathrm{e}^U \mathrm{d}\mu_U = 0 \qquad \Leftrightarrow \qquad \int_{\mathrm{supp}(\mu_U)} (f-I)\mathrm{d}\mu = 0. \tag{8}$$

  Here $\mathrm{supp}(\mu_U) = \mathrm{cl}\{x \in \mathbb{D}^d : U(x) + V(x) < \infty\}$ is the support of the measure μ_U, with cl the closure. In this work, we adopt the usual convention in measure theory that $0 \cdot +\infty = +\infty \cdot 0 = 0$.

- the function $(f-I)\mathrm{e}^U$ is square-integrable with respect to μ_U, so that the central limit theorem can be applied.

We denote by $\mathcal{U}$ the set of functions U that satisfy these conditions. The set $\mathcal{U}$ depends on V and f, but since these are considered to be fixed data of the problem, we do not explicitly indicate this dependence in the notation. If $U \in \mathcal{U}$ and $(X^n)_{n\in\mathbb{N}}$ are i.i.d. samples with law μ_U, then it holds by (8) and the central limit theorem that

$$\frac{1}{\sqrt{N}} \sum_{n=1}^{N} \left((f-I)\mathrm{e}^U\right)(X^n) \xrightarrow[N\to\infty]{\text{Law}} \mathcal{N}\left(0, \int_{\mathbb{D}^d} \left|(f-I)\mathrm{e}^U\right|^2 \mathrm{d}\mu_U\right), \tag{9}$$

where $\mathcal{N}(m, C)$ denotes the Gaussian distribution with mean m and (co)variance C. On the other hand, the law of large numbers gives that

$$\frac{1}{N} \sum_{n=1}^{N} \left(\mathrm{e}^U\right)(X^n) \xrightarrow[N\to\infty]{\text{a.s.}} \int_{\mathbb{D}^d} \mathrm{e}^U \mathrm{d}\mu_U = \frac{1}{Z[U]} \int_{\mathrm{supp}(\mu_U)} \mathrm{e}^{-V} = \frac{\mathscr{Z}[U]}{Z[U]}, \tag{10}$$

where we introduced

$$\mathscr{Z}[U] := \int_{\mathrm{supp}(\mu_U)} \mathrm{e}^{-V}.$$

Note that $\mathscr{Z}[U] \leqslant Z$ in general, with equality if and only if $\mathrm{supp}(\mu_U) = \mathrm{supp}(\mu)$. Combining (9) and (10) and using Slutsky's lemma, we conclude that

$$\sqrt{N}\big(\mu_U^N(f) - I\big) \xrightarrow[N\to\infty]{\text{Law}} \mathcal{N}\big(0, s_f^2[U]\big), \qquad s_f^2[U] := \frac{Z[U]^2}{\mathscr{Z}[U]^2} \int_{\mathbb{D}^d} \left|(f-I)\mathrm{e}^U\right|^2 \mathrm{d}\mu_U. \tag{11}$$

The variance $s_f^2[U]$ of the asymptotic normal distribution is the quantity we wish to minimize. In the next section, we obtain sharp bounds from below on the asymptotic variance $s_f^2[U]$.

2.3 Explicit optimal potential

In order to prepare the proof of the main result of this section, Proposition 4, we first give a preparatory lemma. We introduce the functional $\widehat{s}_f^2 \colon \mathcal{U} \to \mathbb{R} \cup \{\infty\}$ given by

$$\widehat{s}_f^2[U] = \frac{Z[U]}{Z^2} \int_{\mathbb{D}^d} |f-I|^2 \mathrm{e}^{U-V}. \tag{12}$$

Given the convention that $0 \cdot +\infty = +\infty \cdot 0 = 0$, the quantity $\widehat{s}_f^2[U]$ is well defined as an element of $\mathbb{R} \cup \{\infty\}$. Note that $\widehat{s}_f^2[U]$ coincides with the asymptotic variance $s_f^2[U]$ if and only if $\mathrm{supp}(\mu_U) = \mathbb{D}^d$.

Lemma 2. *It holds that*

$$\min_{U\in\mathcal{U}} \widehat{s}_f^2[U] = \frac{1}{Z^2} \left(\int_{\mathbb{D}^d} |f-I| \,\mathrm{d}\mu\right)^2 =: s_f^*. \tag{13}$$

In addition, the minimum is achieved for

$$U = U_*^{\mathrm{iid}} := -\log|f-I| \in \mathcal{U}, \tag{14}$$

with the convention that $\log(0) = -\infty$.

Proof. We first prove that $\widehat{s}_f^2[U] \geqslant s_f^*$ for all $U \in \mathcal{U}$. If $\widehat{s}_f^2[U] = \infty$, then this inequality is clear, so we assume from now on that $\widehat{s}_f^2[U] < \infty$. Using the Cauchy–Schwarz inequality, we have

$$\widehat{s}_f^2[U] = \frac{1}{Z^2} \int_{\mathbb{D}^d} \mathrm{e}^{-U-V} \int_{\mathbb{D}^d} |f - I|^2 \mathrm{e}^{U-V} \geqslant \frac{1}{Z^2} \left(\int_{\mathbb{D}^d} |f - I| \mathrm{e}^{-V} \right)^2 = s_f^*.$$

The statement that the infimum is achieved for U_*^{iid} in (14) follows from a substitution in (12). Note that U_*^{idd} indeed belongs to $\mathcal{U}$. □

Remark 3. The function U_*^{iid} in (14) is not smooth, because $f - I$ admits at least one root in $\mathbb{D}^d$. △

Although $\widehat{s}_f^2[U]$ does not coincide with $s_f^2[U]$ in general, Lemma 2 still contains useful information. Indeed, by regularizing U_*^{iid} in (14), we prove in Proposition 4 that s_f^* is a sharp bound from below on the actual asymptotic variance $s_f^2[U]$ over a class of "nice" biasing potentials. Specifically, let us introduce

$$\mathcal{U}_0 = \Big\{ U \in \mathcal{U} : \mathrm{supp}(|f - I|\mu) \subset \mathrm{supp}(\mu_U) \Big\}.$$

Conditions of the type $\mathrm{supp}(|f - I|\mu) \subset \mathrm{supp}(\mu_U)$ are used in the importance sampling literature; see, for example, equation (1.1) in [7, Section V.1]. Notice that, if this condition is satisfied, then (8) is also satisfied, but the converse is not true; in other words, $\mathcal{U}_0$ is a proper subset of $\mathcal{U}$. We are now ready to state and prove the main result of this section. We discuss in Remark 6 after the proof the existence of an optimal potential achieving the infimum over $\mathcal{U}_0$. Here and in the rest of this paper, the notation $C_{\mathrm{c}}^\infty(\mathbb{D}^d)$ denotes the set of smooth functions with compact support over $\mathbb{D}^d$.

Proposition 4. *Recall that Assumption 1 is assumed to hold throughout this paper. Then,*

- *It holds that* $\inf_{U \in \mathcal{U}} s_f^2[U] = 0$.
- *If* $0 \in \mathcal{U}_0$*, then* $\inf_{U \in \mathcal{U}_0} s_f^2[U] = s_f^*$.
- *If* $0 \in \mathcal{U}_0$*, then* $\inf_{U \in C_{\mathrm{c}}^\infty(\mathbb{D}^d)} s_f^2[U] = s_f^*$.

Remark 5. In view of Assumption 1, the condition $0 \in \mathcal{U}_0$ is equivalent to the condition $f \in L^2(\mu)$. We use the former condition in the statement of Proposition 4 in order to underline the similarity with Proposition 21 in the MCMC setting. △

Proof. We divide the proof into three parts, corresponding to the three items in the statement.
First item. The idea here is to construct an importance distribution μ_U concentrated in a small ball containing a point where $f = I$. Considering balls centered at such a point is usually not sufficient, because the condition (8) may not be satisfied. Take $\varepsilon > 0$ and let $g_\varepsilon \colon \mathbb{D}^d \to \mathbb{R}$ denote the function

$$g_\varepsilon(x) = \frac{1}{|B_\varepsilon(0)|} \int_{B_\varepsilon(x)} (f - I) \mathrm{e}^{-V},$$

where $B_\varepsilon(x) \subset \mathbb{D}^d$ is the open ball of radius ε centered at x and $|B_\varepsilon(0)|$ is the volume of this ball. By Assumption 1, there exists $(x_1, x_2) \in \mathbb{D}^d \times \mathbb{D}^d$ such that $f(x_1) > I$ and $f(x_2) < I$. Since f is smooth, there is $\epsilon > 0$ such that $g_\varepsilon(x_1) > 0$ and $g_\varepsilon(x_2) < 0$ for all $\varepsilon \in (0, \epsilon]$. Therefore, by the intermediate value theorem, there exists for all $\varepsilon \in (0, \epsilon]$ a point $x_\varepsilon \in \mathbb{D}^d$ on the segment joining x_1 and x_2 such that $g_\varepsilon(x_\varepsilon) = 0$. We define

$$U_\varepsilon(x) = \begin{cases} 0 & \text{if } |x - x_\varepsilon| \leqslant \varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

By construction $U_\varepsilon \in \mathcal{U}$, and we calculate from (11) that

$$s_f^2[U_\varepsilon] = \frac{\int_{B_\varepsilon(x_\varepsilon)} |f - I|^2 \mathrm{e}^{-V}}{\int_{B_\varepsilon(x_\varepsilon)} \mathrm{e}^{-V}}.$$

By the mean value theorem, there is $z_\varepsilon \in B_\varepsilon(x_\varepsilon)$ such that $s_f^2[U_\varepsilon] = |f(z_\varepsilon) - I|^2$. Since $g_\varepsilon(x_\varepsilon) = 0$, the function $f - I$ necessarily has a zero in $B_\varepsilon(x_\varepsilon)$. Additionally, since $(x_\varepsilon)_{\varepsilon \in (0,\epsilon]}$ is bounded, the function $f - I$ restricted to $\bigcup_{\varepsilon \in (0,\epsilon]} B_\varepsilon(x_\varepsilon)$ is Lipschitz continuous, with some constant L. From this we obtain that $s_f^2[U_\varepsilon] \leqslant (2L\varepsilon)^2$, and taking the limit $\varepsilon \to 0$ in this equation, we deduce the first item.

Second item. By the Cauchy–Schwarz inequality, the following lower bound holds for all $U \in \mathcal{U}$:

$$s_f^2[U] \geqslant \frac{Z[U]^2}{\mathscr{Z}[U]^2} \left(\int_{\mathbb{D}^d} |f - I| \mathrm{e}^U \, \mathrm{d}\mu_U \right)^2 = \frac{1}{\mathscr{Z}[U]^2} \left(\int_{\mathrm{supp}(\mu_U)} |f - I| \mathrm{e}^{-V} \right)^2. \tag{15}$$

For $U \in \mathcal{U}_0$, the right-most expression in (15) equals

$$\frac{1}{\mathscr{Z}[U]^2} \left(\int_{\mathbb{D}^d} |f - I| \mathrm{e}^{-V} \right)^2 \geqslant s_f^*,$$

where we used that $\mathscr{Z}[U] \leqslant Z$. Therefore, it holds that $s^2[U] \geqslant s_f^*$ for all $U \in \mathcal{U}_0$. That s_f^* is in fact the *infimum* of s_f^2 over $\mathcal{U}_0$ will follow from the third item, because $C_c^\infty \subset \mathcal{U}_0$.

Third item. For $\varepsilon > 0$, let $\varrho_\varepsilon \colon \mathbb{R} \to \mathbb{R}$ denote the mollifier

$$\varrho_\varepsilon(z) = \varepsilon^{-1} \varrho(\varepsilon^{-1} z), \qquad \varrho(z) = \begin{cases} k \exp\left(-\frac{1}{1-|z|^2}\right) & \text{if } |z| \leqslant 1, \\ 0 & \text{if } |z| > 1, \end{cases} \tag{16}$$

with $k > 0$ such that $\int_{\mathbb{R}} \varrho(z) \, \mathrm{d}z = 1$. Let us introduce the smooth regularization of the absolute value function given by $|z|_\varepsilon = \varrho_\varepsilon \star \mathrm{abs}(z)$, where $\mathrm{abs}(z) = |z|$ is the absolute value function. Notice that $|z|_\varepsilon = |z|$ for $|z| \geqslant \varepsilon$ and that

$$\forall z \in \mathbb{R}, \qquad 0 \leqslant |z|_\varepsilon - |z| \leqslant |0|_\varepsilon \leqslant \varepsilon.$$

The first inequality follows from the convexity of the absolute value function, and the second inequality comes from an application of the reverse triangle inequality:

$$|z|_\varepsilon - |z| = \int_{\mathbb{R}} (|z - y| - |z|) \, \varrho_\varepsilon(y) \, \mathrm{d}y \leqslant \int_{\mathbb{R}} |y| \, \varrho_\varepsilon(y) \, \mathrm{d}y = |0|_\varepsilon.$$

Moreover, let $U_\varepsilon \colon \mathbb{D} \to \mathbb{R}$ be the smooth biasing potential given by

$$U_\varepsilon(x) = \begin{cases} \chi_\varepsilon(x) \left(-\log \left| f - I \right|_\varepsilon \right) & \text{if } \mathbb{D} = \mathbb{R}, \\ -\log \left| f - I \right|_\varepsilon & \text{if } \mathbb{D} = \mathbb{T}, \end{cases}$$

where $\chi_\varepsilon = \varrho \star \mathbb{1}_{[-\varepsilon^{-1}, \varepsilon^{-1}]}$. Since $|z|_\varepsilon \geqslant |0|_\varepsilon > 0$ for all $z \in \mathbb{R}$, the function U_ε, which is a regularization of (14), is well-defined everywhere and uniformly bounded from above. The choice of U_*^{iid} as the function we regularize is natural in view of Lemma 2 and the fact that the inequality in (15) is an equality for $U = U_*^{\mathrm{iid}}$.

We now show that $s_f^2[U_\varepsilon]$ converges to the lower bound in (15) in the limit as $\varepsilon \to 0$. We focus in this proof on the case where $\mathbb{D} = \mathbb{R}$, but the reasoning applies verbatim to the case where $\mathbb{D} = \mathbb{T}$. Using (11),

we have that

$$s_f^2[U_\varepsilon] = \frac{Z[U_\varepsilon]}{Z^2} \int_{\mathbb{R}^d} \left(\frac{|f-I|}{|f-I|_\varepsilon^{\chi_\varepsilon}} \right)^2 |f-I|_\varepsilon^{\chi_\varepsilon} \mathrm{e}^{-V}.$$

Since $0 \leqslant \chi_\varepsilon(x) \leqslant 1$ for all $x \in \mathbb{D}^d$, it holds for all $\varepsilon \in (0,1)$ that

$$\begin{cases} |f-I|_\varepsilon^{\chi_\varepsilon} \leqslant (|f-I|+1)^{\chi_\varepsilon} \leqslant |f-I|+1 \\ \dfrac{|f-I|^2}{|f-I|_\varepsilon^{\chi_\varepsilon}} \leqslant |f-I|^{2-\chi_\varepsilon} \leqslant \big(|f-I|+1\big)^{2-\chi_\varepsilon} \leqslant \big(|f-I|+1\big)^2. \end{cases}$$

Since $f \in L^2\left(\mathrm{e}^{-V}\right)$ by assumption, the right-hand sides of these inequalities are integrable. Therefore, using dominated convergence, we obtain that

$$Z[U_\varepsilon] = \int_{\mathbb{R}^d} |f-I|_\varepsilon^{\chi_\varepsilon} \mathrm{e}^{-V} \xrightarrow[\varepsilon \to 0]{} \int_{\mathbb{R}^d} |f-I| \mathrm{e}^{-V}$$

and

$$\int_{\mathbb{R}^d} \left(\frac{|f-I|}{|f-I|_\varepsilon^{\chi_\varepsilon}} \right)^2 |f-I|_\varepsilon^{\chi_\varepsilon} \mathrm{e}^{-V} = \int_{\mathbb{R}^d} \frac{|f-I|^2}{|f-I|_\varepsilon^{\chi_\varepsilon}} \mathrm{e}^{-V} \xrightarrow[\varepsilon \to 0]{} \int_{\mathbb{R}^d} |f-I| \mathrm{e}^{-V}.$$

and so $s_f^2[U_\varepsilon] \to s_f^*$ in the limit as $\varepsilon \to 0$. Since $s_f^2[U] \geqslant s_f^*$ for all $U \in C_\mathrm{c}^\infty(\mathbb{R}^d)$ by (15), we deduce the statement. □

Remark 6. First note that $U_*^{\mathrm{iid}} \in \mathcal{U}_0$. In light of Lemma 2, one may wonder whether $s_f^2[U_*^{\mathrm{iid}}] = s_f^*$. That is to say, is U_*^{iid} *a minimizer* of s_f^2 in $\mathcal{U}_0$? Substitution into (11) reveals that this is not always the case:

$$s_f^2[U_*^{\mathrm{iid}}] = \frac{Z^2}{\mathscr{Z}[U_*^{\mathrm{iid}}]^2} \left(\int_{\mathbb{D}^d} |f-I| \mathrm{d}\mu \right)^2 \geqslant s_f^*. \tag{17}$$

The inequality in this equation is an equality if and only if $\mathscr{Z}[U_*^{\mathrm{iid}}] = Z$ or, equivalently, $f^{-1}(I)$ has zero Lebesgue measure. In particular, if $f^{-1}(I)$ has positive Lebesgue measure, then the biasing potential U_*^{iid} does not achieve the lower bound s_f^*, even though a minimizing sequence that asymptotically achieves the lower bound s_f^* can be constructed by regularizing this potential. △

Example 45 in the appendix illustrates Proposition 4. We explicitly construct in this example a potential function $U \in \mathcal{U} \setminus \mathcal{U}_0$ such that $s_f^2[U] = 0$, as well as a minimizing sequence $(U_\varepsilon)_{\varepsilon>0}$ in $\mathcal{U}_0$ such that $s_f^2[U_\varepsilon] \to s_f^*$ in the limit $\varepsilon \to 0$. The example also illustrates that U_*^{iid} is not necessarily a minimizer in $\mathcal{U}_0$, as mentioned in Remark 6.

This section reveals the difficulties encountered when no regularity of the biasing potential U is assumed. Similar difficulties will be encountered in the analysis of the MCMC estimator (5).

3 Minimizing the asymptotic variance for a single observable

In this section, as in the previous one, we consider a target-oriented approach: we seek the optimal biasing potential U for a given observable f. After presenting the mathematical framework in Subsection 3.1, we first obtain in Subsection 3.2 an expression for the asymptotic variance associated to the estimator (5) in terms of the solution to a Poisson equation where f appears on the right-hand side, and subsequently address the problem of finding the optimal biasing potential U, first in the one-dimensional setting in Subsection 3.3, and then in the multi-dimensional setting in Subsection 3.4.

3.1 Mathematical setting

We will use the following functional spaces:

$$L^2_0(\mu_U) = \left\{ \varphi \in L^2(\mu_U) \,\middle|\, \int_{\mathbb{D}^d} \varphi \, \mathrm{d}\mu_U = 0 \right\}, \qquad H^1(\mu_U) = \left\{ \varphi \in L^2(\mu_U) \,\middle|\, \nabla\varphi \in \left(L^2(\mu_U)\right)^d \right\},$$

where μ_U is the probability measure defined in (4). In the i.i.d. setting, the condition $(f-I)\mathrm{e}^U \in L^2(\mu_U)$ is necessary and sufficient to guarantee that a central limit theorem holds. There does not exist such a simple condition in the MCMC setting, and so, in most of this section, we work under conditions which are only sufficient. Specifically, we denote by $\mathfrak{U}_0 = \mathfrak{U}_0(V, f)$ the set of biasing potentials that satisfy the following assumptions.

Assumption 7.

- *The function U is smooth on $\mathbb{D}^d$.*
- *The function e^{-V-U} is Lebesgue integrable over $\mathbb{D}^d$.*
- *The probability measure μ_U satisfies a Poincaré inequality: there exists $R[U] > 0$ such that*

$$\forall \varphi \in H^1(\mu_U) \cap L^2_0(\mu_U), \qquad \|\varphi\|^2_{L^2(\mu_U)} \leqslant \frac{1}{R[U]} \|\nabla\varphi\|^2_{L^2(\mu_U)}. \tag{18}$$

- *It holds that $(f-I)\,\mathrm{e}^U \in L^2(\mu_U)$.*
- *For any $x_0 \in \mathbb{D}^d$, there exists a unique strong solution X_t to (6) with $X_0 = x_0$.*

In this section, the functions V and f are considered fixed data of the problem, so the dependence of $\mathfrak{U}_0$ on these data is omitted in the notation. However, in Section 4 we will write $\mathfrak{U}_0(V, f)$ to emphasize this dependence where necessary. Just like the set $\mathcal{U}_0$ in Section 2, the set $\mathfrak{U}_0$ in this section contains "nice" biasing potentials. Indeed, the asymptotic behavior of the estimator (5) can be rigorously characterized for $U \in \mathfrak{U}_0$; see Lemma 11.

Remark 8. If $U \in \mathfrak{U}_0$, then the estimator (5) converges to I almost surely as $T \to \infty$ because, by ergodicity,

$$\mu_U^T(f) = \frac{\frac{1}{T}\int_0^T (f\mathrm{e}^U)(X_t)\,\mathrm{d}t}{\frac{1}{T}\int_0^T (\mathrm{e}^U)(X_t)\,\mathrm{d}t} \xrightarrow[T\to\infty]{\text{a.s.}} \frac{\int_{\mathbb{D}^d} (f\mathrm{e}^U)\,\mathrm{d}\mu_U}{\int_{\mathbb{D}^d} (\mathrm{e}^U)\,\mathrm{d}\mu_U} = I.$$

△

Remark 9. In the case where $\mathbb{D} = \mathbb{T}$, a Poincaré inequality of the form (18) always holds provided that $V+U$ is smooth. When $\mathbb{D} = \mathbb{R}$, however, the potential $V+U$ must satisfy appropriate growth conditions to ensure that the inequality holds. For sufficient conditions, see e.g. [5, 8]. We use the Poincaré inequality to establish the central limit theorem, but there are other ways to obtain similar conclusions without directly using the Poincaré inequality, for example by using results of Kipnis–Varadhan or Foster–Lyapunov (see [16] and references within). △

Remark 10. When $\mathbb{D} = \mathbb{T}$, the first item in Assumption 7 implies all the other items, and in this setting $\mathfrak{U}_0 = C^\infty(\mathbb{T}^d) = C^\infty_{\mathrm{c}}(\mathbb{T}^d)$. △

We denote by $\mathcal{L}_U$ the infinitesimal generator on $L^2(\mu_U)$ of the Markov semigroup associated to (6), which is given on $C^\infty_{\mathrm{c}}(\mathbb{D}^d)$ by

$$\mathcal{L}_U = -\nabla(V+U)\cdot\nabla + \Delta = \mathrm{e}^{V+U}\nabla\cdot(\mathrm{e}^{-V-U}\nabla\,\cdot). \tag{19}$$

3.2 Asymptotic variance

The following lemma gives an expression of the asymptotic variance of the estimator $\mu_U^T(f)$ given in (5) in terms of the solution to a Poisson equation.

Lemma 11 (Asymptotic variance)**.** *Suppose that $U \in \mathfrak{U}_0$. Then there exists a unique distributional solution $\phi_U \in H^1(\mu_U) \cap L_0^2(\mu_U)$ to*

$$-\mathcal{L}_U \phi_U = (f - I)\mathrm{e}^U. \tag{20}$$

The solution ϕ_U is smooth and, for Lebesgue almost all initial condition, it holds that

$$\sqrt{T}\big(\mu_U^T(f) - I\big) \xrightarrow[T\to\infty]{\text{Law}} \mathcal{N}\big(0, \sigma_f^2[U]\big),$$

where

$$\sigma_f^2[U] := \frac{2Z[U]^2}{Z^2} \int_{\mathbb{D}^d} |\nabla \phi_U|^2 \mathrm{d}\mu_U = \frac{2Z[U]^2}{Z^2} \int_{\mathbb{D}^d} \phi_U (f - I)\, \mathrm{e}^U \,\mathrm{d}\mu_U. \tag{21}$$

Proof. By density of $C_{\mathrm{c}}^\infty(\mathbb{D}^d)$ in $H^1(\mu_U)$, a function $\phi_U \in H^1(\mu_U) \cap L_0^2(\mu_U)$ is a distributional solution to (20) if and only if

$$\forall \varphi \in H^1(\mu_U) \cap L_0^2(\mu_U), \qquad \int_{\mathbb{D}^d} \nabla \phi_U \cdot \nabla \varphi \,\mathrm{d}\mu_U = \int_{\mathbb{D}^d} (f - I)\mathrm{e}^U \,\varphi \,\mathrm{d}\mu_U. \tag{22}$$

The validity of a Poincaré inequality for μ_U implies that the function space $H^1(\mu_U) \cap L_0^2(\mu_U)$ endowed with the inner product

$$(\varphi_1, \varphi_2) \mapsto \int_{\mathbb{D}^d} \nabla \varphi_1 \cdot \nabla \varphi_2 \,\mathrm{d}\mu_U$$

is a Hilbert space, and that the right-hand side of (22) is a bounded linear functional on this space. Therefore, the Lax–Milgram theorem (or the Riesz representation theorem) yields the existence of a unique solution ϕ_U in $H^1(\mu_U) \cap L_0^2(\mu_U)$. Elliptic regularity theory [20, 18] then implies that $\phi_U \in C^\infty(\mathbb{D}^d)$. From the definition (5) of $\mu_U^T(f)$, we have

$$\sqrt{T}\big(\mu_U^T(f) - I\big) = \frac{\dfrac{1}{\sqrt{T}} \displaystyle\int_0^T \big((f - I)\mathrm{e}^U\big)(X_t)\,\mathrm{d}t}{\dfrac{1}{T} \displaystyle\int_0^T \big(\mathrm{e}^U\big)(X_t)\,\mathrm{d}t}.$$

The numerator converges in law to $\mathcal{N}\big(0, 2\int_{\mathbb{D}^d} |\nabla \phi_U|^2 d\mu_U\big)$, for instance by [10, Theorem 3.1] (the setting there is $\mathbb{R}^d$, but for $\mathbb{T}^d$, the argument using (3) and the martingale central limit theorem, that is essentially [24, Theorem VIII.3.11], works in the same way), while the denominator converges almost surely to $Z/Z[U]$. The claimed convergence in law then follows from Slutsky's lemma. The last equality in (21) follows from the definition (22) of a weak solution. □

Remark 12 (Stability estimate). From the weak formulation (22) and the Poincaré inequality (18), we deduce the stability estimate

$$\|\nabla \phi_U\|_{L^2(\mu_U)} \leqslant \frac{1}{\sqrt{R[U]}} \big\|(f - I)\mathrm{e}^U\big\|_{L^2(\mu_U)}. \tag{23}$$

This standard estimate will be useful in the proof of Lemma 48 in the appendix (for a Poisson equation with a different right-hand side). △

Remark 13. It is instructive to write the counterpart of Lemma 11 for the estimator in the right-most

column and second row of Table 1, which is based on evaluations of the solution to (6) at discrete times:

$$\widetilde{\mu}_U^N := \frac{\sum_{n=0}^{N-1} (f\mathrm{e}^U)(X_{n\tau})}{\sum_{n=0}^{N-1} (\mathrm{e}^U)(X_{n\tau})}. \tag{24}$$

For this estimator, we prove in Lemma 46 that, under appropriate conditions including Assumption 7,

$$\sqrt{N}\left(\widetilde{\mu}_U^N(f) - I\right) \xrightarrow[N\to\infty]{\text{Law}} \mathcal{N}\left(0, \widetilde{\sigma}_f^2[U]\right), \tag{25}$$

with now

$$\widetilde{\sigma}_f^2[U] = \frac{Z[U]^2}{Z^2}\left(2\int_{\mathbb{D}^d} \widetilde{\phi}_U (f-I)\,\mathrm{e}^U\,\mathrm{d}\mu_U - \int_{\mathbb{D}^d} \left|(f-I)\,\mathrm{e}^U\right|^2 \mathrm{d}\mu_U\right), \tag{26}$$

where $\widetilde{\phi}_U$ is the unique solution in $L_0^2(\mu_U)$ to

$$-\widetilde{\mathcal{L}}_U \widetilde{\phi}_U = (f-I)\mathrm{e}^U, \qquad \widetilde{\mathcal{L}}_U := \mathrm{e}^{\tau\mathcal{L}_U} - \mathcal{I}. \tag{27}$$

Here $\mathrm{e}^{t\mathcal{L}_U}$ denotes the Markov semigroup corresponding to the stochastic dynamics (6):

$$\left(\mathrm{e}^{t\mathcal{L}_U}\varphi\right)(x) = \mathbb{E}\big(\varphi(X_t)\big|X_0 = x\big).$$

The asymptotic variance $\widetilde{\sigma}_f^2[U]$ converges to that for the i.i.d. setting given in (11) in the limit as $\tau \to \infty$, and it diverges in the limit as $\tau \to 0$. The latter is not surprising as the correlation between successive samples increases in this limit. However, since formally $\tau\widetilde{\phi}_U \to \phi_U$ in $L_0^2(\mu_U)$ in the limit as $\tau \to 0$, it holds that $\tau\widetilde{\sigma}_f^2[U] \xrightarrow[\tau\to 0]{} \sigma_f^2[U]$. △

3.3 Explicit optimal U in dimension one

In the one-dimensional setting, it is possible to write an explicit expression for the asymptotic variance $\sigma_f^2[U]$, from which an explicit lower bound on $\sigma_f^2[U]$ can be obtained. Our strategy in this section is the following:

- We first obtain an explicit expression for $\sigma_f^2[U]$ for $U \in \mathfrak{U}_0$ (Lemma 14), which we then rewrite in a different form $\widehat{\sigma}_f^2[U]$ given in (34).
- We then observe that $\widehat{\sigma}_f^2[U]$ is defined more generally for $U \in \mathfrak{U} \supset \mathfrak{U}_0$, where $\mathfrak{U}$ is an appropriate superset of $\mathfrak{U}_0$, noting that $\widehat{\sigma}_f^2[U]$ is not necessarily the asymptotic variance of $\mu_U^T(f)$ for $U \in \mathfrak{U}\backslash\mathfrak{U}_0$.
- Next, we show that $\widehat{\sigma}_f^2$ admits an explicit minimizer U_* over $\mathfrak{U}$, with associated minimum σ_f^*. This is proved in Lemma 18.
- Finally, using the expression of U_*, we prove that σ_f^* is the infimum of the actual asymptotic variance $\sigma_f^2[U]$ over $\mathfrak{U}_0$, and that this infimum can be approached within the class of smooth biasing potentials with compact support. This is the content of Proposition 21.

The main result of this section, Proposition 21, and preceding auxiliary result, Lemma 18, should be viewed as the counterparts in the MCMC setting of Proposition 4 and Lemma 2 in the i.i.d. setting.

Lemma 14 (Explicit expression for the asymptotic variance in dimension 1)**.** *For $U \in \mathfrak{U}_0$ and in*

dimension $d = 1$, the asymptotic variance (21) writes

$$\sigma_f^2[U] = \frac{2Z[U]^2}{Z^2} \int_{\mathbb{D}} \left| \left(F - A_{\mathbb{D}}[U]\right) \mathrm{e}^{V+U} \right|^2 \, \mathrm{d}\mu_U, \tag{28}$$

where $F : \mathbb{D} \to \mathbb{R}$ is given by

$$F(x) = \int_0^x \big(f(\xi) - I\big)\mathrm{e}^{-V(\xi)}\mathrm{d}\xi,$$

and

$$A_{\mathbb{D}}[U] = \begin{cases} -\displaystyle\int_{-\infty}^0 \big(f - I\big)\mathrm{e}^{-V} & \text{if } \mathbb{D} = \mathbb{R}, \\ \dfrac{\displaystyle\int_{\mathbb{T}} F\,\mathrm{e}^{V+U}}{\displaystyle\int_{\mathbb{T}} \mathrm{e}^{V+U}} & \text{if } \mathbb{D} = \mathbb{T}. \end{cases} \tag{29}$$

Note that $A_{\mathbb{R}}[U]$ is independent of U; we shall henceforth drop the dependence in the notation. It seems from (29) that $A_{\mathbb{R}}$ and $A_{\mathbb{T}}[U]$ have very different expressions. In fact, the constant $A_{\mathbb{R}}$ may be obtained as a limit of $A_{\mathbb{T}}[U]$ for an increasingly large torus; see Appendix B.

Proof. In dimension one, the Poisson equation (20) reads

$$-\mathrm{e}^{V+U}\left(\mathrm{e}^{-(V+U)}\phi_U'\right)' = (f - I)\mathrm{e}^U. \tag{30}$$

By integration of (30), it holds that

$$\phi_U'(x) = -\left(\int_0^x \big(f(\xi) - I\big)\mathrm{e}^{-V(\xi)}\mathrm{d}\xi - A\right)\mathrm{e}^{(V+U)(x)} = -\big(F(x) - A\big)\mathrm{e}^{(V+U)(x)}, \tag{31}$$

and so

$$\phi_U(x) = B - \int_0^x \big(F(\xi) - A\big)\mathrm{e}^{(V+U)(\xi)}\,\mathrm{d}\xi, \tag{32}$$

for some constants $A \in \mathbb{R}$ and $B \in \mathbb{R}$. The requirement that $\phi_U \in H^1(\mu_U)$ enables to determine the constant A:

- When $\mathbb{D} = \mathbb{T}$, the embedding $H^1(\mu_U) \subset C(\mathbb{T})$ gives that $\phi_U(-\pi) = \phi_U(\pi)$, which leads to the equation for $A_{\mathbb{T}}[U]$ in (29).
- When $\mathbb{D} = \mathbb{R}$, the requirement that $\phi_U \in H^1(\mu_U)$ implies that

$$A = \lim_{x\to\infty} F(x), \tag{33}$$

  where

$$\lim_{x\to\infty} F(x) = \int_0^\infty \big(f(x) - I\big)\mathrm{e}^{-V(x)}\,\mathrm{d}x = -\int_{-\infty}^0 \big(f(x) - I\big)\mathrm{e}^{-V(x)}\,\mathrm{d}x,$$

  because otherwise ϕ_U' in (31) is not in $L^2(\mu_U)$. Indeed, assume for contradiction that

$$\lim_{x\to\infty} F(x) =: L \neq A.$$

  (The limit exists because $(f - I)\mathrm{e}^{-V} \in L^1(\mathbb{R})$ by Assumption 1.) Then there is $K \in \mathbb{R}$ such that

$$\inf_{x \geqslant K} |F(x) - A| \geqslant \frac{1}{2}|L - A|,$$

and so by (31), it holds that

$$\int_{\mathbb{R}} |\phi_U'|^2 \, \mathrm{e}^{-(V+U)} \, \mathrm{d}x \geqslant \frac{1}{4}|L-A|^2 \int_K^\infty \mathrm{e}^{V+U} \, \mathrm{d}x.$$

The right-hand side of this equation is infinite because, by the Cauchy–Schwarz inequality,

$$+\infty = \int_K^\infty \sqrt{\mathrm{e}^{V+U}}\sqrt{\mathrm{e}^{-V-U}} \, \mathrm{d}x \leqslant \int_K^\infty \mathrm{e}^{V+U} \, \mathrm{d}x \int_K^\infty \mathrm{e}^{-V-U} \, \mathrm{d}x.$$

Equation (28) is then obtained by substitution of (31) in (21). □

Remark 15. Once A in (32) has been determined, the value of B can be obtained from the condition that $\phi_U \in L_0^2(\mu_U)$ is mean-zero. This constant is not required for our purposes, because it cancels out in the formula (28) for the asymptotic variance, and so its explicit expression is omitted. △

For all $U \in \mathfrak{U}_0$, the right-hand side of (28) coincides, both when $\mathbb{D} = \mathbb{R}$ and when $\mathbb{D} = \mathbb{T}$, with

$$\widehat{\sigma}_f^2[U] := \frac{2Z[U]}{Z^2} \inf_{A \in \mathbb{R}} \int_{\mathbb{D}} |F-A|^2 \mathrm{e}^{V+U}. \tag{34}$$

Lemma 16. *For all $U \in \mathfrak{U}_0$, it holds that $\sigma_f^2[U] = \widehat{\sigma}_f^2[U]$.*

Proof. When $\mathbb{D} = \mathbb{R}$, the infimum in (34) is achieved for $A = A_{\mathbb{R}}$, because the integral is infinite for any other value of A. Likewise, when $\mathbb{D} = \mathbb{T}$ the infimum in (34) is achieved for $A = A_{\mathbb{T}}[U]$, because the mean under the probability measure proportional to e^{V+U} is the approximation by a constant in the $L^2(\mathrm{e}^{V+U})$ norm; see, for instance, [49, Exercise 1.4.23]. □

With the convention that $0 \cdot +\infty = +\infty \cdot 0 = 0$, the right-hand side of (34) makes sense as an element of $\mathbb{R} \cup \{\infty\}$ for all $U \in \mathfrak{U}$, where $\mathfrak{U} = \mathfrak{U}(V, f)$ is the set of measurable functions $U \colon \mathbb{D} \to \mathbb{R} \cup \{\infty\}$ such that the following assumptions are satisfied:

- It holds that $\mathrm{e}^{-V-U} \in L^1(\mathbb{D}^d)$ and $Z[U] > 0$, so that μ_U is well defined.
- The condition (8) is satisfied.

We emphasize that $\mathfrak{U}$ is a proper superset of $\mathfrak{U}_0$; it contains elements which violate Assumption 7. For biasing potentials not in $\mathfrak{U}_0$, the quantity (34) is not in general an asymptotic variance. In particular, it is possible to construct examples where $\sigma_f^2[U]$ is zero even though $\widehat{\sigma}_f^2[U] > 0$, as we illustrate in Example 17.

Example 17. Consider the setting where $V \colon \mathbb{T} \to \mathbb{R}$ is zero and $f \colon [-\pi, \pi] \to \mathbb{R}$ is given by

$$f(x) = \begin{cases} \operatorname{sgn}(x) & \text{if } |x| \geqslant \frac{\pi}{2}, \\ 0 & \text{otherwise.} \end{cases}, \qquad \operatorname{sgn}(x) := \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x = 0, \\ -1 & \text{if } x < 0. \end{cases} \tag{35}$$

Here we identify $[-\pi, \pi]$ with its image under the quotient map $\mathbb{R} \to \mathbb{T}$. If U is a potential such that (i) there exists a unique strong solution to (6) with initial condition $X_0 = 0$ and (ii) this solution satisfies $X_t \in (-\pi/2, \pi/2)$ with probability 1 for all times, then (5) is a well defined estimator with zero asymptotic variance. However $\widehat{\sigma}_f^2[U] > 0$, which can be viewed from (34) and is confirmed in Lemma 18 hereafter. △

Although $\widehat{\sigma}_f^2$ does not in general correspond to an asymptotic variance, obtaining a bound from below on $\widehat{\sigma}_f^2$ over $\mathfrak{U}$ will be useful in order to motivate the proof of Proposition 21, just like Lemma 2 proved useful for establishing Proposition 4 in the i.i.d. setting.

Lemma 18. *It holds that*

$$\min_{U\in\mathfrak{U}} \widehat{\sigma}_f^2[U] = \frac{2}{Z^2}\bigg(\int_{\mathbb{D}} \big|F(x) - A_{\mathbb{D}}^*\big|\mathrm{d}x\bigg)^2 =: \sigma_f^*, \tag{36}$$

with $A_{\mathbb{R}}^* := A_{\mathbb{R}}$ *and*

$$A_{\mathbb{T}}^* := \sup\bigg\{A \in \mathbb{R} : \int_{\mathbb{T}} \operatorname{sgn}(F - A) \geqslant 0\bigg\}. \tag{37}$$

In addition, the infimum is achieved for

$$U = U_*(x) := -V(x) - \log|F(x) - A_{\mathbb{D}}^*| \in \mathfrak{U}. \tag{38}$$

In this case $\mathrm{e}^{-V-U_*} \propto |F(x) - A_{\mathbb{D}}^*|$.

Proof. It is sufficient to show that, for all $A \in \mathbb{R}$,

$$\frac{2Z[U]}{Z^2}\int_{\mathbb{D}} |F - A|^2 \mathrm{e}^{V+U} \geqslant \frac{2}{Z^2}\bigg(\int_{\mathbb{D}} \big|F(x) - A_{\mathbb{D}}^*\big|\,\mathrm{d}x\bigg)^2. \tag{39}$$

If the left-hand side of (39) is infinite, then the inequality is trivially satisfied. On the other hand, if the left-hand side is finite, in which case the set on which $|F - A|^2\mathrm{e}^{V+U} = \infty$ is of measure zero, then we have by the Cauchy–Schwarz inequality that

$$\frac{2Z[U]}{Z^2}\int_{\mathbb{D}} |F - A|^2 \mathrm{e}^{V+U} = \frac{2}{Z^2}\int_{\mathbb{D}} \mathrm{e}^{-V-U}\int_{\mathbb{D}} |F - A|^2 \mathrm{e}^{V+U} \geqslant \frac{2}{Z^2}\left(\int_{\mathbb{D}} |F - A|\right)^2.$$

In the case $\mathbb{D} = \mathbb{R}$, the right-hand side is finite only if $A = A_{\mathbb{R}}$, which leads to (36). In the case $\mathbb{D} = \mathbb{T}$, the inequality (36) is obtained by noting that

$$\int_{\mathbb{D}} \big|F - A\big| = \mathbb{E}\big|F(X) - A\big|,$$

where $X \sim \mathcal{U}(\mathbb{T})$ is a random variable uniformly distributed on the torus. It is well known, see for example [49, Exercise 1.4.23], that the expectation on the right-hand side is minimized for any A that is a median of $F(X)$. Here F is continuous, so the median of $F(X)$ is unique and given by $A_{\mathbb{T}}^*$, which implies that (36) holds.

The fact that the lower bound is achieved for U in (38) follows from the inequality

$$\begin{aligned}\widehat{\sigma}_f^2[U_*] &= \frac{2Z[U_*]}{Z^2}\inf_{A\in\mathbb{R}}\int_{\mathbb{D}} |F - A|^2\,\mathrm{e}^{V+U_*} \\ &\leqslant \frac{2Z[U_*]}{Z^2}\int_{\mathbb{D}} |F - A_{\mathbb{D}}^*|^2\,\mathrm{e}^{V+U_*} = \frac{2}{Z^2}\left(\int_{\mathbb{D}} |F - A_{\mathbb{D}}^*|\right)^2,\end{aligned}$$

which concludes the proof. □

Remark 19. The singularities in the biasing potential U_* coincide with zeros of the function $F(x) - A_{\mathbb{D}}^*$. Consider for simplicity the case where $\mathbb{D} = \mathbb{R}$. If x_* denotes a zero of the function $F(x) - A_{\mathbb{R}}^*$, then it holds by definition of $F(x)$ that

$$0 = F(x_*) - A_{\mathbb{R}}^* = \int_{-\infty}^{x_*} (f(x) - I)\mathrm{e}^{-V(x)}\,\mathrm{d}x.$$

Rearranging this equation, we obtain

$$\frac{\displaystyle\int_{-\infty}^{x_*} f(x)\,\mathrm{e}^{-V(x)}\,\mathrm{d}x}{\displaystyle\int_{-\infty}^{x_*} \mathrm{e}^{-V(x)}\,\mathrm{d}x} = I.$$

In other words, the average of f with respect to the measure μ restricted to $[-\infty, x_*]$ coincides with its average with respect to μ over the real line. When singular, the biasing potential (38) effectively divides the domain into regions that suffice for the estimation of I. Several numerical experiments illustrating this behavior are presented in Section 5. △

Remark 20. Equation (37) implies that $A^*_{\mathbb{T}}$ is the median associated with $F(X)$, where X is a random variable with uniform distribution over $\mathbb{T}$. Just as $A_{\mathbb{R}}$ is obtained as a limit of $A_{\mathbb{T}}$ for an increasingly large torus, so too $A^*_{\mathbb{R}} = A_{\mathbb{R}}$ is recovered as a limit of $A^*_{\mathbb{T}}$; see Appendix B. △

The potential U_* defined by (38) does not necessarily satisfy Assumption 7, and the measure μ_{U_*} may not have full support. However, regularizing U_* enables to show that σ^*_f is the *infimum* of the asymptotic variance $\sigma^2_f[U]$, not only over $\mathfrak{U}_0$, but also over the smaller subset $C^\infty_{\mathrm{c}} \subset \mathfrak{U}_0$ of smooth and compactly supported biasing potentials. This is the content of the following result. Table 2 after the proof summarizes the main results obtained in this section and presents a comparison with the i.i.d. setting.

Proposition 21. *Suppose that* $0 \in \mathfrak{U}_0$. *Then,*

- *It holds that* $\inf_{U\in\mathfrak{U}_0} \sigma^2_f[U] = \sigma^*_f$.
- *It holds that* $\inf_{U\in C^\infty_{\mathrm{c}}(\mathbb{D})} \sigma^2_f[U] = \sigma^*_f$.

Proof. Since $\sigma^2_f[U] = \widehat{\sigma}^2_f[U]$ for $U \in \mathfrak{U}_0$ and $C^\infty_{\mathrm{c}}(\mathbb{D}^d) \subset \mathfrak{U}_0$, Lemma 18 and the second statement of Proposition 21 imply the first statement. In order to prove the second statement, we use the same notation in this proof as in Proposition 4. Let $U_\varepsilon \colon \mathbb{D} \to \mathbb{R}$ be the smooth biasing potential given by

$$U_\varepsilon(x) = \begin{cases} -\chi_\varepsilon(x)\Big(V(x) + \log\big|F(x) - A^*_{\mathbb{R}}\big|_\varepsilon\Big) & \text{if } \mathbb{D} = \mathbb{R}, \\ -V(x) - \log\big|F(x) - A^*_{\mathbb{T}}\big|_\varepsilon & \text{if } \mathbb{D} = \mathbb{T}, \end{cases}$$

where for $\varepsilon \in (0,1)$, $\chi_\varepsilon = \varrho \star \mathbb{1}_{[-\ell_\varepsilon,\ell_\varepsilon]}$ with $\ell_\varepsilon = \varepsilon^{-1/2} - 1$. (This choice of ℓ_ε enables to write the bound in (42) below.) The probability distribution μ_{U_ε}, with density proportional to $\mathrm{e}^{-V-U_\varepsilon}$, satisfies a Poincaré inequality. This follows from the fact that $\mathrm{e}^{-V-U_\varepsilon}$ is uniformly bounded from below when $\mathbb{D} = \mathbb{T}$, and from the classical Holley–Stroock biasing argument when $\mathbb{D} = \mathbb{R}$; see [23], as for example reviewed in [31, Theorem 2.11]. Therefore $U_\varepsilon \in \mathfrak{U}_0$ and so, by Lemma 14, the associated asymptotic variance is given by

$$\sigma^2_f[U_\varepsilon] = \frac{2Z[U_\varepsilon]}{Z^2} \int_{\mathbb{D}} \big(F - A_\varepsilon\big)^2\,\mathrm{e}^{V+U_\varepsilon}, \tag{40}$$

where $A_\varepsilon := A_{\mathbb{D}}[U_\varepsilon]$ is given by (29) with $U = U_\varepsilon$. We now prove, separately for $\mathbb{D} = \mathbb{T}$ and $\mathbb{D} = \mathbb{R}$, that

$$\lim_{\varepsilon\to 0} Z[U_\varepsilon] \to \int_{\mathbb{D}} |F - A^*_{\mathbb{D}}| \qquad \text{and} \qquad \limsup_{\varepsilon\to 0} \int_{\mathbb{D}} \big(F - A_\varepsilon\big)^2\,\mathrm{e}^{V+U_\varepsilon} \leqslant \int_{\mathbb{D}} \big|F(x) - A^*_{\mathbb{D}}\big|\,\mathrm{d}x.$$

Given these results, taking the limit superior as $\varepsilon \to 0$ in (40) gives

$$\limsup_{\varepsilon\to 0} \sigma^2_f[U_\varepsilon] \leqslant \frac{2}{Z^2}\left(\int_{\mathbb{D}} \big|F(x) - A^*_{\mathbb{D}}\big|\,\mathrm{d}x\right)^2.$$

Since the right-hand side is a lower bound on $\sigma_f^2[U_\varepsilon] = \widehat{\sigma}_f^2[U_\varepsilon]$ by (36), the result will be proved.

Case $\mathbb{D} = \mathbb{T}$. In this setting, it holds by dominated convergence, with an argument similar to the one used to prove the third item of Proposition 4, that

$$Z[U_\varepsilon] = \int_{\mathbb{T}} \big|F - A_{\mathbb{T}}^*\big|_\varepsilon \xrightarrow[\varepsilon\to 0]{} \int_{\mathbb{T}} \big|F - A_{\mathbb{T}}^*\big|.$$

In addition, since A_ε is the average of F over $\mathbb{T}$ with respect to the probability measure with density proportional to $\mathrm{e}^{V+U_\varepsilon}$, it holds for all $\varepsilon \in (0,1)$ that

$$\begin{aligned}\int_{\mathbb{T}} \big|F - A_\varepsilon\big|^2 \mathrm{e}^{V+U_\varepsilon} &= \inf_{C\in\mathbb{R}} \int_{\mathbb{T}} \big|F - C\big|^2 \mathrm{e}^{V+U_\varepsilon} \\ &\leqslant \int_{\mathbb{T}} \big|F - A_{\mathbb{T}}^*\big|^2 \mathrm{e}^{V+U_\varepsilon} = \int_{\mathbb{T}} \frac{\big|F - A_{\mathbb{T}}^*\big|^2}{\big|F - A_{\mathbb{T}}^*\big|_\varepsilon} \leqslant \int_{\mathbb{T}} \big|F - A_{\mathbb{T}}^*\big|,\end{aligned}$$

which enables to conclude.

Case $\mathbb{D} = \mathbb{R}$. The numerator of the fraction on the right-hand side of (40) can be written as

$$\begin{aligned}Z[U_\varepsilon] &= \int_{\mathbb{R}} \exp\Big(- V(x) + \chi_\varepsilon(x)\big(V(x) + \log\big|F(x) - A_{\mathbb{R}}^*\big|_\varepsilon\big)\Big)\,\mathrm{d}x \\ &= \int_{\mathbb{R}} \exp\big((\chi_\varepsilon - 1)V\big)|F - A_{\mathbb{R}}^*|_\varepsilon^{\chi_\varepsilon}. \end{aligned} \tag{41}$$

By convexity of the exponential function, it holds that

$$\begin{aligned}\exp\big((1-\chi_\varepsilon)(-V) + \chi_\varepsilon \log|F - A_{\mathbb{R}}^*|_\varepsilon\big) &\leqslant (1-\chi_\varepsilon)\mathrm{e}^{-V} + \chi_\varepsilon|F - A_{\mathbb{R}}^*|_\varepsilon \\ &\leqslant \mathrm{e}^{-V} + \chi_\varepsilon\big(|F - A_{\mathbb{R}}^*| + \varepsilon\big) \\ &\leqslant \mathrm{e}^{-V} + |F - A_{\mathbb{R}}^*| + \varepsilon\chi_\varepsilon.\end{aligned}$$

Since $\varepsilon = (\ell_\varepsilon + 1)^{-2}$, all three terms on the right-hand side are dominated by an integrable function over $\mathbb{R}$ independent of ε, because

$$\forall x \in \mathbb{R}, \qquad \varepsilon\chi_\varepsilon(x) \leqslant \frac{\mathbb{1}_{[-\ell_\varepsilon-1,\ell_\varepsilon+1]}(x)}{(\ell_\varepsilon+1)^2} \leqslant \min\left\{1, \frac{1}{x^2}\right\}. \tag{42}$$

Therefore, by dominated convergence, we deduce from (41) that $Z[U_\varepsilon] \to \int_{\mathbb{R}}|F - A_{\mathbb{R}}^*|$ in the limit as $\varepsilon = (\ell_\varepsilon+1)^{-2} \to 0$. For the integral on the right-hand side of (40), noting that $A_\varepsilon = A_{\mathbb{R}}^*$ and recalling that this constant is independent of U, we have that

$$\begin{aligned}\int_{\mathbb{R}} (F - A_\varepsilon)^2 \mathrm{e}^{V+U_\varepsilon} &= \int_{\mathbb{R}} |F - A_{\mathbb{R}}^*|^2 \exp\Big((1-\chi_\varepsilon)V + \chi_\varepsilon\big(-\log|F - A_{\mathbb{R}}^*|_\varepsilon\big)\Big) \\ &\leqslant \int_{\mathbb{R}} |F - A_{\mathbb{R}}^*|^2 \left((1-\chi_\varepsilon)\mathrm{e}^V + \frac{\chi_\varepsilon}{|F - A_{\mathbb{R}}^*|_\varepsilon}\right) \\ &\leqslant \int_{\mathbb{R}\setminus B_{\ell_\varepsilon-1}} |F - A_{\mathbb{R}}^*|^2 \mathrm{e}^V + \int_{\mathbb{R}} |F - A_{\mathbb{R}}^*|,\end{aligned} \tag{43}$$

where we used the convexity of the exponential function and the notation $B_{\ell_\varepsilon-1} = [-\ell_\varepsilon + 1, \ell_\varepsilon - 1]$. Since $\sigma_f^2[0]$ is finite, so is $\int_{\mathbb{R}}|F - A_{\mathbb{R}}^*|^2\mathrm{e}^V$, implying that the first term on the right-hand side of (43) converges to 0 in the limit $\varepsilon \to 0$. □

	Minimal assumptions	"Nice" biasing potentials	C_c^∞
i.i.d. setting (any d)	$\inf_{U\in\mathcal{U}} s_f^2[U] = 0$	$\inf_{U\in\mathcal{U}_0} s_f^2[U] = s_f^*$	$\inf_{U\in C_c^\infty(\mathbb{D}^d)} s_f^2[U] = s_f^*$
MCMC setting ($d = 1$)	$\inf_{U\in\mathfrak{U}} \sigma_f^2[U] \leqslant \sigma_f^*$	$\inf_{U\in\mathfrak{U}_0} \sigma_f^2[U] = \sigma_f^*$	$\inf_{U\in C_c^\infty(\mathbb{D})} \sigma_f^2[U] = \sigma_f^*$

Table 2: Summary of the main results obtained in Subsection 3.3, and comparison with the corresponding results in the i.i.d. setting obtained in Section 2. See (13) and (36) respectively for the definitions of s_f^* and σ_f^*. Concerning the infimum of the asymptotic variance under minimal assumptions in the MCMC setting and $d = 1$, we showed in Example 17 that there are cases where $\sigma_f^* > 0$ but the minimum over $\mathfrak{U}$ of the asymptotic variance for the MCMC estimator is 0. It may be possible to prove, by extending the reasoning in the proof of Proposition 4, that the infimum of the asymptotic variance of the MCMC estimator (5) is 0 for any potential V and observable f satisfying Assumption 1, but we do not address this question here.

Remark 22. The results in Proposition 21 parallel the second and third items in Proposition 4. We do not aim at rigorously establishing an analogue of the first item in Proposition 4, which would require analyzing the well-posedness of (6) and the properties of the estimator (5) when the biasing potential is irregular and unbounded. △

Remark 23. Since $U_* \in \mathfrak{U}$ defined in (38) is a minimizer of $\widehat{\sigma}_f^2$, and since the lower bound σ_f^* on $\sigma_f^2[U]$ may be approached by regularizing this potential, we often refer to U_* as *the optimal biasing potential*. This is, of course, a slight abuse of terminology given that U_* is not in general a minimizer of the actual asymptotic variance $\sigma_f^2[U]$, neither on $\mathfrak{U}$ (because an asymptotic variance smaller than σ_f^* can sometimes be achieved) nor on $\mathfrak{U}_0$ (because it does not hold that $U_* \in \mathfrak{U}_0$ in general). △

Remark 24. To conclude this section, we note that the parallel between the i.i.d. and MCMC settings is not perfect: while $\sigma_f^2[U]$ and $\widehat{\sigma}_f^2[U]$ coincide for $U \in \mathfrak{U}_0$ in the MCMC setting, $s_f^2[U]$ and $\widehat{s}_f^2[U]$ do not generally coincide for $U \in \mathcal{U}_0$ in the i.i.d. setting. △

3.4 Optimal U in the multi-dimensional setting via steepest descent

In the multi-dimensional setting, obtaining an explicit expression for the optimal biasing U is not possible. However, analogously to [12], the functional derivative of the asymptotic variance with respect to the biasing potential can be expressed in terms of the solution to a Poisson equation. This enables a numerical strategy based on a steepest descent for finding a good biasing potential.

Computation of the functional derivative

In the following, the directional derivative of a functional $E : C^\infty(\mathbb{D}^d) \to \mathbb{R}$ at $U \in C^\infty(\mathbb{D}^d)$ in the direction $\delta U \in C_c^\infty(\mathbb{D}^d)$ is denoted by

$$\mathrm{d}E[U] \cdot \delta U = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\big(E[U + \varepsilon\delta U] - E[U]\big), \tag{44}$$

whenever the limit exists.

Theorem 25 (Functional derivative of the asymptotic variance)**.** *Suppose that $U \in \mathfrak{U}_0$ and let ϕ_U be as in Lemma 11. Then for all $\delta U \in C_c^\infty(\mathbb{D}^d)$, it holds that*

$$\begin{aligned}\frac{1}{2}\mathrm{d}\sigma_f^2[U]\cdot\delta U &:= \frac{1}{2}\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\big(\sigma_f^2[U+\varepsilon\delta U]-\sigma_f^2[U]\big)\\ &= \frac{Z[U]^2}{Z^2}\int_{\mathbb{D}^d}\delta U\left(|\nabla\phi_U|^2-\int_{\mathbb{D}^d}|\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{d}\mu_U. \end{aligned}\tag{45}$$

Proof. We first rewrite (21) as

$$\sigma_f^2[U]=\frac{2Z[U]^2}{Z^2}\int_{\mathbb{D}^d}\phi_U(f-I)\mathrm{e}^U\,\mathrm{d}\mu_U=\frac{2Z[U]}{Z^2}\int_{\mathbb{D}^d}\phi_U(f-I)\mathrm{e}^{-V},$$

so that the only factors depending on U are $Z[U]$ and ϕ_U. By definition of the functional derivative, using (22) for the first integral term on the right-hand side, we have

$$\frac{1}{2}\mathrm{d}\sigma_f^2[U]\cdot\delta U=\frac{\mathrm{d}Z[U]\cdot\delta U}{Z^2}\int_{\mathbb{D}^d}|\nabla\phi_U|^2\mathrm{e}^{-V-U}+\lim_{\varepsilon\to 0}\frac{Z[U]}{\varepsilon Z^2}\int_{\mathbb{D}^d}(\phi_{U+\varepsilon\delta U}-\phi_U)(f-I)\mathrm{e}^{-V},\tag{46}$$

where $\phi_{U+\varepsilon\delta U}$ is the solution to the perturbed Poisson equation

$$-\mathcal{L}_{U+\varepsilon\delta U}\phi_{U+\varepsilon\delta U}=(f-I)\mathrm{e}^{U+\varepsilon\delta U}.\tag{47}$$

The function $(f-I)\mathrm{e}^{U+\varepsilon\delta U}$ has zero mean with respect to $\mu_{U+\varepsilon\delta U}$. By Assumption 7 and the fact that $\delta U\in C_c^\infty(\mathbb{D}^d)$, it holds that $(f-I)\mathrm{e}^{U+\varepsilon\delta U}\in L^2(\mathrm{e}^{-V-U-\varepsilon\delta U})$ and that $\mu_{U+\varepsilon\delta U}$ satisfies a Poincaré inequality, by the Holley–Stroock theorem. Consequently, there exists a unique solution in $L_0^2(\mathrm{e}^{-V-U-\varepsilon\delta U})$ to (47) by Lemma 11. A simple calculation using the fact that $\delta U\in C_c^\infty(\mathbb{D}^d)$ gives

$$\mathrm{d}Z[U]\cdot\delta U=-\int_{\mathbb{D}^d}\delta U\mathrm{e}^{-V-U}.\tag{48}$$

For the second term on the right-hand side of (46), we have by Lemma 48 that

$$\begin{aligned}\frac{1}{\varepsilon}\int_{\mathbb{D}^d}(\phi_{U+\varepsilon\delta U}-\phi_U)(f-I)\mathrm{e}^{-V} &= -\frac{1}{\varepsilon}\int_{\mathbb{D}^d}(\phi_{U+\varepsilon\delta U}-\phi_U)(\mathcal{L}_U\phi_U)\,\mathrm{e}^{-V-U}\\ &= \frac{1}{\varepsilon}\int_{\mathbb{D}^d}\nabla(\phi_{U+\varepsilon\delta U}-\phi_U)\cdot\nabla\phi_U\,\mathrm{e}^{-V-U}\xrightarrow[\varepsilon\to 0]{}\int_{\mathbb{D}^d}\nabla\psi_{U,\delta U}\cdot\nabla\phi_U\,\mathrm{e}^{-V-U}\\ &= \int_{\mathbb{D}^d}(\mathcal{L}_U\psi_{U,\delta U})\phi_U\,\mathrm{e}^{-V-U}=\int_{\mathbb{D}^d}\Big(-\mathrm{e}^{U+V}\nabla\cdot\big(\mathrm{e}^{-U-V}\delta U\nabla\phi_U\big)\Big)\phi_U\,\mathrm{e}^{-V-U}\\ &= \int_{\mathbb{D}^d}\delta U|\nabla\phi_U|^2\,\mathrm{e}^{-V-U},\end{aligned}$$

where $\psi_{U,\delta U}$ is the solution to the Poisson equation (62). The equalities before and after the limit follow from the definitions of ϕ_U and $\psi_{U,\delta U}$ as weak solutions to (20) and (62), respectively. The last inequality is obtained by integration by parts, which is justified because δU is compactly supported. Combining this equation with (46) and (48), we deduce (45). □

Before presenting the numerical method for approaching the optimal biasing potential U, we mention two corollaries of Theorem 25.

Corollary 26 (Critical points)**.** *Suppose that $U\in\mathfrak{U}_0$. Then U is a critical point of the asymptotic variance viewed as a functional of U if and only if the corresponding solution to the Poisson equation (20) satisfies*

$$|\nabla\phi_U|^2=\int_{\mathbb{D}^d}|\nabla\phi_U|^2\mathrm{d}\mu_U.\tag{49}$$

In other words, the norm of $\nabla\phi_U$ is constant over $\mathbb{D}^d$.

Corollary 27 (No smooth minimizer)**.** *Let $\mathbb{D} = \mathbb{T}$. Then there is no biasing potential $U \in C^\infty(\mathbb{T}^d)$ that is a critical point of the asymptotic variance $\sigma_f^2[U]$.*

Proof. Assume for contradiction that there is a smooth biasing potential U for which (49) holds. By elliptic regularity, the corresponding solution ϕ_U to the Poisson equation (20) is also smooth and so, by the extreme value theorem, it attains its minimum at some point in $\mathbb{T}^d$, where $\nabla\phi_U$ vanishes. By (49), this implies that $\nabla\phi_U = 0$ for all $x \in \mathbb{T}^d$ and, therefore, $-\mathcal{L}_U\phi_U = 0 = (f - I)\,\mathrm{e}^U$. This is a contradiction because, by Assumption 1, the observable f is not everywhere equal to I. □

Corollary 27 highlights a limitation of the target-oriented approach taken in this section, as singular potentials are impractical at the numerical level and unlikely to be of any use for different observables. This motivates the approach taken in Section 4, which aims at finding a biasing potential U that leads to a reduction in variance for not just one but a family of observables.

Steepest descent method

To conclude this section, we present an iterative approach for approximating a minimizer of $\sigma_f^2[U]$. We focus on the case where $\mathbb{D} = \mathbb{T}$ for simplicity, but the approach is easy to generalize to other settings (see Subsection 4.2). Since an expression for the functional derivative of $\sigma_f^2[U]$ is available by Theorem 25, we employ a method based on steepest descent. Each step of the method may be decomposed into three stages:

- First, an approximate solution to the Poisson equation (20) is computed. A number of numerical methods can be employed to this end. Given that the optimal potential always exhibits singularities when $\mathbb{D} = \mathbb{T}$, we opt for a finite difference approach rather than, for example, a spectral method [2, 48]. The details of the finite difference method are presented in Appendix D, together with a convergence proof in the setting where U is regular.
- Then, from the solution to (20), an approximation of the gradient G of the asymptotic variance is calculated based on Theorem 25.
- Finally, the potential U is updated according to $U \leftarrow U - \eta\, G$, where η is found by backtracking line search following Armijo's method [6].

These steps are repeated until the $L^2(\mathbb{T})$ norm of the gradient is sufficiently small. A couple of comments are in order. First, the expression of G depends on the considered Hilbert functional space. By (45), the functions

$$G_{L^2(\mathrm{e}^{-V-U})} = \frac{Z[U]}{Z^2}\left(|\nabla\phi_U|^2 - \int |\nabla\phi_U|^2\,\mathrm{d}\mu_U\right),$$

$$G_{L^2(\mathrm{e}^{-V})} = \frac{Z[U]}{Z^2}\left(|\nabla\phi_U|^2 - \int |\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-U}, \tag{50}$$

$$G_{L^2(\mathbb{T})} = \frac{Z[U]}{Z^2}\left(|\nabla\phi_U|^2 - \int |\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-U-V}, \tag{51}$$

are all ascent directions for $\sigma_f^2[U]$, corresponding to the gradients in $L^2(\mathrm{e}^{-V-U})$, in $L^2(\mathrm{e}^{-V})$ and in $L^2(\mathbb{T})$, respectively. Of these three options, the latter two are better suited for use in an optimization method. Indeed, employing the $L^2(\mathrm{e}^{-V-U})$ derivative would lead to a change of metric with each update of U, which precludes the use of methods that rely on information from multiple steps, such as the Barzilai–Borwein method [9]. In the numerical experiments presented in Section 5, we use (51), but good results can also be obtained by using (50).

Second, the gradient needs to be discretized in practice. In order to avoid convergence issues, it is desirable that the discretized gradient is itself the gradient of a function. Therefore, we use the discretization given in (88), which is guaranteed to be the gradient of an appropriate discretization of the asymptotic variance; see Proposition 63.

4 Minimizing the asymptotic variance for a class of observables

Assume that the set of observables of which we want to compute the expectation is well described by a Gaussian random field

$$f = \sum_{j=1}^{J} \sqrt{\lambda_j} u_j f_j, \qquad u_j \sim \mathcal{N}(0,1), \qquad \lambda_j \in (0,\infty), \tag{52}$$

where $(f_j)_{1 \leqslant j \leqslant J}$ are given functions from $\mathbb{D}^d$ to $\mathbb{R}$ and the random variables $(u_j)_{1 \leqslant j \leqslant J}$ are independent. This equation defines a probability distribution $\mathcal{F}$ on the space of observables as the pushforward of the finite-dimensional Gaussian measure $\mathcal{G} = \mathcal{N}(0, \mathrm{id}_J)$ on $\mathbb{R}^J$; the probability measure $\mathcal{F}$ assigns a probability 1 to $\mathrm{Span}(f_1, \ldots, f_J)$. One may wonder whether it is possible to minimize the average asymptotic variance for observables drawn from this distribution. For clarity, we denote by $\mathbb{E}_{\mathcal{F}}$ expectations with respect to observables. Within this section, we also use the notation

$$\mathfrak{U}_0 = \bigcap_{j=1}^{J} \mathfrak{U}_0(V, f_j), \qquad \mathfrak{U} = \bigcap_{j=1}^{J} \mathfrak{U}(V, f_j),$$

where $\mathfrak{U}_0(V, f_j)$ and $\mathfrak{U}(V, f_j)$ are the sets defined before Assumption 7 and after (34), respectively. These sets are assumed to be non-empty in this section. Denoting by ϕ the solution in $H^1(\mu_U) \cap L^2_0(\mu_U)$ to

$$-\mathcal{L}_U \phi = (f - I)\mathrm{e}^U,$$

and assuming that $U \in \mathfrak{U}_0$, we have by Lemma 11 that

$$\begin{aligned} \mathbb{E}_{\mathcal{F}}\left[\sigma_f^2[U]\right] &= \mathbb{E}_{\mathcal{F}}\left[\frac{2Z[U]}{Z^2} \int_{\mathbb{D}^d} \phi(f - I)\mathrm{e}^{-V}\right] \\ &= \frac{2Z[U]}{Z^2} \mathbb{E}_{\mathcal{G}}\left[\sum_{j=1}^{J}\sum_{k=1}^{J} u_j u_k \sqrt{\lambda_j \lambda_k} \int_{\mathbb{D}^d} \phi_k (f_j - I_j)\mathrm{e}^{-V}\right], \end{aligned}$$

where, for $1 \leqslant j \leqslant J$, the function ϕ_j is the unique solution in $H^1(\mu_U) \cap L^2_0(\mu_U)$ to the Poisson equation $-\mathcal{L}_U \phi_j = (f_j - I_j)\mathrm{e}^U$, with $I_j := \mu(f_j)$. Since $\mathbb{E}_{\mathcal{G}}[u_j u_k] = \delta_{jk}$, we obtain by rearranging the previous expression that

$$\sigma^2[U] := \mathbb{E}_{\mathcal{F}}\left[\sigma_f^2[U]\right] = \frac{2Z[U]}{Z^2} \sum_{j=1}^{J} \lambda_j \int_{\mathbb{D}^d} \phi_j (f_j - I_j)\mathrm{e}^{-V} = \sum_{j=1}^{J} \lambda_j \sigma_{f_j}^2[U]. \tag{53}$$

Therefore, minimizing the expectation $\mathbb{E}_{\mathcal{F}}[\sigma_f^2]$ amounts to minimizing the sum on the right-hand side of (53).

4.1 Optimal biasing potential in the one-dimensional setting with $\mathbb{D} = \mathbb{R}$

In the one-dimensional setting with $\mathbb{D} = \mathbb{R}$, an explicit expression for the infimum of the asymptotic variance can be obtained, similar to that Lemma 18 in the case of a single observable. In order to state

a precise result, we introduce the notation

$$\widehat{\sigma}^2[U] = \sum_{j=1}^{J} \lambda_j \widehat{\sigma}^2_{f_j}[U],$$

where $\widehat{\sigma}^2_g$ for an observable g was defined in (34). Let us recall that, by the reasoning in Subsection 3.3, the quantity $\widehat{\sigma}^2[U]$ coincides with $\sigma^2[U]$ in (53) when $U \in \mathfrak{U}_0$, but $\widehat{\sigma}[U]$ is well-defined more generally for any $U \in \mathfrak{U}$. In Lemma 29 below, we give a bound from below on $\widehat{\sigma}^2[U]$ in the particular case where $d = 1$ and $\mathbb{D} = \mathbb{R}$. Before presenting this result, we introduce the notation

$$F_j(x) = \int_0^x \big(f_j(\xi) - I_j\big)\mathrm{e}^{-V(\xi)}\mathrm{d}\xi, \qquad A_{\mathbb{R},j} = -\int_{-\infty}^0 \big(f_j(\xi) - I_j\big)\mathrm{e}^{-V(\xi)}\mathrm{d}\xi.$$

Remark 28. In the rest of this section, F_j and $A_{\mathbb{R},j}$ always appear together as $F_j - A_{\mathbb{R},j}$, which can be rewritten as an integral over $(-\infty, x]$ with the same integrand as in the definition of F_j, that is to say

$$F_j(x) - A_{\mathbb{R},j} = \int_{-\infty}^x \big(f_j(\xi) - I_j\big)\mathrm{e}^{-V(\xi)}\,\mathrm{d}\xi.$$

For the sake of conciseness, we could introduce a new notation to refer to $F_j - A_{\mathbb{R},j}$, but we refrain from doing so in order to keep the notation consistent with that used in Section 3. △

Lemma 29. *Assume that $d = 1$ and $\mathbb{D} = \mathbb{R}$. Then, for all $U \in \mathfrak{U}$, it holds that*

$$\min_{U\in\mathfrak{U}} \widehat{\sigma}^2(U) = \frac{2}{Z^2}\left(\int_{\mathbb{R}} \sqrt{\sum_{j=1}^{J} \lambda_j |F_j - A_{\mathbb{R},j}|^2}\right)^2. \tag{54}$$

The minimum is achieved for

$$U = U_* := -V - \log\left(\sqrt{\sum_{j=1}^{J} \lambda_j |F_j - A_{\mathbb{R},j}|^2}\right) \in \mathfrak{U}. \tag{55}$$

In this case e^{-V-U_*} is proportional to $\sqrt{\sum_{j=1}^J \lambda_j |F_j - A_{\mathbb{R},j}|^2}$.

Proof. We first show that $\widehat{\sigma}^2[U]$ is bounded from below by the right-hand side of (54). This is trivial if $\widehat{\sigma}^2[U]$ is infinite, so we assume from now on that $\widehat{\sigma}^2[U] < \infty$. Using the definition of $\widehat{\sigma}^2[U]$, we have

$$\widehat{\sigma}^2[U] = \sum_{j=1}^{J} \lambda_j \widehat{\sigma}^2_{f_j}[U] = \frac{2Z[U]}{Z^2}\int_{\mathbb{R}} \left(\sum_{j=1}^{J} \lambda_j |F_j - A_{\mathbb{R},j}|^2\right)\mathrm{e}^{V+U}. \tag{56}$$

Here, we used that the infimum in the definition (34) of $\widehat{\sigma}^2_{f_j}$ is achieved for $A = A_{\mathbb{R},j}$, as explained in Lemma 16. Let us introduce the notation

$$G = \sqrt{\sum_{j=1}^{J} \int_{\mathbb{R}} \lambda_j |F_j - A_{\mathbb{R},j}|^2}.$$

Since $\widehat{\sigma}^2[U] < \infty$ by assumption, the set over which $G^2\mathrm{e}^{V+U}$ takes an infinite value is of zero Lebesgue measure. Therefore, by the Cauchy–Schwarz inequality,

$$\widehat{\sigma}^2[U] = \frac{2Z[U]}{Z^2}\int_{\mathbb{R}} |G|^2\mathrm{e}^{U+V} \geqslant \frac{2}{Z^2}\left(\int_{\mathbb{R}} |G|\sqrt{\mathrm{e}^{U+V}}\sqrt{\mathrm{e}^{-V-U}}\right)^2 = \frac{2}{Z^2}\left(\int_{\mathbb{R}} G\right)^2.$$

The claim that U_* in (55) achieves the lower bound can be verified by substitution in (56). $\square$

Remark 30. Notice that, unless the functions $(F_j - A_{\mathbb{R},j})_{1\leqslant j\leqslant J}$ share a common root, the optimal biasing potential U_* in (55) is a smooth function. $\triangle$

In the same way that we obtained Proposition 21 from Lemma 18, we deduce from Lemma 29 the following result. The proof is a simple adaptation of that of Proposition 21, so we omit it.

Proposition 31. *Assume that $d = 1$ and $\mathbb{D} = \mathbb{R}$, and suppose that $0 \in \mathfrak{U}_0$. Then*

$$\inf_{U\in\mathfrak{U}_0} \sigma^2[U] = \inf_{U\in C_c^\infty(\mathbb{R})} \sigma^2[U] = \frac{2}{Z^2}\left(\int_{\mathbb{R}} \sqrt{\sum_{j=1}^J \lambda_j |F_j - A_{\mathbb{R},j}|^2}\right)^2 .$$

4.2 Numerical optimization

A result similar to Lemma 29 is not easily available when $d = 1$ and $\mathbb{D} = \mathbb{T}$, because the constant $A_{\mathbb{T}}$ given in (29) depends on U. In this case or in the multi-dimensional setting, one can resort to a steepest descent approach in order to find the optimal biasing potential. It is easy to prove, based on Theorem 25, that the functional derivative of $\sigma^2[U]$ is given by

$$\frac{1}{2}\mathrm{d}\sigma^2[U]\cdot\delta U = \frac{Z[U]^2}{Z^2}\int_{\mathbb{D}^d}\left(\delta U - \int_{\mathbb{D}^d}\delta U\,\mathrm{d}\mu_U\right)\left(\sum_{j=1}^J \lambda_j|\nabla\phi_j|^2\right)\mathrm{d}\mu_U. \tag{57}$$

The approach presented in Subsection 3.4 can then be applied *mutatis mutandis*. Numerical experiments illustrating the potential found as a result of this procedure are presented in Section 5.

4.3 Free energy biasing

In the molecular dynamics literature, variance reduction over a compact state space is often achieved by *free energy biasing*, a heuristic approach which, in the absence of coarse graining via a reaction coordinate, amounts to setting $U = -V$; see [31] and the references therein. To conclude this section, we address the following related question: is there a probability distribution $\mathcal{F}$ on observables such that $U = -V$ is a minimizer of the average asymptotic variance $\sigma^2[U]$, i.e. for which energy biasing is optimal? While we will not be able to provide a definite answer to this question, we shall prove in Proposition 32 that, for an appropriate probability measure on observables, the biasing $U = -V$ corresponds to a critical point of $\sigma^2[U]$. This does not imply that $U = -V$ is necessarily optimal, because $\sigma^2[U]$ is not convex in general; see Remark 56 in Appendix C.

Proposition 32. *Suppose that $\mathbb{D} = \mathbb{T}$ with $d = 1$ and assume, for $J \in 2\mathbb{N}_{>0}$, that $(f_j, \lambda_j)_{1\leqslant j\leqslant J}$ are the J first eigenfunctions and eigenvalues of the operator $\mathcal{K} = \mathrm{e}^V(-\Delta + \tau^2\mathcal{I})^{-\alpha}\mathrm{e}^{-V}$, where $\alpha \in (0,\infty)$ and $\tau \in \mathbb{R}$ are parameters of the random field and $\mathcal{K}$ is viewed as a compact self-adjoint operator on the following space of functions defined on $\mathbb{T}$:*

$$\left\{f \in L^2\left(\mathrm{e}^{-2V}\right) : \int_{\mathbb{T}} f\mathrm{e}^{-V} = 0\right\}.$$

Then the average asymptotic variance $\sigma^2[U]$ admits a critical point for $U = -V$.

Proof. The eigenfunctions of the operator $\mathcal{K}$ are given by

$$f_j(x) = \mathrm{e}^V \begin{cases} \sin\left(\dfrac{j+1}{2}x\right), & \text{if } j \text{ is odd,} \\ \cos\left(\dfrac{j}{2}x\right), & \text{if } j \text{ is even.} \end{cases} \tag{58}$$

Note that $I_j = 0$ for all $1 \leqslant j \leqslant J$. When $U = -V$, the generator of the Markov semigroup associated with (6) is just the Laplacian operator. Therefore, for a given $j \in \{1, \ldots, J\}$, the solution to the Poisson equation $-\mathcal{L}_U \phi_j = (f_j - I_j)\mathrm{e}^U$ is given by

$$\phi_j(x) = \left\lceil \frac{j}{2} \right\rceil^{-2} f_j(x).$$

Since $\lambda_j = \lambda_{j+1}$ for all odd values of j and since $\sin^2 + \cos^2 = 1$, we deduce that the sum on the right-hand side of (57) is constant, implying that the functional derivative of $\sigma^2[U]$ is zero when evaluated at the biasing potential $U = -V$. □

Remark 33. The choice of the operator $\mathcal{K}$ is motivated by the form (48) of the desired observables, which is itself motivated by the fact that these observables lead to Poisson equations with explicit trigonometric solutions when $U = -V$. △

Remark 34. In this section, we assumed for simplicity that the random observable admitted a finite expansion of the form (52). The results we obtained could in principle be extended to the case of a more general Gaussian field, with an infinite Karhunen–Loève series. For background on Gaussian variables in infinite dimension, see for example [41, Section 1.5]. The reference [13] is also useful for understanding the regularity of infinite series of the form (52). △

5 Examples and numerical experiments

We begin in Subsection 5.1 by presenting examples and numerical experiments in dimension 1. Then, in Subsection 5.2, we present numerical experiments for the case where the state space is $\mathbb{T}^2$ and the optimal biasing potential is approximated by steepest descent. Finally, in Subsection 5.3, we illustrate the approach proposed in Section 4.

5.1 One-dimensional examples

In this subsection, we present a few examples illustrating the optimal biasing potential U for various observables and underlying potentials V. In all the figures, the optimal potential depicted is calculated numerically using the steepest descent approach presented in Subsection 3.3. It is apparent in Examples 36 and 37 that this approach indeed yields the optimal biasing potential (38), an explicit expression of which is given in these examples.

The first few examples aim at illustrating settings where the optimal biasing potential exhibits different levels of singularity. The optimal potential is smooth in Example 35, it exhibits two singularity points in Example 36, and it blows up over a whole interval in Example 37. In these examples, the reference probability measure is unimodal, and the gain in asymptotic variance obtained from using the optimal potential is small. Finally, in example Example 38, a multi-modal reference probability measure is considered, and it is observed that importance sampling enables a considerable decrease in asymptotic variance in this case. Without loss of generality, we normalize in the figures the potentials U so that the minimum value of $V + U$ over the domain considered is 0.

Example 35. Assume that $\mathbb{D} = \mathbb{R}$ and $f = V'$. Then $I = 0$ and $F(x) - A_{\mathbb{R}} = \mathrm{e}^{-V(x)}$; in this case, the optimal biasing potential (38) is $U_* = 0$. $\triangle$

Example 36. Assume that $\mathbb{D} = \mathbb{T}$, $V = 0$ and $f(x) = \cos(x)$. Then $I = 0$ and $F(x) = \sin(x)$. The constant $A^*_{\mathbb{T}}$ in (37) is 0, and so the optimal biasing potential (38) is given by

$$U_*(x) = -\log|\sin(x)|.$$

This potential is illustrated in Figure 1 together with the corresponding measure μ_{U_*}. Notice that the singularities divide the domain into the two regions $[-\pi, 0]$ and $[0, \pi]$, but the average of f with respect to e^{-V} conditioned to either region is equal to $I = 0$, in accordance with the discussion in Remark 19.

When $U = 0$, the solution to the Poisson equation (20) is given by $\phi(x) = \cos(x)$ and $Z = 1$, so the asymptotic variance (28) is given by

$$\sigma_f^2[U = 0] = 2 \int_{-\pi}^{\pi} |\sin(x)|^2 \, \frac{\mathrm{d}x}{2\pi} = 1.$$

The infimum (36) of the asymptotic variance, on the other hand, is given by

$$\frac{2}{Z^2} \left(\int_{\mathbb{T}} \big| F(x) - A^*_{\mathbb{T}} \big| \mathrm{d}x \right)^2 = 2 \left(\int_{\mathbb{T}} \big| \sin(x) \big| \frac{\mathrm{d}x}{2\pi} \right)^2 = \frac{8}{\pi^2} = 0.810\ldots$$

The optimal biasing potential therefore leads a reduction in variance of about 19%. $\triangle$

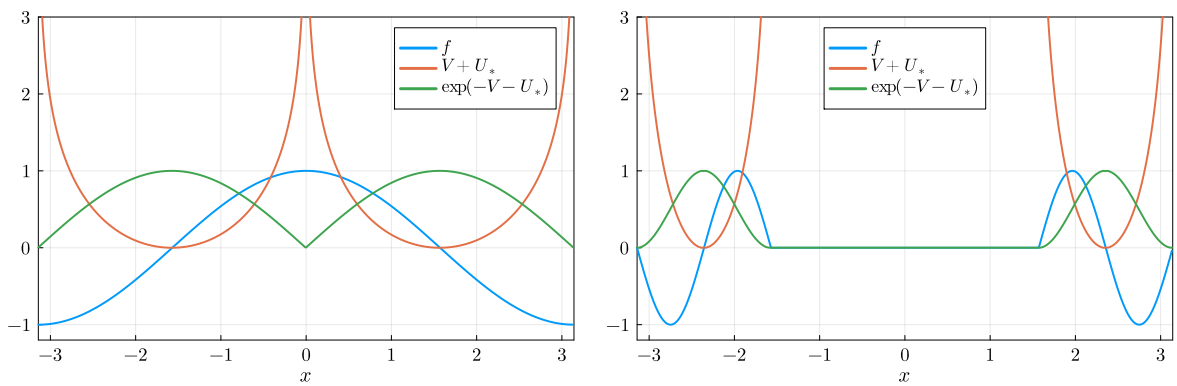

Figure 1: Optimal potential for Example 36 (left) and Example 37 (right).

As we show above in Corollary 27, singularities in the optimal biasing potential are inevitable when the state space is the torus in any dimension. Moreover, it is possible to construct examples where the optimal measure μ_{U_*} is supported on a subset of $\mathbb{T}$, as shown in the following example.

Example 37. Consider the case where $\mathbb{D} = \mathbb{T}$ and $V(x) = 0$, with the observable

$$f(x) = \begin{cases} \sin(4|x|) & \text{if } |x| \geqslant \frac{\pi}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

Then $I = 0$ and

$$F(x) = \int_0^x f(\xi)\, \mathrm{e}^{-V(\xi)} \, \mathrm{d}\xi = \begin{cases} \frac{1}{4}\big(-1 + \cos(4x)\big) & \text{if } x \leqslant -\frac{\pi}{2}, \\ \frac{1}{4}\big(1 - \cos(4x)\big) & \text{if } x \geqslant \frac{\pi}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

The constant $A^*_{\mathbb{T}}$ in (37) is again zero, and so the optimal biasing potential is $U_*(x) = -\log|F(x)|$. The optimal biasing potential and the corresponding measure μ_{U_*} for this example are depicted in Figure 1. As the figure illustrates, the Lebesgue density of μ_{U_*} with respect to the Lebesgue measure is zero over the interval $[-\pi/2, \pi/2]$. △

To conclude this section, we present an example where using the biasing potential U_* leads to a significant decrease of the variance.

Example 38. Consider again the case where $\mathbb{D} = \mathbb{T}$, with this time $V(x) = 5\cos(2x)$ and the observable $f(x) = \sin(x)$. The reference dynamics, i.e. the dynamics (6) with $U = 0$, is metastable in view of the high potential barrier; the asymptotic variance when $U = 0$ for the observable considered, estimated numerically from (28), is equal to 3459 after rounding to the closest integer.

The optimal total potential $V + U_*$ and probability distribution μ_{U_*} are depicted in Figure 2. The asymptotic variance associated with U_* is about 3.64, roughly 1000 times smaller than the asymptotic variance for the reference dynamics. △

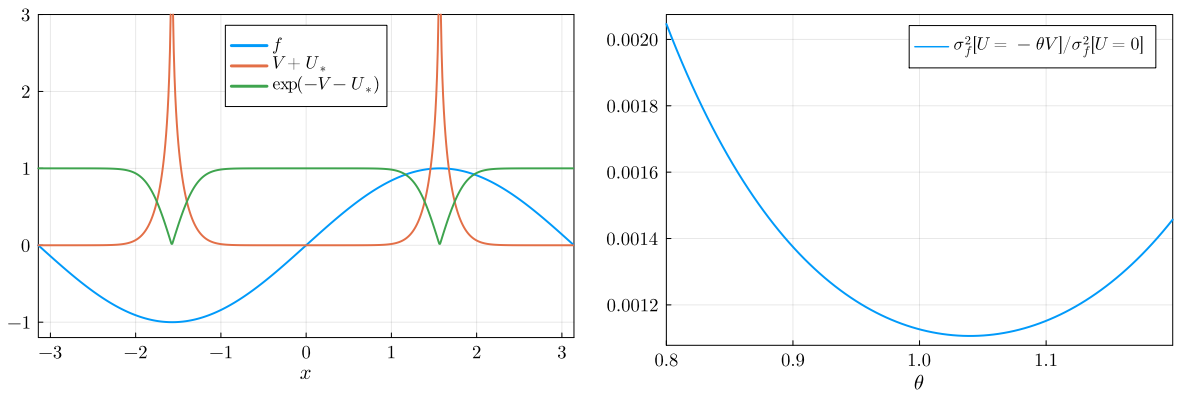

Figure 2: Optimal potential for Example 38 (left), and asymptotic variance corresponding to the biasing potential $U = -\theta V$ over the range $[0.8, 1.2]$ of values for θ.

The numerical values of the asymptotic variance for the examples considered in this section and different choices of U are summarized in Table 3. We also present in this table, for each of the examples, the value of the asymptotic variance corresponding to case where $U = -\theta V$, for the value of θ that yields the largest variance reduction. This approach is found to yield a variance reduction close to the optimal one in the setting of Example 38.

Test case	$U = 0$	$U = -V$	$U = -\theta_* V$	Optimal U
Example 36	1	1	1	0.811
Example 37	1	1	1	0.334
Example 38	1	0.00113	0.00111 ($\theta_* = 1.038$)	0.00105

Table 3: Ratio of the asymptotic variance of the importance sampling estimator (5) relative to its value in the case where $U = 0$, for different choices of the biasing potential U and in the one-dimensional setting. The parameter θ_* is the minimizer of $\sigma_f^2[-\theta_* V]$, calculated by using the `Optim.jl` [40] implementation of the LBFGS solver. The numbers are rounded to 3 significant digits.

5.2 Two-dimensional examples

By Corollary 27, the optimal potential when the domain is the two-dimensional torus $\mathbb{T}^2$ also exhibits singularities. In all the examples presented hereafter, these are line singularities. In order to approximate

the optimal potential in the numerical experiments presented in this section, we use the steepest descent approach presented in Subsection 3.4 with 150×150 discretization points. We begin in Examples 39 and 40 by considering cases where the reference dynamics does not suffer from metastability. The gain in asymptotic variance provided by importance sampling is small in these settings. Then, in Example 41, we consider a setting where the reference measure is multi-modal, for which importance sampling leads to a considerable decrease in asymptotic variance.

Example 39. We consider the case where the potential is $V(x) = 0$ and the observable is $f(x) = \sin(x_1) + \sin(x_2)$. This observable has average zero not only with respect to μ, but also with respect to the restrictions of this measure to the subsets $[-\pi/2, \pi/2] \times [-\pi/2, \pi/2]$, $[-\pi/2, \pi/2] \times [\pi/2, 3\pi/2]$, $[\pi/2, 3\pi/2] \times [-\pi/2, \pi/2]$, and $[\pi/2, 3\pi/2] \times [\pi/2, 3\pi/2]$ which together form a partition of $\mathbb{T}^2$. Here we identify subsets of $\mathbb{R}^2$ with their image under the quotient map $\mathbb{R}^2 \to \mathbb{T}^2$. Interestingly, the total potential $V + U$ corresponding to the optimal biasing potential exhibits singularities precisely at the boundaries between these regions, effectively dividing the state space into four separate regions; see Figure 3. It appears clearly from the right panel in the same figure that, in agreement with Corollary 26, the solution to the corresponding Poisson equation (20) is affine by parts, with discontinuities of the first derivative at singularities of $V + U$. The reduction in asymptotic variance corresponding to the optimal potential in this case is only about 19%. △

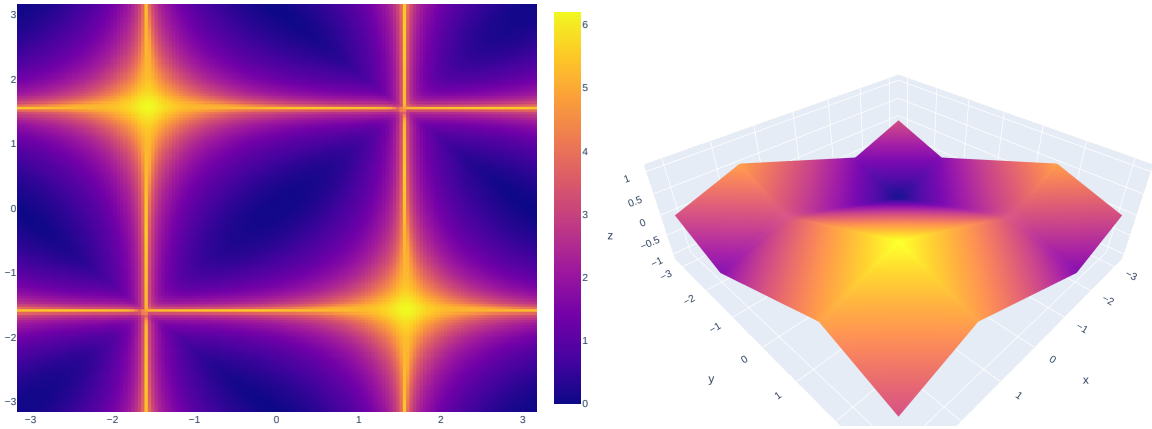

Figure 3: Optimal potential $V + U$ for Example 39 (left), together with the solution to the associated Poisson equation (20) (right).

We now present an example with a non-uniform reference distribution μ.

Example 40. In this example, we consider that the potential and observable are given by

$$V(x) = \exp\left(\cos(x_1)\sin(x_2) + \frac{1}{5}\cos(3x_1)\right), \qquad f(x) = \sin\Big(x_1 + \cos(x_2)\Big)^3.$$

The potential V and observable f are illustrated respectively in the top left and right panels of Figure 4. The corresponding optimal total potential $V + U$, together with the associated solution to the Poisson equation (20), are depicted in the bottom left and right panels respectively. Once again, it appears that the optimal potential divides the domain into two separate regions where the averages of f are the same. The reduction in asymptotic variance obtained by employing the perturbed dynamics (6) is about 20%. △

To conclude this section, we present an example where the target probability distribution is multi-modal, in which case a considerable reduction of the asymptotic variance can be achieved.

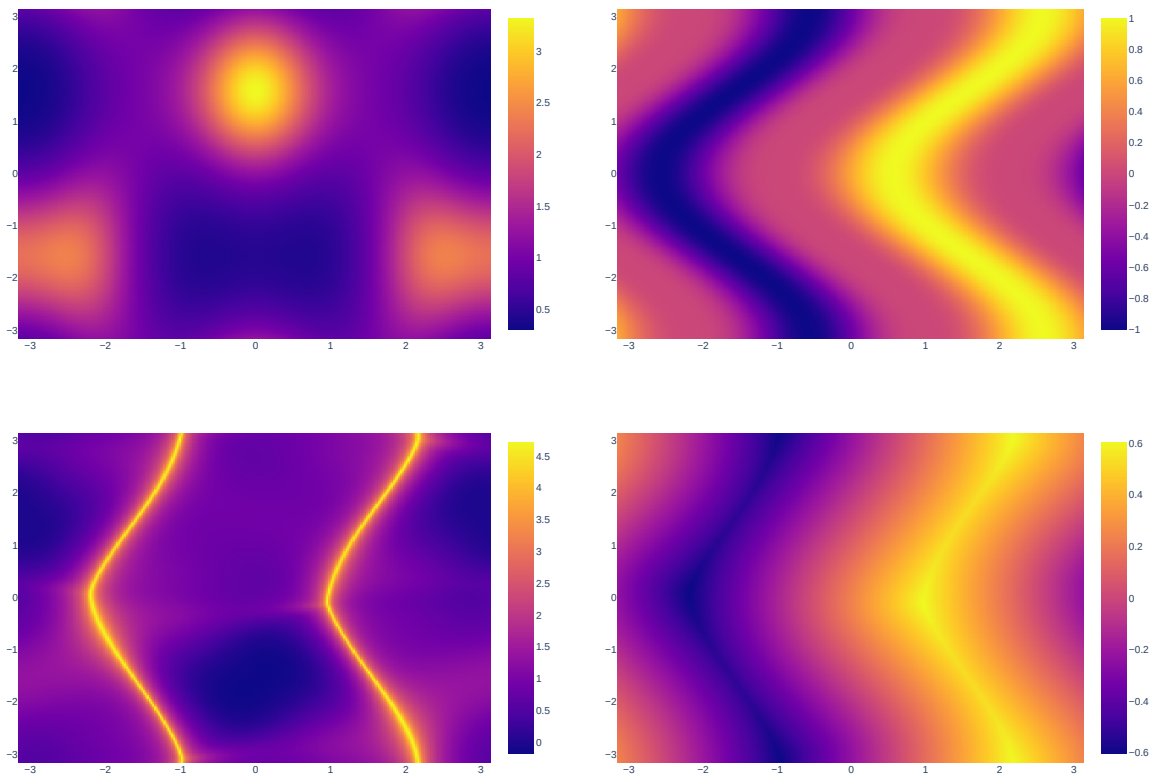

Figure 4: Unperturbed potential V (top left), observable f (top right), optimal potential $V + U_*$ (bottom left), and corresponding solution to the Poisson equation ϕ_U (bottom right) for Example 40.

Example 41. We consider the case where $V(x) = 2\cos(2x_1) - \cos(x_2)$ and $f(x) = \sin(x_1)$. The potential $V(x)$ has two global minima located at $(\pi/2, 0)$ and $(-\pi/2, 0)$, and the observable $f(x)$ takes different values when evaluated at these points. The optimal total potential $V + U$ is illustrated in Figure 5. We observe two line singularities which effectively divide the domain into two separate regions where the average of f is equal to $I = 0$. The reduction in asymptotic variance obtained by employing the perturbed dynamics (6) is about 86%. △

The numerical values of the asymptotic variances for the examples considered in this section and different choices of U are collated in Table 4. The asymptotic variances corresponding to the simple biasing with $U = -\theta V$ with optimal θ are also presented. This approach is found to perform quite well in the multimodal setting of Example 41.

Test case	$U = 0$	$U = -V$	$U = -\theta_* V$	Optimal U
Example 39	1	1	1	0.811
Example 40	1	0.997	0.987 ($\theta_* = 0.614$)	0.804
Example 41	1	0.177	0.177 ($\theta_* = 0.994$)	0.132

Table 4: Ratio of the asymptotic variance of the importance sampling estimator (5) relative to its value in the case where $U = 0$, for different choices of the biasing potential U and in the two-dimensional setting. The parameter θ_* is the minimizer of $\sigma_f^2[-\theta_* V]$, calculated by using the `Optim.jl` [40] implementation of the LBFGS solver. The numbers are rounded to 3 significant digits.

Remark 42. In all the examples presented in this subsection, the optimal biasing potential effectively partitions the domain into several regions that suffice for the estimation of I. It is natural to wonder whether this observation holds true in general: is it *always* the case that, when such partitioning of

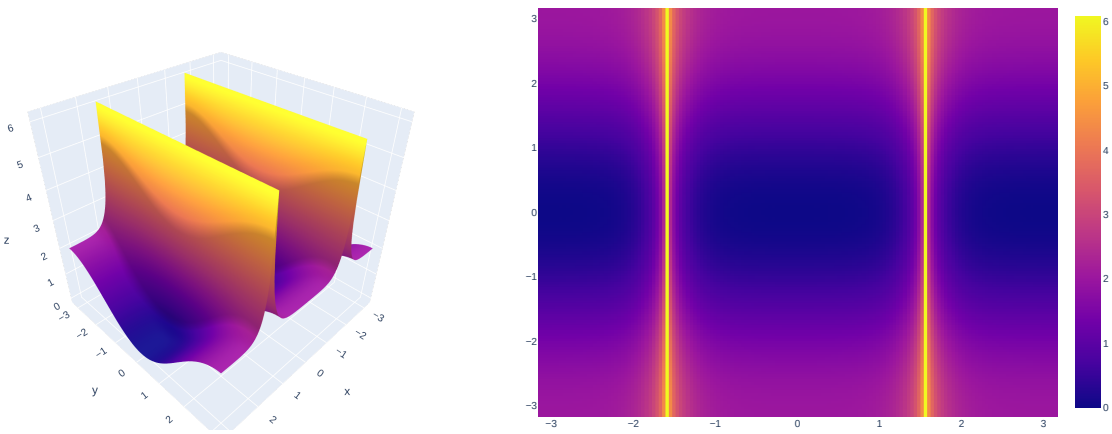

Figure 5: Optimal potential $V + U_*$ for Example 41.

the domain occurs, averages of the observable with respect to the corresponding conditioned measures coincide with the target average I? We gave in Remark 19 a positive answer to this question in the one-dimensional setting. Although we are not able to provide an equally rigorous answer in the multi-dimensional setting, we motivate hereafter our belief that the answer is also positive in this case. To this end, suppose that U_* partitions the domain into a number of regions, corresponding to the connected components of $\{U_* < \infty\}$. Suppose also that there exists an ensemble $(U_\varepsilon)_{\varepsilon>0}$ of smooth biasing potentials such that $\sigma_f^2[U_\varepsilon] \to \sigma_f^2[U_*]$ and $\mathrm{e}^{-V-U_\varepsilon} \to \mathrm{e}^{-V-U_*}$ in $L^\infty(\mathbb{D}^d)$ as $\varepsilon \to 0$. In particular, it holds under this assumption that $U_\varepsilon(x) \to U_*(x)$ for almost all $x \in \{U_* < \infty\}$. It is well known, see e.g. [41, Section 7.3], that the average escape time from a potential well for the overdamped Langevin dynamics (6) scales exponentially with respect to the height of the potential barrier. Therefore, for very small ε, it would take a very long time for the dynamics to visit all the regions of the state space. In these conditions, the asymptotic variance would be very large, unless the averages of the observable with respect to the probability measure μ conditioned to each of the regions happen to coincide. More precisely, if $\sigma_f^2[U_\varepsilon]$ does not diverge as $\varepsilon \to 0$, then the conditional averages in all the regions must necessarily coincide. △

5.3 Minimizing the asymptotic variance for a class of observables

In this section, we illustrate the approach proposed in Section 4, first for a one-dimensional example and then for a two-dimensional example.

Example 43. We consider the same potential as in Example 38, i.e. $V(x) = 5\cos(2x)$, and a set-up similar to that of Proposition 32. Specifically, the observables and associated weights, denoted by $(\lambda_j)_{1\leqslant j\leqslant J}$ in (52), are given by the first $J = 21$ eigenpairs of the operator $(-\Delta+\mathcal{I})^{-1}$, equipped with periodic boundary conditions on the space of mean-zero functions with respect to the Lebesgue measure. The associated Gaussian random field f is stationary, in the sense that the covariance $\mathrm{cov}\big(f(x_1), f(x_2)\big)$ depends only on the difference $x_1 - x_2$. The optimal potential in this case is illustrated in the left panel of Figure 6. In contrast with the examples of Subsection 5.1, the optimal potential is smooth and, therefore, more easily usable in an MCMC scheme. The average asymptotic variance $\sigma^2[U]$ given in (53) is reduced by a factor equal to about 900.

In the right-panel of Figure 6, we illustrate the optimal potential when the observables are instead the eigenfunctions of $\mathrm{e}^V(-\Delta+\mathcal{I})^{-1}\mathrm{e}^{-V}$ equipped with periodic boundary conditions, which is precisely the setting considered in Proposition 32. In this case, the optimal potential is indeed $V + U = 0$, in agreement with the latter result. The average asymptotic variance $\sigma^2[U]$ is reduced by a factor equal to

about 700. △

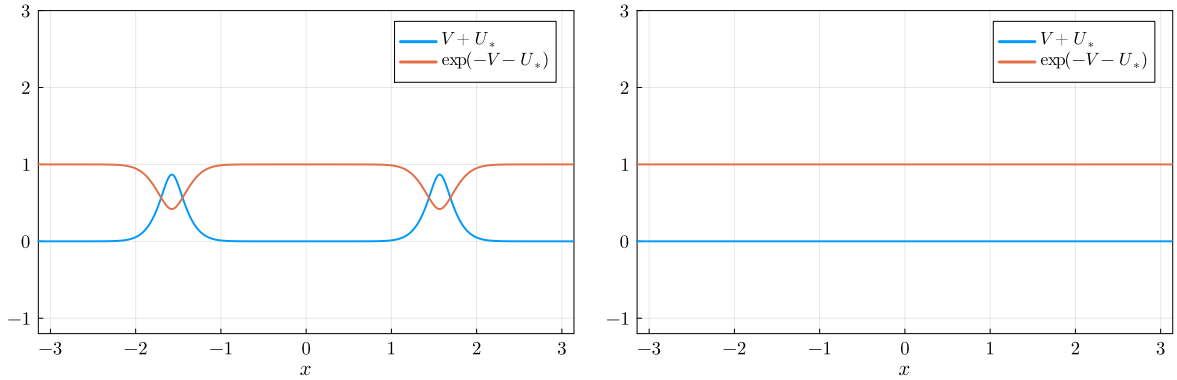

Figure 6: Optimal potentials for Example 43, when different probability measures are placed on the observables.

Example 44. We consider the same potential as in Example 41, i.e. $V(x) = 2\cos(2x_1) - \cos(x_2)$. For the observables and corresponding weights in (52), we take the eigenpairs of the operator $(-\Delta + \mathcal{I})^{-1}$ with periodic boundary conditions on the space of mean-zero functions with respect to the Lebesgue measure. The eigenfunctions are of the form

$$\cos(mx_1)\cos(nx_2), \qquad \cos(mx_1)\sin(nx_2), \qquad \sin(mx_1)\cos(nx_2), \qquad \sin(mx_1)\sin(nx_2).$$

We consider all the eigenpairs with $m \leqslant 4$ and $n \leqslant 4$. The optimal potential $V + U_*$ in this case is depicted in Figure 7, together with the initial potential V. We observe that the potential has been flattened in the direction x. The resulting reduction in the average asymptotic variance is about 70%. △

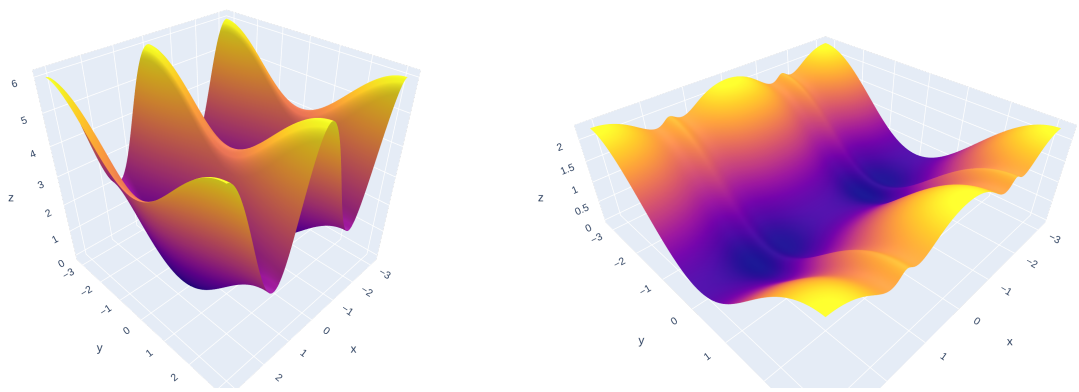

Figure 7: Potential V (left) and optimal potential $V + U_*$ (right) corresponding to Example 44.

6 Conclusions and perspectives for future works

In this work, we considered an importance sampling method based on the overdamped Langevin dynamics in a perturbed potential and present a novel approach for constructing the biasing potential. Under appropriate assumptions, this potential is optimal, in the sense that it leads to the minimum asymptotic variance when employed for calculating the average of one or a class of observables with respect to

the target probability measure. The optimal biasing potential is explicit in dimension 1, and may be approximated by steepest descent in higher dimensions.

We demonstrated the performance of the method by means of numerical experiments in dimensions 1 and 2. In the multimodal setting, in particular, using the optimal importance distribution enables a considerable reduction in asymptotic variance. Finally, our numerical experiments show that, while minimizing the asymptotic variance for just one observable leads to singularities in the potential, targeting a number of observables simultaneously leads to smooth potentials which can more easily be employed in numerical schemes.

A drawback of the proposed methodology is that the construction of the optimal biasing potential relies on an iterative method which, at each step, requires the solution of a Poisson equation. While feasible in low dimension, this approach is computationally too costly in a high-dimensional setting. A possible approach in this case is to reduce the dimension of the problem by requiring that the biasing potential is a function of only a few well-chosen degrees of freedom (so-called collective variables), which ideally capture the metastable behavior of the dynamics. This corresponds to the setting of free energy computation [30], and suggests to consider the variance as a functional of some free energy, which particularly makes sense when the observable under investigation itself depends only on the collective variables. Investigation of this approach will be the subject of future work. Another direction for future work would be to investigate whether a similar approach can be employed to minimize the asymptotic variance of estimators based on discrete-time MCMC schemes using overdamped Langevin dynamics. We expect the resulting optimal biasing potentials in that case to be close to those considered here.

A Technical auxiliary results

In this section, we collect technical auxiliary results used in Sections 2 and 3.

Example 45. Consider the setting where $\mathbb{D} = \mathbb{T}$ in dimension $d = 1$ and $V = 0$, with the observable $f\colon [-\pi, \pi] \to \mathbb{R}$ given by

$$f(x) = \begin{cases} \operatorname{sgn}(x) & \text{if } |x| \geqslant \frac{\pi}{2}, \\ 0 & \text{otherwise.} \end{cases}$$

where the sgn function is defined in (35). Here we identify $[-\pi, \pi]$ with its image under the quotient map $\mathbb{R} \to \mathbb{T}$. In this case $I = 0$ and we have the following:

- If U is such that $\mathrm{e}^{-U} = \mathbb{1}_{[-\pi/4,\pi/4]}$, where $\mathbb{1}_S$ is the indicator function of the set S, then it holds that $f(X^n) = I$ and $\mathrm{e}^U(X^n)$ with probability 1 for $X^n \sim \mu_U$, and so

$$s_f^2[U] = 0.$$

  This is in agreement with the first item in Proposition 4. In this particular case, 0 is not only the infimum but also the minimum of the asymptotic variance over $\mathcal{U}$.

- The variance in (13) is given by

$$s_f^* := \left(\frac{1}{2\pi}\int_{\mathbb{T}} |f - I|\right)^2 = \frac{1}{4}.$$

- The potential U_*^{iid} in (14) is given by $U_*^{\mathrm{iid}} = -\log|f|$. If $X^n \sim \mu_{U_*^{\mathrm{iid}}}$, then the random variable $f(X^n)$ is equal to either -1 and 1, each with probability $1/2$, and the random variable $(\mathrm{e}^U)(X^n)$

is equal to 1 almost surely. Therefore, the associated asymptotic variance is given by

$$s_f^2[U_*^{\mathrm{iid}}] = 1.$$

This equation can also be obtained from (11). We observe that $s_f^2[U_*^{\mathrm{iid}}] > s_f^*$, which is consistent with the discussion in Remark 6.

- Let $U_\varepsilon := -\log(|f| + \varepsilon)$, which may be viewed as a discontinuous but bounded regularization of U_*^{iid}. Then, for $X^n \sim \mu_{U_\varepsilon}$, using the notation w. p. to mean "with probability", we have that

$$\left(f\mathrm{e}^{U_\varepsilon}\right)(X^n) = \begin{cases} \frac{1}{1+\varepsilon} & \text{w. p. } \frac{1+\varepsilon}{2+4\varepsilon} \\ 0 & \text{w. p. } \frac{2\varepsilon}{2+4\varepsilon} \\ -\frac{1}{1+\varepsilon} & \text{w. p. } \frac{1+\varepsilon}{2+4\varepsilon} \end{cases}, \qquad \left(\mathrm{e}^{U_\varepsilon}\right)(X^n) = \begin{cases} \frac{1}{1+\varepsilon} & \text{w. p. } \frac{1+\varepsilon}{2+4\varepsilon} \\ \frac{1}{\varepsilon} & \text{w. p. } \frac{2\varepsilon}{2+4\varepsilon} \\ \frac{1}{1+\varepsilon} & \text{w. p. } \frac{1+\varepsilon}{2+4\varepsilon} \end{cases}.$$

It follows that the variance of $\left(f\mathrm{e}^{U_\varepsilon}\right)(X^n)$ is given by

$$\frac{1+\varepsilon}{1+2\varepsilon}\left(\frac{1}{1+\varepsilon}\right)^2 = \frac{1}{(1+2\varepsilon)(1+\varepsilon)},$$

and that $\mathbb{E}\left[\mathrm{e}^{U_\varepsilon}(X^n)\right] = \frac{2}{1+2\varepsilon}$. Therefore, by Slutsky's lemma, or from Equation (11), we obtain that

$$s_f^2[U_\varepsilon] = \frac{1+2\varepsilon}{4+4\varepsilon}.$$

We observe that $s_f^2[U_\varepsilon] \to s_f^*$ in the limit as $\varepsilon \to 0$.

This example shows that the biasing potential U_*^{iid} is sometimes suboptimal in $\mathcal{U}_0$; here we constructed a regularized biasing potential associated with a smaller asymptotic variance than that associated with U_*^{iid}. Furthermore, this example illustrates that the quantity s_f^* is not in general a lower bound on the asymptotic variance over the set of biasing potentials in $\mathcal{U}$. △

Lemma 46 (Asymptotic variance for the estimator given in (24))**.** *Suppose that Assumption 7 is satisfied, that $\mathbb{D} = \mathbb{T}$ and that $X_0 \sim \mu_U$. Then there exists a unique solution $\widetilde{\phi}_U$ in $L_0^2(\mu_U)$ to (27) and it holds that*

$$\sqrt{N}\left(\widetilde{\mu}_U^N(f) - I\right) \xrightarrow[N\to\infty]{\text{Law}} \mathcal{N}\left(0, \widetilde{\sigma}_f^2[U]\right),$$

where $\widetilde{\sigma}_f^2[U]$ is given by (26).

Remark 47. The assumptions that $\mathbb{D} = \mathbb{T}$ and $X_0 \sim \mu$ should be viewed as technical; it should in principle be possible to relax them. △

Proof. We begin by showing the existence and uniqueness of a solution in $L_0^2(\mu_U)$ to the Poisson equation (27). To this end, we recall that, under Assumption 7,

$$\|\mathrm{e}^{t\mathcal{L}_U}\|_{\mathcal{B}\left(L_0^2(\mu_U)\right)} \leqslant \mathrm{e}^{-R[U]t}, \tag{59}$$

where $\mathcal{B}\left(L_0^2(\mu_U)\right)$ is the Banach space of continuous linear operators on $L_0^2(\mu_U)$ and $R[U]$ is the Poincaré constant in (18) associated with μ_U; see e.g. [31, Proposition 2.3] and [41, Theorem 4.4]. Therefore, the Neumann series $\sum_{n=0}^{\infty} \mathrm{e}^{n\tau\mathcal{L}_U}$ is convergent in $L_0^2(\mu_U)$, which implies that $\mathcal{I} - \mathrm{e}^{\tau\mathcal{L}_U}$ is invertible with inverse $(\mathcal{I} - \mathrm{e}^{\tau\mathcal{L}_U})^{-1}$ equal to the series. Therefore, there exists a unique solution $\widetilde{\phi}_U \in L_0^2(\mu_U)$ to (27).

The estimator (7) may be rewritten as

$$\widetilde{\mu}_U^N(f) = I + \frac{\sum_{n=0}^{N-1} g(X_{n\tau})}{\sum_{n=0}^{N-1} (\mathrm{e}^U)(X_{n\tau})}, \qquad g := (f - I)\mathrm{e}^U. \tag{60}$$

The key idea in order to understand the asymptotic behavior of the numerator in (60) is to rewrite the sum as

$$\begin{aligned}\sum_{n=0}^{N-1} g(X_{n\tau}) &= \sum_{n=0}^{N-1} \left(\left(\mathcal{I} - \mathrm{e}^{\tau \mathcal{L}_U} \right) \widetilde{\phi}_U \right) (X_{n\tau}) \\ &= \sum_{n=0}^{N-1} \left(\widetilde{\phi}_U \left(X_{(n+1)\tau} \right) - \mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U \left(X_{n\tau} \right) \right) - \widetilde{\phi}_U \left(X_{N\tau} \right) + \widetilde{\phi}_U(X_0).\end{aligned}$$

This approach dates back to the work of Kipnis and Varadhan [25]. The first term is a sum of uncorrelated, identically distributed random variables with mean zero and variance

$$\begin{aligned}\gamma_f^2[U] := \mathbb{E}\left(\left| \widetilde{\phi}_U \left(X_\tau \right) - \mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U \left(X_0 \right) \right|^2 \right) &= \int_{\mathbb{D}^d} \left(\left(\mathrm{e}^{\tau \mathcal{L}_U} \left| \widetilde{\phi}_U \right|^2 \right)(x) - \left| \left(\mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U \right)(x) \right|^2 \right) \mu_U(\mathrm{d}x) \\ &= \int_{\mathbb{D}^d} \left(\left| \widetilde{\phi}_U(x) \right|^2 - \left| \left(\mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U \right)(x) \right|^2 \right) \mu_U(\mathrm{d}x),\end{aligned}$$

where we used the invariance of μ_U by the dynamics with generator $\mathcal{L}_U$ for the first term in the last integral. Since $\widetilde{\phi}_U$ is a solution to (27), it holds that $\mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U = \widetilde{\phi}_U - g$, which by substitution gives that

$$\gamma_f^2[U] = \int_{\mathbb{D}^d} 2\widetilde{\phi}_U g - g^2 \, \mathrm{d}\mu_U.$$

Using an approach similar to that in [39, Theorem 17.4.4], we can show that the conditions of the martingale central limit theorem [22] (see also [34] for a detailed pedagogical proof) are satisfied, and so it holds that

$$\frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \left(\widetilde{\phi}_U \left(X_{(n+1)\tau} \right) - \mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\phi}_U \left(X_{n\tau} \right) \right) \xrightarrow[N \to \infty]{\text{Law}} \mathcal{N}\left(0, \gamma_f^2[U]\right).$$

Hence, since it is clear in the setting where $\mathbb{D} = \mathbb{T}$ that

$$\frac{1}{\sqrt{N}} \left(\widetilde{\phi}_U \left(X_{N\tau} \right) - \widetilde{\phi}_U(X_0) \right) \xrightarrow[N \to \infty]{\text{Law}} 0,$$

it follows from Slutsky's lemma that

$$\frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} g(X_{n\tau}) \xrightarrow[N \to \infty]{\text{Law}} \mathcal{N}\left(0, \gamma_f^2[U]\right).$$

A similar approach, based on the Poisson equation

$$-\widetilde{\mathcal{L}}_U \widetilde{\psi}_U = \left(\mathrm{e}^U - \frac{Z}{Z[U]} \right),$$

of which the right-hand side is in $L_0^2(\mu_U)$ by the assumption that $\mathbb{D} = \mathbb{T}$, can be employed to understand the asymptotic behavior of the denominator in (60). Specifically, it holds that

$$\frac{1}{N} \sum_{n=0}^{N-1} \left(\mathrm{e}^{U(X_{n\tau})} - \frac{Z}{Z[U]} \right) = \frac{1}{N} \sum_{n=0}^{N-1} \left(\widetilde{\psi}_U \left(X_{(n+1)\tau} \right) - \mathrm{e}^{\tau \mathcal{L}_U} \widetilde{\psi}_U \left(X_{n\tau} \right) \right) - \frac{\widetilde{\psi}_U \left(X_{N\tau} \right) + \widetilde{\psi}_U(X_0)}{N}.$$

An explicit calculation, using that the first term on the right-hand side is a sum of uncorrelated, identically distributed random variables, gives that the variance of the right-hand side converges to 0 in the limit as $N \to \infty$, implying the convergence

$$\frac{1}{N}\sum_{n=0}^{N-1} \mathrm{e}^{U(X_{n\tau})} \xrightarrow[N\to\infty]{\text{Law}} \frac{Z}{Z[U]}.$$

The proof can then be concluded by using Slutsky's lemma once more. □

Lemma 48 (Solution to the perturbed Poisson equation)**.** *Suppose that Assumption 7 is satisfied and that $\delta U \in C_{\mathrm{c}}^{\infty}(\mathbb{D}^d)$, and let $\phi_{U+\varepsilon\delta U}$ denote the solution to the Poisson equation (47) posed in $L_0^2(\mathrm{e}^{-V-U-\varepsilon\delta U})$. Then*

$$\frac{\nabla\phi_{U+\varepsilon\delta U} - \nabla\phi_U}{\varepsilon} \xrightarrow[\varepsilon\to 0]{} \nabla\psi_{U,\delta U} \text{ in } L^2(\mu_U), \tag{61}$$

where $\psi_{U,\delta U}$ denotes the unique solution in $H^1(\mu_U)\cap L_0^2(\mu_U)$ to

$$\begin{aligned} -\mathcal{L}_U\psi_{U,\delta U} &= (f-I)\mathrm{e}^U\delta U - \nabla(\delta U)\cdot\nabla\phi_U \\ &= -\mathrm{e}^{U+V}\nabla\cdot\left(\mathrm{e}^{-U-V}\delta U\nabla\phi_U\right). \end{aligned} \tag{62}$$

Remark 49. By integration by parts, which is allowed since $\phi_U \in C^\infty(\mathbb{D}^d)$ and $\delta U \in C_{\mathrm{c}}^\infty(\mathbb{D}^d)$, we can check that the right-hand side of (62) is indeed mean zero with respect to μ_U:

$$-\int_{\mathbb{D}^d} \mathrm{e}^{U+V}\nabla\cdot\left(\mathrm{e}^{-U-V}\delta U\nabla\phi_U\right)\,\mathrm{d}\mu_U = \frac{1}{Z[U]}\int_{\mathbb{D}^d}\nabla\cdot\left(\mathrm{e}^{-U-V}\delta U\nabla\phi_U\right)\,\mathrm{d}x = 0.$$

Therefore, there indeed exists a unique distributional solution in $H^1(\mu_U)\cap L_0^2(\mu_U)$ to (62) by the Lax–Milgram theorem. △

Proof of Lemma 48. Between the Poisson equations (20) and (47), both the operator and the right-hand side differ. We begin by rewriting

$$\mathcal{L}_{U+\varepsilon\delta U} = \mathcal{L}_U - \varepsilon\nabla(\delta U)\cdot\nabla. \tag{63}$$

Let $\psi_\varepsilon = \varepsilon^{-1}(\phi_{U+\varepsilon\delta U} - \phi_U)$. It holds that

$$-\mathcal{L}_{U+\varepsilon\delta U}\psi_\varepsilon = (f-I)\frac{\mathrm{e}^{U+\varepsilon\delta U} - \mathrm{e}^U}{\varepsilon} - \nabla(\delta U)\cdot\nabla\phi_U. \tag{64}$$

The right-hand side is mean zero with respect to $\mu_{U+\varepsilon\delta U}$ by construction, and so by the Lax–Milgram theorem there exists a unique distributional solution in $H^1(\mu_{U+\varepsilon\delta U})\cap L_0^2(\mu_{U+\varepsilon\delta U})$ to (64), which coincides with ψ_ε up to an additive constant. Subtracting (62) from (64), we deduce that

$$-\mathcal{L}_{U+\varepsilon\delta U}(\psi_\varepsilon - \psi_{U,\delta U}) = -(\mathcal{L}_U - \mathcal{L}_{U+\varepsilon\delta U})\psi_{U,\delta U} + (f-I)\left(\frac{\mathrm{e}^{U+\varepsilon\delta U} - \mathrm{e}^U}{\varepsilon} - \mathrm{e}^U\delta U\right) =: \zeta_\varepsilon.$$

The second term on the right-hand side converges to 0 in $L^2(\mu_U)$ in the limit as $\varepsilon \to 0$, as does the first term in view of (63). By the Holley–Stroock theorem, the probability measure $\mu_{U+\varepsilon\delta U}$ satisfies the Poincaré inequality (18) with a constant $R[U+\varepsilon\delta U]$ that converges to $R[U]$ in the limit $\varepsilon \to 0$. Consequently, we deduce from the standard stability estimate (23) that

$$\|\nabla(\psi_\varepsilon - \psi_{U,\delta U})\|_{L^2(\mu_{U+\varepsilon\delta U})} \leqslant \frac{\|\zeta_\varepsilon\|_{L^2(\mu_{U+\varepsilon\delta U})}}{R[U+\varepsilon\delta U]}.$$

Since the right-hand side converges to 0 in the limit $\varepsilon \to 0$, so must the left-hand side, which leads to the convergence $\|\nabla(\psi_\varepsilon - \psi_{U,\delta U})\|_{L^2(\mu_U)} \to 0$ given the equivalence between the norms of $L^2(\mu_U)$ and $L^2(\mu_{U+\varepsilon\delta U})$. This concludes the proof. □

Remark 50. One may wonder whether the statement (61) can be strengthened to

$$\frac{\phi_{U+\varepsilon\delta U} - \phi_U}{\varepsilon} \xrightarrow[\varepsilon\to 0]{} \psi_{U,\delta U} \text{ in } H^1(\mu_U). \tag{65}$$

The answer to this question is negative. Indeed, assume by contradiction that (65) holds. Then in particular $\phi_{U+\varepsilon\delta U} - \phi_U \to 0$ in $L^2(\mu_U)$ in the limit as $\varepsilon \to 0$ and so

$$\begin{aligned}\int_{\mathbb{D}^d} \frac{\phi_{U+\varepsilon\delta U} - \phi_U}{\varepsilon} \mathrm{d}\mu_U &= \frac{1}{\varepsilon}\int_{\mathbb{D}^d} \phi_{U+\varepsilon\delta U}\mathrm{d}\mu_U \\ &= \frac{1}{Z[U]}\int_{\mathbb{D}^d} \phi_{U+\varepsilon\delta U}\left(\frac{\mathrm{e}^{-V-U} - \mathrm{e}^{-V-U-\varepsilon\delta U}}{\varepsilon}\right) \\ &\xrightarrow[\varepsilon\to 0]{} \int_{\mathbb{D}^d} \phi_U \delta U \mathrm{d}\mu_U,\end{aligned} \tag{66}$$

where we used that ϕ_U and $\phi_{U+\varepsilon\delta U}$ are mean-zero with respect to e^{-V-U} and $\mathrm{e}^{-V-U-\varepsilon\delta U}$, respectively. This is a contradiction because (65) implies that

$$\int_{\mathbb{D}^d} \frac{\phi_{U+\varepsilon\delta U} - \phi_U}{\varepsilon}\mathrm{d}\mu_U \xrightarrow[\varepsilon\to 0]{} \int_{\mathbb{D}^d} \psi_{U,\delta U}\mathrm{d}\mu_U = 0,$$

and so (65) does not hold.

It is, however, simple to show that $\phi_{U+\varepsilon\delta U} \to \phi_U$ in $L^2(\mu_U)$ in the limit as $\varepsilon \to 0$. Additionally, it holds by Lemma 48 and the Poincaré inequality that

$$\frac{\phi_{U+\varepsilon\delta U} - \phi_U}{\varepsilon} - \int_{\mathbb{D}^d} \frac{\phi_{U+\varepsilon\delta U} - \phi_U}{\varepsilon}\,\mathrm{d}\mu_U \xrightarrow[\varepsilon\to 0]{} \psi_{U,\delta U} \text{ in } H^1(\mu_U),$$

but these statements are not useful for our purposes in this paper. △

Remark 51. Since $\psi_{U,\delta U}$ is a weak solution to (62), it holds for every $\delta W \in C_c^\infty(\mathbb{D}^d)$ that

$$\begin{aligned}\int_{\mathbb{D}^d} \nabla\psi_{U,\delta W}\cdot\nabla\psi_{U,\delta U}\,d\mu_U &= \int_{\mathbb{D}^d} \psi_{U,\delta W}\Big(-\mathrm{e}^{U+V}\nabla\cdot\big(\mathrm{e}^{-U-V}\delta U\nabla\phi_U\big)\Big)\,\mathrm{d}\mu_U \\ &= \int_{\mathbb{D}^d} \delta U\nabla\phi_U\cdot\nabla\psi_{U,\delta W}\,\mathrm{d}\mu_U,\end{aligned} \tag{67}$$

where integration by parts is justified because $\delta U \in C_c^\infty(\mathbb{D}^d)$. This equality, where the roles of δU and δW can be reversed, is useful in the proof of Proposition 53 below. △

Remark 52. In dimension $d = 1$, it follows from (62) that

$$\psi'_{U,\delta U} = \delta U\phi'_U + C_{\mathbb{D}}[U,\delta U]\mathrm{e}^{V+U}, \tag{68}$$

for some constant $C_{\mathbb{D}}[U,\delta U]$ such that $\psi'_{U,\delta U} \in L^2(\mu_U)$. Clearly $C_{\mathbb{R}}[U,\delta U] = 0$. When $\mathbb{D} = \mathbb{T}$, we obtain the value of $C_{\mathbb{T}}[U,\delta U]$ by requiring periodicity, that is

$$0 = \int_{\mathbb{T}} \psi'_{U,\delta U} = \int_{\mathbb{T}} \delta_U\phi'_U + C_{\mathbb{T}}[U,\delta U]\int_{\mathbb{T}} \mathrm{e}^{V+U},$$

which leads to

$$C_{\mathbb{T}}[U,\delta U] = -\frac{\displaystyle\int_{\mathbb{T}} \delta U \phi_U'}{\displaystyle\int_{\mathbb{T}} \mathrm{e}^{V+U}}.$$

We note that this formula may also be obtained by considering the differential of (31) viewed as a functional of U, an approach which reveals that $C_{\mathbb{D}}[U,\delta U] = \mathrm{d}A_{\mathbb{D}}[U]\cdot\delta U$. △

B Connection between $(A_{\mathbb{R}}, A_{\mathbb{R}}^*)$ and $(A_{\mathbb{T}}, A_{\mathbb{T}}^*)$

In this section, we discuss the links between the constants defined in (29) and (37).

Connection between $A_{\mathbb{R}}$ and $A_{\mathbb{T}}$. The constant $A_{\mathbb{R}}^* = A_{\mathbb{R}}$ is recovered as a limit of $A_{\mathbb{T}}^*$ for an increasingly large torus. More precisely, it holds that

$$A_{\mathbb{R}} = \lim_{L\to\infty} \frac{\displaystyle\int_{-L}^{L} F\,\mathrm{e}^{V+U}}{\displaystyle\int_{-L}^{L} \mathrm{e}^{V+U}}. \tag{69}$$

Indeed, for any $\ell > 0$ and $L > \ell$, it holds that

$$\begin{aligned}\frac{\displaystyle\int_{-L}^{L} (F-A_{\mathbb{R}})\,\mathrm{e}^{V+U}}{\displaystyle\int_{-L}^{L} \mathrm{e}^{V+U}} &= \frac{\displaystyle\int_{[-L,-\ell)\cup(\ell,L]} (F-A_{\mathbb{R}})\,\mathrm{e}^{V+U}}{\displaystyle\int_{[-L,-\ell)\cup(\ell,L]} \mathrm{e}^{V+U}} \frac{\displaystyle\int_{[-L,-\ell)\cup(\ell,L]} \mathrm{e}^{V+U}}{\displaystyle\int_{[-L,L]} \mathrm{e}^{V+U}} \\ &\quad + \frac{\displaystyle\int_{[-\ell,\ell]} (F-A_{\mathbb{R}})\,\mathrm{e}^{V+U}}{\displaystyle\int_{[-\ell,\ell]} \mathrm{e}^{V+U}} \frac{\displaystyle\int_{[-\ell,\ell]} \mathrm{e}^{V+U}}{\displaystyle\int_{[-L,L]} \mathrm{e}^{V+U}}.\end{aligned} \tag{70}$$

The right-hand side is a convex combination of the averages of $F - A_{\mathbb{R}}$ restricted to the sets $[-L,-\ell)\cup(\ell,L]$, for the first term, and $[-\ell,\ell]$, for the second term. In the proof of Lemma 14, we proved that

$$\int_{\mathbb{R}} \mathrm{e}^{U+V} = \infty.$$

Therefore, since F is uniformly bounded, the second summand on the right-hand side of (70) converges to 0 in the limit as $L\to\infty$, and so

$$\limsup_{L\to\infty} \left| \frac{\displaystyle\int_{-L}^{L} F\,\mathrm{e}^{V+U}}{\displaystyle\int_{-L}^{L} \mathrm{e}^{V+U}} - A_{\mathbb{R}} \right| = \limsup_{L\to\infty} \left| \frac{\displaystyle\int_{[-L,-\ell)\cup(\ell,L]} (F-A_{\mathbb{R}})\,\mathrm{e}^{V+U}}{\displaystyle\int_{[-L,-\ell)\cup(\ell,L]} \mathrm{e}^{V+U}} \right| \leqslant \sup_{|x|\geqslant\ell} |F(x) - A_{\mathbb{R}}|.$$

Since $\lim_{|x|\to\infty} F(x) = A_{\mathbb{R}}$ by definition of $A_{\mathbb{R}}$ in (33), the right-hand side of this equation can be made arbitrarily small by taking ℓ sufficiently large, and so the limit (69) follows.

Connection between $A_{\mathbb{R}}^*$ and $A_{\mathbb{T}}^*$. The constant $A_{\mathbb{R}}^* = A_{\mathbb{R}}$ coincides with

$$\lim_{\ell\to\infty} \sup \left\{ A \in \mathbb{R} : \int_{-\ell}^{\ell} \operatorname{sgn}(F-A) \geqslant 0 \right\}. \tag{71}$$

Indeed, since $\lim_{|x|\to\infty} F(x) = A_{\mathbb{R}}$, there exists for any $\varepsilon > 0$ a constant $\ell_\varepsilon > 0$ such that

$$\forall \ell \geqslant \ell_\varepsilon, \qquad \int_{-\ell}^{\ell} \operatorname{sgn}(F - A_{\mathbb{R}} + \varepsilon) > 0 \qquad \text{and} \qquad \int_{-\ell}^{\ell} \operatorname{sgn}(F - A_{\mathbb{R}} - \varepsilon) < 0.$$

Therefore, for all $\ell \geqslant \ell_\varepsilon$, the supremum in (71) is contained in the interval $[A_{\mathbb{R}} - \varepsilon, A_{\mathbb{R}} + \varepsilon]$. Since ε was arbitrary, the claim is proved.

C Second variation of the asymptotic variance

Since the method we propose in Subsection 3.4 relies on a steepest descent for the asymptotic variance viewed as a functional of U, it is natural to wonder whether this functional is convex, in order to provide guarantees on the convergence of the method. We provide a partial answer to this question in Proposition 53 and Remark 56 below. Specifically, we prove that the asymptotic variance is convex when the domain is the one-dimensional real line but possibly non-convex when the domain is $\mathbb{T}$. We have not managed to prove or rule out the convexity of the asymptotic variance in the multi-dimensional setting.

We emphasize that the convexity of the asymptotic variance in the case where the domain is $\mathbb{R}$ does not imply the uniqueness (up to an additive constant) of the minimizer. The most straightforward example is that of the constant observable, in which case the asymptotic variance is equal to 0 for any smooth biasing potential U.

Proposition 53. *Suppose that Assumption 7 is satisfied and let ϕ_U be the solution to the Poisson equation as in Lemma 11. Then, for all $\delta U, \delta W \in C_{\mathrm{c}}^\infty(\mathbb{D}^d)$, it holds that*

$$\begin{aligned}\frac{1}{2}\mathrm{d}(\mathrm{d}\sigma_f^2[U]\cdot\delta U)\cdot\delta W = \frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U_0\delta W_0\left(|\nabla\phi_U|^2 + \int_{\mathbb{D}^d}|\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-V-U} \\ - \frac{2Z[U]}{Z^2}\int_{\mathbb{D}^d}\left(\nabla\psi_{U,\delta U_0} - \delta U_0\nabla\phi_U\right)\cdot\left(\nabla\psi_{U,\delta W_0} - \delta W_0\nabla\phi_U\right)\mathrm{e}^{-V-U},\end{aligned} \tag{72}$$

where, for a perturbation $\delta X \in \{\delta U, \delta W\}$,

$$\delta X_0 := \delta X - \mu_U(\delta X), \qquad \mu_U(\delta X) := \int_{\mathbb{D}^d}\delta X\,\mathrm{d}\mu_U.$$

and $\psi_{U,\delta X_0} \in H^1(\mu_U)\cap L_0^2(\mu_U)$ is the solution to (62) with $\delta U = \delta X_0$. In addition, the second term in (72) is zero in dimension 1 when $\mathbb{D} = \mathbb{R}$, and so the asymptotic variance $\sigma_f^2[U]$ is a convex functional in this case.

Proof. We begin by rewriting the expression (45) as

$$\begin{aligned}\frac{1}{2}\mathrm{d}\sigma_f^2[U]\cdot\delta U &= \frac{1}{Z^2}\int_{\mathbb{D}^d}\left(Z[U]\delta U - \int_{\mathbb{D}^d}\delta U\,\mathrm{e}^{-V-U}\right)|\nabla\phi_U|^2\mathrm{e}^{-V-U} \\ &= \frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U|\nabla\phi_U|^2\mathrm{e}^{-V-U} - \left(\int_{\mathbb{D}^d}\delta U\,\mathrm{e}^{-V-U}\right)\frac{\sigma_f^2[U]}{2Z[U]} =: T_1[U;\delta U] + T_2[U;\delta U].\end{aligned}$$

Using the chain rule, we have

$$\begin{aligned}\mathrm{d}T_1[U;\delta U]\cdot\delta W = &-\frac{1}{Z^2}\int_{\mathbb{D}^d}\delta W\mathrm{e}^{-V-U}\int_{\mathbb{D}^d}\delta U|\nabla\phi_U|^2\mathrm{e}^{-V-U} \\ &+ \lim_{\varepsilon\to 0}\frac{Z[U]}{\varepsilon Z^2}\int_{\mathbb{D}^d}\delta U\left(|\nabla\phi_{U+\varepsilon\delta W}|^2 - |\nabla\phi_U|^2\right)\mathrm{e}^{-V-U} - \frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\delta W|\nabla\phi_U|^2\mathrm{e}^{-V-U}.\end{aligned}$$

Similarly, for the second term we obtain

$$\mathrm{d}T_2[U;\delta U]\cdot\delta W = \frac{1}{Z^2}\int_{\mathbb{D}^d}\delta U\delta W\mathrm{e}^{-V-U}\int_{\mathbb{D}^d}|\nabla\phi_U|^2\mathrm{e}^{-V-U} - \int_{\mathbb{D}^d}\delta U\mathrm{e}^{-V-U}\mathrm{d}\left(\frac{\sigma_f^2[U]}{2Z[U]}\right)\cdot\delta W.$$

The functional derivative in the last term on the right-hand side is calculated as in the proof of Theorem 25; specifically,

$$\mathrm{d}\left(\frac{\sigma_f^2[U]}{2Z[U]}\right)\cdot\delta W = \mathrm{d}\left(\frac{1}{Z^2}\int_{\mathbb{D}^d}\phi_U(f-I)\mathrm{e}^{-V}\right)\cdot\delta W = \frac{1}{Z^2}\int_{\mathbb{D}^d}\delta W|\nabla\phi_U|^2\mathrm{e}^{-V-U}.$$

By Lemma 48 and the fact that $\delta U\in C_{\mathrm{c}}^\infty(\mathbb{D}^d)$, we have that

$$\begin{aligned}
&\frac{1}{\varepsilon}\int_{\mathbb{D}^d}\delta U\left(|\nabla\phi_{U+\varepsilon\delta W}|^2-|\nabla\phi_U|^2\right)\mathrm{e}^{-V-U}\\
&\qquad=\int_{\mathbb{D}^d}\delta U\left(\frac{\nabla\phi_{U+\varepsilon\delta W}-\nabla\phi_U}{\varepsilon}\right)\cdot\left(\nabla\phi_{U+\varepsilon\delta W}+\nabla\phi_U\right)\mathrm{e}^{-V-U}\\
&\qquad\xrightarrow[\varepsilon\to 0]{}2\int_{\mathbb{D}^d}\delta U\nabla\psi_{U,\delta W}\cdot\nabla\phi_U\,\mathrm{e}^{-V-U}.
\end{aligned}$$

Collecting all the terms, we obtain

$$\begin{aligned}
\frac{1}{2}\mathrm{d}(\mathrm{d}\sigma_f^2[U]\cdot\delta U)\cdot\delta W = &-\frac{1}{Z^2}\int_{\mathbb{D}^d}\delta U\mathrm{e}^{-V-U}\int_{\mathbb{D}^d}\delta W|\nabla\phi_U|^2\mathrm{e}^{-V-U}\\
&-\frac{1}{Z^2}\int_{\mathbb{D}^d}\delta W\mathrm{e}^{-V-U}\int_{\mathbb{D}^d}\delta U|\nabla\phi_U|^2\mathrm{e}^{-V-U}\\
&+\frac{2Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\nabla\psi_{U,\delta W}\cdot\nabla\phi_U\mathrm{e}^{-V-U}\\
&+\frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\delta W\left(-|\nabla\phi_U|^2+\int_{\mathbb{D}^d}|\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-V-U}.
\end{aligned}\tag{73}$$

By rewriting the last term on the right-hand side as

$$\frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\delta W\left(|\nabla\phi_U|^2+\int_{\mathbb{D}^d}|\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-V-U}-\frac{2Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\delta W|\nabla\phi_U|^2\mathrm{e}^{-V-U},$$

and substituting $\delta U\delta W=\delta U_0\delta W_0+\delta U\mu_U(\delta W)+\delta W\mu_U(\delta U)-\mu_U(\delta U)\mu_U(\delta W)$ in the first term of the latter expression, the second variation may be further simplified to

$$\begin{aligned}
\frac{1}{2}\mathrm{d}(\mathrm{d}\sigma_f^2[U]\cdot\delta U)\cdot\delta W = &\frac{Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U_0\delta W_0\left(|\nabla\phi_U|^2+\int_{\mathbb{D}^d}|\nabla\phi_U|^2\,\mathrm{d}\mu_U\right)\mathrm{e}^{-V-U}\\
&+\frac{2Z[U]}{Z^2}\int_{\mathbb{D}^d}\delta U\nabla\phi_U\cdot\left(\nabla\psi_{U,\delta W}-\delta W\nabla\phi_U\right)\mathrm{e}^{-V-U}.
\end{aligned}\tag{74}$$

Using (67), both for $\psi_{U,\delta U}$ and $\psi_{U,\delta W}$, we obtain

$$\begin{aligned}
&\int_{\mathbb{D}^d}\delta U\nabla\phi_U\cdot\left(\nabla\psi_{U,\delta W}-\delta W\nabla\phi_U\right)\mathrm{e}^{-V-U}\\
&\qquad=-\int_{\mathbb{D}^d}\left(\nabla\psi_{U,\delta U}-\delta U\nabla\phi_U\right)\cdot\left(\nabla\psi_{U,\delta W}-\delta W\nabla\phi_U\right)\mathrm{e}^{-V-U}.
\end{aligned}$$

From (62), it is simple to see that $\nabla\psi_{U,\delta U}=\nabla\psi_{U,\delta U_0}+\nabla\psi_{U,\mu_U(\delta U)}=\nabla\psi_{U,\delta U_0}+\mu_U(\delta U)\nabla\phi_U$. Similarly, $\nabla\psi_{U,\delta W}=\nabla\psi_{U,\delta W_0}+\mu_U(\delta W)\nabla\phi_U$. Substituting these expressions in (74) leads to the claimed result (72).

One-dimensional setting. In dimension 1 when $\mathbb{D} = \mathbb{R}$, it holds that $\psi'_{U,\delta W} = \delta W \phi'_U$ by (68), and so the second term in (74) cancels out, which proves the last part of the statement. $\square$

Remark 54. Since all the terms on the right-hand side of (72) depend only on δU_0, the second variation is invariant under vertical shift of δU, in the sense that, formally,

$$\forall C \in \mathbb{R}, \qquad \mathrm{d}\big(\mathrm{d}\sigma_f^2[U] \cdot (\delta U + C)\big) \cdot (\delta U + C) = \mathrm{d}(\mathrm{d}\sigma_f^2[U] \cdot \delta U) \cdot \delta U.$$

This property had to hold a priori because $\sigma_f^2[U]$ is itself invariant under addition of constants to U, and so we could have assumed that $\mu_U(\delta U) = 0$ from the beginning of the proof without loss of generality. $\triangle$

Remark 55. The optimal biasing potential is known explicitly by Lemma 14 in the one-dimensional setting, so Proposition 53 is of little direct importance in this case. Nonetheless, the result provides understanding for the numerical experiments using the formula of the directional derivative. $\triangle$

Remark 56 (One-dimensional case with $\mathbb{D} = \mathbb{T}$). The asymptotic variance is not a convex functional when $\mathbb{D} = \mathbb{T}$ and $d = 1$. Indeed, we construct in this remark a potential V, a smooth function ϕ, and a direction δU such that the second variation of the asymptotic variance σ_f^2 for the observable $f = -\mathcal{L}\phi$ (with $\mathcal{L}$ the generator $\mathcal{L}_U$ given in (19) with $U = 0$) in the direction δU is negative when evaluated at the biasing potential $U = 0$. In the setting we consider, since ϕ is the solution to (20) when $U = 0$, it holds by Remark 52 that

$$\psi'_{U=0,\delta U_0} = \delta U_0 \phi' - \left(\frac{\int_{\mathbb{T}} \delta U_0 \phi'}{\int_{\mathbb{T}} \mathrm{e}^V}\right) \mathrm{e}^V.$$

Here $\delta U_0 := \delta U - \mu(\delta U)$. Therefore, by substitution in (72) we have that

$$\frac{1}{2}\mathrm{d}\big(\mathrm{d}\sigma_f^2[0] \cdot \delta U\big) \cdot \delta U = \frac{1}{Z}\left(\int_{\mathbb{T}} \delta U_0^2 \left(|\phi'|^2 + \int_{\mathbb{T}} |\phi'|^2 \mathrm{d}\mu\right) \mathrm{e}^{-V} - 2\frac{\big(\int_{\mathbb{T}} \delta U_0 \phi'\big)^2}{\int_{\mathbb{T}} \mathrm{e}^V}\right),$$

The right-hand side of this equation is not always positive. In order to show this, consider the case where $\delta U_0 = \phi' \mathrm{e}^V$. Note that δU_0 indeed has average 0 with respect to μ since $\int_{\mathbb{T}} \delta U_0 \mathrm{e}^{-V} = \int_{\mathbb{T}} \phi' = 0$. Then, we have

$$\frac{Z}{2}\mathrm{d}\big(\mathrm{d}\sigma_f^2[0] \cdot \delta U\big) \cdot \delta U = \int_{\mathbb{T}} |\phi'|^4 \mathrm{e}^V + \frac{\int_{\mathbb{T}} |\phi'|^2 \mathrm{e}^{-V}}{\int_{\mathbb{T}} \mathrm{e}^{-V}} \int_{\mathbb{T}} |\phi'|^2 \mathrm{e}^V - 2\frac{\big(\int_{\mathbb{T}} |\phi'|^2 \mathrm{e}^V\big)^2}{\int_{\mathbb{T}} \mathrm{e}^V}.$$

Assume that $\phi = \varrho_\varepsilon \star h + C$ is a regularization of a hat function $h \colon \mathbb{T} \to \mathbb{R}$ given on the interval $[-\pi, \pi]$, which we identify with its image under the quotient map $\mathbb{R} \to \mathbb{T}$, by

$$h(x) := \begin{cases} 1 - |x|, & |x| < 1, \\ 0 & \text{otherwise}, \end{cases}$$

with ϱ_ε the standard mollifier (16) and $C \in \mathbb{R}$ the constant such that ϕ has average 0 with respect to μ. Then, letting ν denote the probability measure with Lebesgue density proportional to e^V and $\mathcal{I} = [-1, 1]$, we obtain that, in the limit as $\varepsilon \to 0$,

$$\int_{\mathbb{T}} |\phi'|^4 \mathrm{d}\nu \to \nu(\mathcal{I}), \qquad \int_{\mathbb{T}} |\phi'|^2 \mathrm{d}\mu \to \mu(\mathcal{I}), \qquad \int_{\mathbb{T}} |\phi'|^2 \mathrm{d}\nu \to \nu(\mathcal{I}).$$

Therefore, it holds in this limit that

$$\frac{Z}{2}\mathrm{d}(\mathrm{d}\sigma_f^2[0] \cdot \delta U) \cdot \delta U \to \big(\nu(\mathcal{I}) + \mu(\mathcal{I})\nu(\mathcal{I}) - 2\nu(\mathcal{I})^2\big) \int_{\mathbb{T}} \mathrm{e}^V.$$

Now let $V(x) = K\cos(x)$ for all x. In the limit as $K \to \infty$, it holds that $\mu(\mathcal{I}) \to 0$ and $\nu(\mathcal{I}) \to 1$. We conclude that, for sufficiently large K and sufficiently small ε, the second variation of the asymptotic variance in direction δU is negative. $\triangle$

D Numerical discretization of the Poisson equation

We consider here the case where the domain is $\mathbb{T}^2$ for simplicity, noting that the method may be generalized to any spatial dimension. In order to numerically solve the Poisson equation (20), we use a finite difference approach on a grid of size $N \times N$. For a given $\delta > 0$, the discretization nodes are arranged linearly according to

$$\mathbf{x}_\ell := (-\pi + i\delta, -\pi + j\delta) \in \mathbb{T}^2, \qquad j = \left\lfloor \frac{\ell - 1}{N} \right\rfloor, \qquad i = \ell - 1 - jN, \qquad \delta = \frac{2\pi}{N}, \tag{75}$$

for $\ell \in \{1, \dots, N^2\}$. Note that the indices i and j each run from 0 to $N-1$; the largest value of either coordinate over the set of discretization nodes is $\pi - \delta$, which is sufficient given that $-\pi$ and π coincide under the quotient map $\mathbb{R}^2 \to \mathbb{T}^2$.

Before we present the method, we introduce additional notation. We denote by Π_N the discretization operator which associates to a function its values at the grid points (75), and for a function $h\colon \mathbb{T}^2 \to \mathbb{R}$, we write $\mathbf{h} = \Pi_N h \in \mathbb{R}^{N^2}$. The notation $\exp.(\mathbf{h})$ refers the vector obtained by applying the exponential function element-wise to $\mathbf{h}$, and $\mathrm{diag}(\mathbf{h})$ refers to the diagonal matrix with diagonal entries given by $\mathbf{h}$. The notation $\mathbf{1} \in \mathbb{R}^{N^2}$ refers to a column vector containing only ones. We also introduce the one-dimensional backward and forward difference operators, which act on vectors in $\mathbb{R}^N$:

$$D_{\mathrm{B}} = \frac{1}{\delta}\begin{pmatrix} 1 & & & & -1 \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix}, \qquad D_{\mathrm{F}} = \frac{1}{\delta}\begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \\ 1 & & & & -1 \end{pmatrix}.$$

From these operators, we construct difference operators along the x and y directions by taking Kronecker products with the $\mathbb{R}^{N\times N}$ identity matrix id_N:

$$D_{\mathrm{B}}^x = \mathrm{id}_N \otimes D_{\mathrm{B}}, \qquad D_{\mathrm{B}}^y = D_{\mathrm{B}} \otimes \mathrm{id}_N, \qquad D_{\mathrm{F}}^x = \mathrm{id}_N \otimes D_{\mathrm{F}}, \qquad D_{\mathrm{F}}^y = D_{\mathrm{F}} \otimes \mathrm{id}_N.$$

We recall that, for two matrices $A, B \in \mathbb{R}^{N\times N}$, the Kronecker product $A \otimes B$ is defined as

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1N}B \\ \vdots & \ddots & \vdots \\ a_{N1}B & \cdots & a_{NN}B \end{pmatrix}.$$

We denote by $\nabla_{\mathrm{F}}\mathbf{h}$ the $N^2 \times 2$ matrix $\nabla_{\mathrm{F}}\mathbf{h} = \begin{pmatrix} D_{\mathrm{F}}^x\mathbf{h} & D_{\mathrm{F}}^y\mathbf{h} \end{pmatrix}$. For a weight function $w\colon \mathbb{T}^2 \to \mathbb{R}$, we introduce the weighted inner product $\langle\,\cdot\,,\,\cdot\,\rangle_w\colon \mathbb{R}^{N^2} \times \mathbb{R}^{N^2} \to \mathbb{R}$ given for $\mathbf{g}, \mathbf{h} \in \mathbb{R}^{N^2}$ by

$$\langle \mathbf{g}, \mathbf{h}\rangle_w = \delta^2\, \mathbf{g}^{\mathsf{T}}\, \mathrm{diag}(\mathbf{w})\mathbf{h} = \delta^2 \sum_{\ell=1}^{N^2} \mathbf{g}_\ell \mathbf{h}_\ell\, w(\mathbf{x}_\ell), \tag{76}$$

with corresponding norm $\|\cdot\|_w$. We include the factor δ^2 in this definition so that, if $\mathbf{g}$ and $\mathbf{h}$ contain

the values taken by continuous functions g and h when evaluated at the discretization points and w is continuous, then

$$\langle \mathbf{g}, \mathbf{h} \rangle_w \xrightarrow[N\to\infty]{} \int_{\mathbb{T}^2} g(x)h(x)w(x)\,\mathrm{d}x.$$

Finally, let $\|\nabla_{\mathrm{F}}\mathbf{h}\|_w^2 = \|D_{\mathrm{F}}^x\mathbf{h}\|_w^2 + \|D_{\mathrm{F}}^y\mathbf{h}\|_w^2$ and let $|\nabla_{\mathrm{F}}\mathbf{h}|^2$ denote the $N^2 \times 1$ column vector obtained by taking the squared Euclidean norm of each row of $\nabla_{\mathrm{F}}\mathbf{h}$. In the remainder of this section, the notation (76) and corresponding norm are usually employed with the weight function $w = \mathrm{e}^{-V-U}$ and so, in order to simplify notation, we omit the subscript in this case. We are now ready to write the discrete formulation of the Poisson equation (20).

Proposition 57. *For $V, U, f\colon \mathbb{T}^2 \to \mathbb{R}$, there exists a unique solution $(\boldsymbol{\phi}_N, I_N) \in \mathbb{R}^{N^2} \times \mathbb{R}$ to*

$$-\widetilde{L}\begin{pmatrix}\boldsymbol{\phi}_N\\ I_N\end{pmatrix} := \begin{pmatrix}-L & \exp.(\mathbf{U})\\ \delta^2 \exp.(-\mathbf{V}-\mathbf{U})^{\mathsf{T}} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{\phi}_N\\ I_N\end{pmatrix} = \begin{pmatrix}\mathrm{diag}\big(\exp.(\mathbf{U})\big)\mathbf{f}\\ 0\end{pmatrix}, \tag{77}$$

where

$$\begin{aligned} L = {} & \mathrm{diag}\big(\exp.(\mathbf{V}+\mathbf{U})\big) D_{\mathrm{B}}^x \,\mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big) D_{\mathrm{F}}^x \\ & + \mathrm{diag}\big(\exp.(\mathbf{V}+\mathbf{U})\big) D_{\mathrm{B}}^y \,\mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big) D_{\mathrm{F}}^y. \end{aligned} \tag{78}$$

Remark 58. The first rows in (77) may be rewritten as

$$-L\boldsymbol{\phi}_N = \mathrm{diag}\big(\exp.(\mathbf{U})\big)(\mathbf{f} - I_N\mathbf{1}),$$

which resembles the Poisson equation (20). The last row in (77) may be rewritten as

$$\delta^2 \exp.(-\mathbf{V}-\mathbf{U})^{\mathsf{T}}\boldsymbol{\phi}_N = \langle \mathbf{1}, \boldsymbol{\phi}_N \rangle = 0.$$

It expresses the requirement that the vector $\boldsymbol{\phi}_N$ should be mean-zero with respect to the discrete measure $\exp.(-\mathbf{V}-\mathbf{U})$. △

Remark 59. We use the notation I_N for the scalar unknown in (77) because solving (77) yields both an approximate solution to the Poisson equation and an approximation of $I = \mu(f)$. △

Proof. In order to prove the statement, it is sufficient to show that the homogeneous equation

$$\begin{pmatrix}-L & \exp.(\mathbf{U})\\ \delta^2 \exp.(-\mathbf{V}-\mathbf{U})^{\mathsf{T}} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{\gamma}\\ \sigma\end{pmatrix} = \begin{pmatrix}\mathbf{0}\\ 0\end{pmatrix} \tag{79}$$

admits only the trivial solution $= (\mathbf{0}, 0)$. We assume by contradiction that $(\boldsymbol{\gamma}, \sigma)$ is a nonzero solution. Then

$$-L\boldsymbol{\gamma} + \sigma \exp.(\mathbf{U}) = \mathbf{0},$$

implying that

$$-\langle L\boldsymbol{\gamma}, \mathbf{1} \rangle + \sigma \langle \exp.(\mathbf{U}), \mathbf{1} \rangle = 0. \tag{80}$$

The linear operator on $\mathbb{R}^{N^2 \times N^2}$ induced by L is self-adjoint for the inner product $\langle\,\cdot\,,\,\cdot\,\rangle$, because

$$\begin{aligned} -\langle \mathbf{g}, L\mathbf{h} \rangle &= -\delta^2 \mathbf{g}^{\mathsf{T}} \left(D_{\mathrm{B}}^x \,\mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big) D_{\mathrm{F}}^x + D_{\mathrm{B}}^y \,\mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big) D_{\mathrm{F}}^y \right) \mathbf{h} \\ &= \langle D_{\mathrm{F}}^x \mathbf{g}, D_{\mathrm{F}}^x \mathbf{h} \rangle + \langle D_{\mathrm{F}}^y \mathbf{g}, D_{\mathrm{F}}^y \mathbf{h} \rangle, \end{aligned} \tag{81}$$

where we used the relation $D_{\mathrm{B}}^{\mathsf{T}} = -D_{\mathrm{F}}$. Therefore, going back to (80), we deduce that

$$0 = -\langle \boldsymbol{\gamma}, L\mathbf{1}\rangle + \sigma\langle \exp.(\mathbf{U}), \mathbf{1}\rangle = \sigma\langle \exp.(\mathbf{U}), \mathbf{1}\rangle = \delta^2\sigma\mathbf{1}^{\mathsf{T}}\exp.(-\mathbf{V}).$$

Therefore $\sigma = 0$, but then $L\boldsymbol{\gamma} = \mathbf{0}$ by (79) and so $\langle \boldsymbol{\gamma}, L\boldsymbol{\gamma}\rangle = 0$. By the relation (81), this implies that $D_{\mathrm{F}}^x\boldsymbol{\gamma} = D_{\mathrm{F}}^y\boldsymbol{\gamma} = 0$, so the vector $\boldsymbol{\gamma}$ is constant. The last equation in (79) then implies that $\boldsymbol{\gamma} = \mathbf{0}$. Note that (81) implies that $\mathrm{Ker}(L^{\mathsf{T}}) = \mathrm{Span}\big\{\exp.(-\mathbf{V} - \mathbf{U})\big\}$, which will be useful in the proof of Lemma 61. □

It is possible to prove the convergence of the solution to (77) to the exact solution of the Poisson equation (20) in the limit as $N \to \infty$. To this end, we begin by showing the following Poincaré-like inequality.

Lemma 60 (Discrete Poincaré inequality)**.** *Assume that $V + U \colon \mathbb{T}^2 \to \mathbb{R}$ is uniformly bounded. Then there exists a constant $R_{\mathrm{disc}}[U] > 0$ independent of N such that*

$$\forall \mathbf{g} \in \Big\{\mathbf{h} \in \mathbb{R}^{N^2} : \mathbf{h}^{\mathsf{T}}\exp.(-\mathbf{V} - \mathbf{U}) = 0\Big\}, \qquad \|\nabla_{\mathrm{F}}\mathbf{g}\|^2 \geqslant R_{\mathrm{disc}}[U]\|\mathbf{g}\|^2. \tag{82}$$

Proof. It is sufficient to show (82) for $V + U = 0$. Indeed, assuming that the inequality holds in this particular case and denoting by C a constant which depends only on $V + U$ and is allowed to change from line to line, we have that

$$\begin{aligned}\forall \mathbf{g} \in \mathbb{R}^{N^2}, \qquad &\langle D_{\mathrm{F}}^x\mathbf{g}, D_{\mathrm{F}}^x\mathbf{g}\rangle + \langle D_{\mathrm{F}}^y\mathbf{g}, D_{\mathrm{F}}^y\mathbf{g}\rangle \\ &\geqslant C\Big(\langle D_{\mathrm{F}}^x\mathbf{g}, D_{\mathrm{F}}^x\mathbf{g}\rangle_1 + \langle D_{\mathrm{F}}^y\mathbf{g}, D_{\mathrm{F}}^y\mathbf{g}\rangle_1\Big) \\ &\geqslant C\langle \mathbf{g} - \widetilde{\mathbf{g}}, \mathbf{g} - \widetilde{\mathbf{g}}\rangle_1, \qquad \widetilde{\mathbf{g}} = \frac{\langle \mathbf{g}, \mathbf{1}\rangle_1}{\langle \mathbf{1}, \mathbf{1}\rangle_1}\mathbf{1},\end{aligned}$$

where we employed the equivalence between $\langle\,\cdot\,,\,\cdot\,\rangle_1$, which is given by (76) in the particular case where $V + U = 0$, and $\langle\,\cdot\,,\,\cdot\,\rangle_{\mathrm{e}^{-V-U}}$, noting that both constants in this equivalence can be fixed independently of N. Using this equivalence in the other direction, we obtain

$$\begin{aligned}\langle \mathbf{g} - \widetilde{\mathbf{g}}, \mathbf{g} - \widetilde{\mathbf{g}}\rangle_1 &\geqslant C\langle \mathbf{g} - \widetilde{\mathbf{g}}, \mathbf{g} - \widetilde{\mathbf{g}}\rangle \geqslant C\inf_{s\in\mathbb{R}}\langle \mathbf{g} - s\mathbf{1}, \mathbf{g} - s\mathbf{1}\rangle \\ &= C\langle \mathbf{g} - \overline{\mathbf{g}}, \mathbf{g} - \overline{\mathbf{g}}\rangle, \qquad \overline{\mathbf{g}} = \frac{\langle \mathbf{g}, \mathbf{1}\rangle}{\langle \mathbf{1}, \mathbf{1}\rangle}\mathbf{1}.\end{aligned}$$

Finally, equation (82) when $V + U = 0$ follows from its one-dimensional counterpart by using a standard tensorization argument (as for the proof of [31, Proposition 2.6] for instance). It only remains to show the one-dimensional inequality

$$\forall \mathbf{g} \in \mathbb{R}^N, \qquad \langle D_{\mathrm{F}}\mathbf{g}, D_{\mathrm{F}}\mathbf{g}\rangle_1 \geqslant R_{\mathrm{disc}}[U]\langle \mathbf{g} - \widetilde{\mathbf{g}}, \mathbf{g} - \widetilde{\mathbf{g}}\rangle_1, \qquad \widetilde{\mathbf{g}} = \frac{\langle \mathbf{g}, \mathbf{1}\rangle_1}{\langle \mathbf{1}, \mathbf{1}\rangle_1}\mathbf{1}, \tag{83}$$

for a constant $R_{\mathrm{disc}}[U]$ independent of N for sufficiently large N. To this end, we notice that

$$\big\langle D_{\mathrm{F}}\mathbf{g}, D_{\mathrm{F}}\mathbf{g}\big\rangle_1 = \big\langle D_{\mathrm{B}}D_{\mathrm{F}}(\mathbf{g} - \widetilde{\mathbf{g}}), \mathbf{g} - \widetilde{\mathbf{g}}\big\rangle_1.$$

The matrix $D_{\mathrm{B}} D_{\mathrm{F}}$ is given by

$$D_{\mathrm{B}} D_{\mathrm{F}} = \frac{1}{\delta^2} \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ -1 & & & -1 & 2 \end{pmatrix}.$$

This is a circulant matrix [14] with explicit eigenvalues given by

$$\lambda_k = \frac{4}{\delta^2} \sin^2\left(\frac{\pi k}{N}\right) = \frac{N^2}{\pi^2} \sin^2\left(\frac{\pi k}{N}\right), \qquad k = 0, 1, \ldots, N-1.$$

The minimum eigenvalue of this matrix is $\lambda_0 = 0$, and the associated eigenvector is $\mathbf{1}$, to which $\mathbf{g} - \widetilde{\mathbf{g}}$ is orthogonal. Therefore, equation (83) implies that

$$\forall \mathbf{g} \in \mathbb{R}^N, \qquad \left\langle D_{\mathrm{F}} \mathbf{g}, D_{\mathrm{F}} \mathbf{g} \right\rangle_1 \geqslant \lambda_1 \left\langle \mathbf{g} - \widetilde{\mathbf{g}}, \mathbf{g} - \widetilde{\mathbf{g}} \right\rangle_1,$$

which implies that, for fixed N, equation (83) holds with constant $R_{\mathrm{disc}}(N) = (N/\pi)^2 \sin^2(\pi/N)$, which converges to 1 in the limit $N \to \infty$. See also [42, Lemma 12.2] for a Poincaré inequality for discrete functions on a bounded interval that are zero at the endpoints. □

Proposition 57 implies that $\widetilde{L}$ is invertible. Using Lemma 60, we show that $\widetilde{L}^{-1}$ does not diverge in the limit as $N \to \infty$, in an appropriate norm.

Lemma 61. *Assume that $V, U \colon \mathbb{T}^2 \to \mathbb{R}$ are continuous. Then the matrix $\widetilde{L}^{-1}$ is bounded uniformly in $N \in \mathbb{N}$, for the operator norm induced by the following norm on $\mathbb{R}^{N^2} \times \mathbb{R}$:*

$$(\boldsymbol{\gamma}, \sigma) \mapsto \|\boldsymbol{\gamma}\|_{\mathrm{e}^{-U-V}} + |\sigma|. \tag{84}$$

Proof. The strategy of proof is similar to that used in [47, Section 2.2]. Since by the Fredholm alternative $\mathrm{Ran}(L) = \mathrm{Ker}(L^{\mathsf{T}})^{\perp}$, the range of L is given by $\left\{\mathbf{h} \in \mathbb{R}^{N^2} : \mathbf{h}^{\mathsf{T}} \exp.(-\mathbf{V} - \mathbf{U}) = 0\right\}$. It then follows by Lemma 60 that the following inequality holds for all $\mathbf{g} \in \mathrm{Ran}(L)$:

$$\|L\mathbf{g}\| \|\mathbf{g}\| \geqslant -\langle L\mathbf{g}, \mathbf{g}\rangle = \|D_{\mathrm{F}}^x \mathbf{g}\|^2 + \|D_{\mathrm{F}}^y \mathbf{g}\|^2 \geqslant R_{\mathrm{disc}}[U] \|\mathbf{g}\|^2,$$

and so we deduce that that $\|L^{-1}\| \leqslant \frac{1}{R_{\mathrm{disc}}[U]}$ over $\mathrm{Ran}(L)$. Denote by $(\boldsymbol{\gamma}, \sigma)$ the solution to

$$\begin{pmatrix} -L & \exp.(\mathbf{U}) \\ \delta^2 \exp.(-\mathbf{V} - \mathbf{U})^{\mathsf{T}} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\gamma} \\ \sigma \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ s \end{pmatrix}. \tag{85}$$

This solution satisfies

$$-\langle L\boldsymbol{\gamma}, \mathbf{1}\rangle + \sigma \langle \exp.(\mathbf{U}), \mathbf{1}\rangle = \langle \mathbf{g}, \mathbf{1}\rangle, \tag{86}$$

and since $\langle L\boldsymbol{\gamma}, \mathbf{1}\rangle = \langle \boldsymbol{\gamma}, L\mathbf{1}\rangle = 0$, this implies

$$|\sigma| = \left| \frac{\langle \mathbf{g}, \mathbf{1}\rangle}{\langle \exp.(\mathbf{U}), \mathbf{1}\rangle} \right| \leqslant \frac{\|\mathbf{g}\| \|\mathbf{1}\|}{\langle \exp.(\mathbf{U}), \mathbf{1}\rangle}.$$

We then deduce that

$$\boldsymbol{\gamma} - \overline{\boldsymbol{\gamma}} = -L^{-1}\big(\mathbf{g} - \sigma \exp.(\mathbf{U})\big), \qquad \overline{\boldsymbol{\gamma}} = \frac{\langle \boldsymbol{\gamma}, \mathbf{1}\rangle}{\langle \mathbf{1}, \mathbf{1}\rangle} \mathbf{1},$$

and then the last equation in (85) gives $\overline{\boldsymbol{\gamma}} = s\mathbf{1}/\|\mathbf{1}\|^2$. This leads to the bound

$$\begin{aligned}\|\boldsymbol{\gamma}\| &\leqslant \|\boldsymbol{\gamma} - \overline{\boldsymbol{\gamma}}\| + \|\overline{\boldsymbol{\gamma}}\| \\ &\leqslant \frac{1}{R_{\mathrm{disc}}[U]}\big(\|\mathbf{g}\| + |\sigma|\|\exp.(\mathbf{U})\|\big) + |s|\frac{\|\mathbf{1}\|}{\|\mathbf{1}\|^2} \leqslant \frac{\|\mathbf{g}\|}{R_{\mathrm{disc}}[U]}\left(1 + \frac{\|\exp.(\mathbf{U})\|\|\mathbf{1}\|}{\langle \exp.(\mathbf{U}), \mathbf{1}\rangle}\right) + |s|\frac{\|\mathbf{1}\|}{\|\mathbf{1}\|^2}.\end{aligned}$$

In the limit $N \to \infty$, it holds that

$$\|\mathbf{1}\| \to \sqrt{\int_{\mathbb{T}^2} \mathrm{e}^{-V-U}}, \qquad \|\exp.(\mathbf{U})\| \to \sqrt{\int_{\mathbb{T}^2} \mathrm{e}^{-V+U}}, \qquad \langle \exp.(\mathbf{U}), \mathbf{1}\rangle \to \int_{\mathbb{T}^2} \mathrm{e}^{-V},$$

which enables to conclude the proof. □

We are now ready to prove the convergence of the solution of the discretized Poisson equation (77) in the limit $N \to \infty$.

Proposition 62. *Suppose that Assumption 7 is satisfied. Let ϕ denote the exact solution to (20) and let $I = \mu(f)$. Let also $(\boldsymbol{\phi}_N, I_N)$ denote the solution to the discretized equation (77). Then it holds that*

$$\|\boldsymbol{\phi}_N - \Pi_N \phi\| \xrightarrow[N\to\infty]{} 0, \qquad I_N \xrightarrow[N\to\infty]{} I.$$

Proof. The proof is an application of the standard Lax equivalence theorem. We denote the matrix of the linear system (77) by $\widetilde{L}_N$ to emphasize its dependence on N. Convergence follows from the usual argument:

$$\left\|\begin{pmatrix}\Pi_N\phi - \boldsymbol{\phi}_N \\ I - I_N\end{pmatrix}\right\| \leqslant C\left\|\widetilde{L}_N\begin{pmatrix}\Pi_N\phi - \boldsymbol{\phi}_N \\ I - I_N\end{pmatrix}\right\| = \left\|\widetilde{L}_N\begin{pmatrix}\Pi_N\phi \\ I\end{pmatrix} - \begin{pmatrix}\Pi_N\left(f\mathrm{e}^U\right) \\ 0\end{pmatrix}\right\| \xrightarrow[N\to\infty]{} 0,$$

where the norm in this equation is that defined in (84). The first inequality follows from the stability statement of Lemma 61, while the limit follows from the consistency of the discretization, which is simple to check given that ϕ is a smooth function under Assumption 7, and relying on the presence of the factor δ^2 in the definition (76). □

The main interest of the discretization (77) lies in the following statement, which may be viewed as a result on the commutation of the discretization and derivative operators. In order to be more precise, we denote by $(\boldsymbol{\phi}_N, I_N)$ the solution to (77) and let

$$\sigma^2_{f,N}[\mathbf{U}] = \frac{2Z_N[\mathbf{U}]}{Z_N^2}\|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N\|^2, \qquad \text{where} \begin{cases} Z_N := \delta^2\mathbf{1}^{\mathsf{T}}\exp.(-\mathbf{V}), \\ Z_N[\mathbf{U}] := \delta^2\mathbf{1}^{\mathsf{T}}\exp.(-\mathbf{V}-\mathbf{U}). \end{cases} \tag{87}$$

The following statement shows that the functional derivative of $\widehat{\sigma}^2_f[\mathbf{U}]$ has a structure similar to that of $\sigma^2_f[U]$ given in (21); it may be viewed as a discretization thereof.

Proposition 63 (Functional derivative of $\sigma^2_{f,N}$)**.** *Suppose that $V, U\colon \mathbb{T}^2 \to \mathbb{R}$ are uniformly bounded. The functional derivative with respect to $\mathbf{U}$ of $\sigma^2_{f,N}$ is given by*

$$\frac{1}{2}\mathrm{d}\sigma^2_{f,N}[\mathbf{U}]\cdot\boldsymbol{\delta U} = \frac{Z_N[\mathbf{U}]}{Z_N^2}\left\langle \boldsymbol{\delta U}, |\nabla_{\mathrm{F}}\boldsymbol{\phi}_N|^2 - \overline{|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N|^2}\right\rangle, \qquad \overline{|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N|^2} := \frac{\|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N\|^2}{Z_N[\mathbf{U}]}. \tag{88}$$

Notice that (88) is very similar to the formula (45) for the functional derivative of $\sigma^2_f[U]$.

Proof. The proof mirrors that of Theorem 25. In view of (81), we first rewrite

$$\begin{aligned}\sigma^2_{f,N}[\mathbf{U}] &= \frac{2Z_N[\mathbf{U}]}{Z_N^2}\|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N\|^2 = -\frac{2Z_N[\mathbf{U}]}{Z_N^2}\langle\boldsymbol{\phi}_N, L\boldsymbol{\phi}_N\rangle \\ &= \frac{2Z_N[\mathbf{U}]}{Z_N^2}\langle\boldsymbol{\phi}_N, \mathrm{diag}\big(\exp.(\mathbf{U})\big)(\mathbf{f}-I_N\mathbf{1})\rangle = \frac{2Z_N[\mathbf{U}]}{Z_N^2}\langle\boldsymbol{\phi}_N, \mathbf{f}-I_N\mathbf{1}\rangle_{\mathrm{e}^{-V}}.\end{aligned}$$

Let $(\boldsymbol{\phi}_N^\varepsilon, I_N^\varepsilon)$ denote the solution to (77) with $\mathbf{U}+\varepsilon\boldsymbol{\delta U}$ in place of $\mathbf{U}$ everywhere and L^ε the corresponding matrix (78). It is simple to check, using a reasoning similar to (86) as well as the equation $\langle L^\varepsilon\boldsymbol{\phi}_N^\varepsilon, \mathbf{1}\rangle = 0$, that the scalar term $I_N^\varepsilon = I_N$ is fact independent of the potential $\mathbf{U}$. Therefore, we obtain that

$$-L^\varepsilon\boldsymbol{\phi}_N^\varepsilon = \mathrm{diag}\big(\exp.(\mathbf{U}+\varepsilon\boldsymbol{\delta U})\big)(\mathbf{f}-I_N\mathbf{1}).$$

By definition of the functional derivative, we then have

$$\frac{1}{2}\mathrm{d}\sigma^2_{f,N}[\mathbf{U}]\cdot\boldsymbol{\delta U} = \frac{\mathrm{d}Z_N[\mathbf{U}]\cdot\boldsymbol{\delta U}}{Z_N^2}\|\nabla_{\mathrm{F}}\boldsymbol{\phi}_N\|^2 + \lim_{\varepsilon\to 0}\frac{Z_N[\mathbf{U}]}{\varepsilon Z_N^2}\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, \mathbf{f}-I_N\mathbf{1}\rangle_{\mathrm{e}^{-V}}. \tag{89}$$

The functional derivative in the first term is given by

$$\mathrm{d}Z_N[\mathbf{U}]\cdot\boldsymbol{\delta}U = -\langle\boldsymbol{\delta U}, \mathbf{1}\rangle. \tag{90}$$

For the second term in (89), we obtain

$$\begin{aligned}\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, \mathbf{f}-I_N\mathbf{1}\rangle_{\mathrm{e}^{-V}} &= \big\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, \mathrm{diag}\big(\exp.(\mathbf{U})\big)(\mathbf{f}-I_N\mathbf{1})\big\rangle_{\mathrm{e}^{-V-U}} \\ &= -\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, L\boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U}} \\ &= -\langle L(\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N), \boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U}} \\ &= -\langle L^\varepsilon\boldsymbol{\phi}_N^\varepsilon, \boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U-\varepsilon\delta U}} + \langle L\boldsymbol{\phi}_N, \boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U}} \\ &\quad - \langle L\boldsymbol{\phi}_N^\varepsilon, \boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U}} + \langle L^\varepsilon\boldsymbol{\phi}_N^\varepsilon, \boldsymbol{\phi}_N\rangle_{\mathrm{e}^{-V-U-\varepsilon\delta U}}.\end{aligned}$$

The first two terms in the last expression cancel out, and after substituting the expressions of L and L^ε given in (78) in the other two terms, we obtain

$$\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, \mathbf{f}-I_N\mathbf{1}\rangle_{\mathrm{e}^{-V}} = -\langle D_{\mathrm{B}}^x(M-M^\varepsilon)D_{\mathrm{F}}^x\boldsymbol{\phi}_N^\varepsilon, \boldsymbol{\phi}_N\rangle_1 - \langle D_{\mathrm{B}}^y(M-M^\varepsilon)D_{\mathrm{F}}^y\boldsymbol{\phi}_N^\varepsilon, \boldsymbol{\phi}_N\rangle_1,$$

where

$$M - M^\varepsilon := \mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big) - \mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U}-\varepsilon\boldsymbol{\delta U})\big).$$

Noting that

$$\lim_{\varepsilon\to 0}\frac{M-M^\varepsilon}{\varepsilon} = \mathrm{diag}\big(\exp.(-\mathbf{V}-\mathbf{U})\big)\,\mathrm{diag}(\boldsymbol{\delta U}),$$

we deduce that

$$\lim_{\varepsilon\to 0}\frac{Z_N[\mathbf{U}]}{\varepsilon Z_N^2}\langle\boldsymbol{\phi}_N^\varepsilon-\boldsymbol{\phi}_N, \mathbf{f}-I_N\mathbf{1}\rangle_{\mathrm{e}^{-V}} = \frac{Z_N[\mathbf{U}]}{Z_N^2}\big\langle\boldsymbol{\delta U}, |\nabla_{\mathrm{F}}\boldsymbol{\phi}_N|^2\big\rangle_{\mathrm{e}^{-V-U}}.$$

Combining this equation with (89) and (90), we deduce (88). □

Acknowledgements. We are grateful to Andrew Duncan and Grigorios Pavliotis for useful discussions and for sharing with us their preliminary calculations on this problem. The work of MC was supported by the Agence Nationale de la Recherche under grant ANR-20-CE40-0022 (SWIDIMS). The work of TL,

GS and UV was partially funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 810367), and by the Agence Nationale de la Recherche (ANR) under grants ANR-21-CE40-0006 (SINEQ) and ANR-19-CE40-0010 (QuAMProcs).

References

[1] A. Abdulle, G. Vilmart, and K. C. Zygalakis. Long time accuracy of Lie–Trotter splitting methods for Langevin dynamics. *SIAM J. Numer. Anal.*, **53**:1–16, 2015.

[2] A. Abdulle, G. A. Pavliotis, and U. Vaes. Spectral methods for multiscale stochastic differential equations. *SIAM/ASA J. Uncertain. Quantif.*, **5**(1):720–761, 2017.

[3] S. Agapiou, O. Papaspiliopoulos, D. Sanz-Alonso, and A. M. Stuart. Importance sampling: intrinsic dimension and computational cost. *Statist. Sci.*, **32**(3):405–431, 2017.

[4] M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids*. Oxford University Press, Inc., 2nd edition, 2017.

[5] C. Ané, S. Blachère, D. Chafaï, P. Fougères, I. Gentil, F. Malrieu, C. Roberto, and G. Scheffer. *Sur les Inégalités de Sobolev Logarithmiques*, volume **10** of *Panoramas et Synthèses*. Société Mathématique de France, Paris, 2000.

[6] L. Armijo. Minimization of functions having Lipschitz continuous first partial derivatives. *Pacific J. Math.*, **16**:1–3, 1966.

[7] S. Asmussen and P. W. Glynn. *Stochastic Simulation: Algorithms and Analysis*, volume **57** of *Stochastic Modelling and Applied Probability*. Springer, New York, 2007.

[8] D. Bakry, F. Barthe, P. Cattiaux, and A. Guillin. A simple proof of the Poincaré inequality for a large class of probability measures including the log-concave case. *Electron. Commun. Probab.*, **13**:60–66, 2008.

[9] J. Barzilai and J. M. Borwein. Two-point step size gradient methods. *IMA J. Numer. Anal.*, **8**(1):141–148, 1988.

[10] P. Cattiaux, D. Chafaï, and A. Guillin. Central limit theorems for additive functionals of ergodic Markov diffusions processes. *ALEA Lat. Am. J. Probab. Math. Stat.*, **9**(2):337–382, 2012.

[11] F. Cérou, P. Héas, and M. Rousset. Entropy minimizing distributions are worst-case optimal importance proposals. *arXiv preprint*, **2212.04292**, 2022.

[12] M. Chak, N. Kantas, T. Lelièvre, and G. A. Pavliotis. Optimal friction matrix for underdamped Langevin sampling. *arXiv preprint*, **2112.06844**, 2021.

[13] M. Dashti and A. M. Stuart. *The Bayesian approach to inverse problems*. In *Handbook of Uncertainty Quantification*. R. Ghanem, D. Higdon, and H. Owhadi, editors. Springer International Publishing, Cham, 2017, pages 311–428.

[14] P. J. Davis. *Circulant Matrices*. A Wiley-Interscience Publication. John Wiley & Sons, New York-Chichester-Brisbane, 1979.

[15] A. Debussche and E. Faou. Weak backward error analysis for SDEs. *SIAM J. Numer. Anal.*, **50**(3):1735–1752, 2012.

[16] A. B. Duncan, T. Lelièvre, and G. A. Pavliotis. Variance reduction using nonreversible Langevin samplers. *J. Stat. Phys.*, **163**(3):457–491, 2016.

[17] D. J. Evans and G. P. Morriss. *Statistical Mechanics of Nonequilibrium Liquids*. Cambridge University Press, 2008.

[18] L. C. Evans. *Partial Differential Equations*, volume **19** of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, second edition, 2010.

[19] E. García-Portugués, M. Sørensen, K. V. Mardia, and T. Hamelryck. Langevin diffusions on the torus: Estimation and applications. *Stat. Comput.*, **29**(1):1–22, 2019.

[20] D. Gilbarg and N. S. Trudinger. *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics. Springer-Verlag, Berlin, 2001.

[21] W. K. Hastings. Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, **57**(1):97–109, 1970.

[22] I. S. Helland. Central limit theorems for martingales with discrete or continuous time. *Scand. J. Statist.*, **9**(2):79–94, 1982.

[23] R. Holley and D. Stroock. Logarithmic Sobolev inequalities and stochastic Ising models. *J. Statist. Phys.*, **46**(5-6):1159–1194, 1987.

[24] J. Jacod and A. N. Shiryaev. *Limit Theorems for Stochastic Processes*, volume **288** of *Grundlehren der mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, second edition, 2003.

[25] C. Kipnis and S. R. S. Varadhan. Central limit theorem for additive functionals of reversible Markov processes and applications to simple exclusions. *Comm. Math. Phys.*, **104**(1):1–19, 1986.

[26] W. Kliemann. Recurrence and invariant measures for degenerate diffusions. *Ann. Probab.*, **15**(2):690–707, 1987.

[27] K. Law, A. Stuart, and K. Zygalakis. *Data Assimilation*, volume **62** of *Texts in Applied Mathematics*. Springer, Cham, 2015.

[28] B. Leimkuhler, C. Matthews, and G. Stoltz. The computation of averages from equilibrium and nonequilibrium Langevin molecular dynamics. *IMA J. Numer. Anal.*, **36**(1):13–79, 2016.

[29] B. Leimkuhler and C. Matthews. *Molecular Dynamics*, volume **39** of *Interdisciplinary Applied Mathematics*. Springer, Cham, 2015.

[30] T. Lelièvre, M. Rousset, and G. Stoltz. *Free Energy Computations*. Imperial College Press, London, 2010.

[31] T. Lelièvre and G. Stoltz. Partial differential equations and stochastic methods in molecular dynamics. *Acta Numer.*, **25**:681–880, 2016.

[32] L. Lorenzi. *Analytical Methods for Kolmogorov Equations*. Monographs and Research Notes in Mathematics. CRC Press, Boca Raton, FL, 2017.

[33] M. Tuckerman. *Statistical Mechanics: Theory and Molecular Simulation*. Oxford University Press, 2010.

[34] P. Major. Central limit theorems for martingales. *Technical report, Mathematical Institute of the Hungarian Academy of Science*, 2013.

[35] G. Maruyama and H. Tanaka. Ergodic property of N-dimensional recurrent Markov processes. *Mem. Fac. Sci. Kyushu Univ. Ser. A*, **13**:157–172, 1959.

[36] J. C. Mattingly, A. M. Stuart, and D. J. Higham. Ergodicity for SDEs and approximations: locally Lipschitz vector fields and degenerate noise. *Stochastic Process. Appl.*, **101**(2):185–232, 2002.

[37] J. C. Mattingly, A. M. Stuart, and M. V. Tretyakov. Convergence of numerical time-averaging and stationary measures via Poisson equations. *SIAM J. Numer. Anal.*, **48**(2):552–577, 2010.

[38] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller. Equation of state calculations by fast computing machines. *J. Chem. Phys.*, **21**(6):1087–1092, 1953.

[39] S. Meyn and R. L. Tweedie. *Markov Chains and Stochastic Stability*. Cambridge University Press, Cambridge, second edition, 2009.

[40] P. K. Mogensen and A. N. Riseth. Optim: A mathematical optimization package for Julia. *J. Open Source Softw.*, **3**(24):615, 2018.

[41] G. A. Pavliotis. *Stochastic Processes and Applications*, volume **60** of *Texts in Applied Mathematics*. Springer, New York, 2014.

[42] A. Quarteroni, R. Sacco, and F. Saleri. *Numerical Mathematics*, volume **37** of *Texts in Applied Mathematics*. Springer-Verlag, Berlin, second edition, 2007.

[43] L. Rey-Bellet. *Ergodic properties of Markov processes*. In *Open Quantum Systems II: The Markovian Approach*. S. Attal, A. Joye, and C.-A. Pillet, editors. Springer Berlin Heidelberg, Berlin, Heidelberg, 2006, pages 1–39.

[44] G. O. Roberts and J. S. Rosenthal. Optimal scaling of discrete approximations to Langevin diffusions. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, **60**(1):255–268, 1998.

[45] G. O. Roberts and R. L. Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli*, **2**(4), 1996.

[46] P. J. Rossky, J. D. Doll, and H. L. Friedman. Brownian dynamics as smart Monte Carlo simulation. *J. Chem. Phys.*, **69**(10):4628–4633, 1978.

[47] J. Roussel and G. Stoltz. Spectral methods for Langevin dynamics and associated error estimates. *ESAIM Math. Model. Numer. Anal.*, **52**(3):1051–1083, 2018.

[48] J. Shen, T. Tang, and L.-L. Wang. *Spectral Methods*, volume **41** of *Springer Series in Computational Mathematics*. Springer, Heidelberg, 2011.

[49] D. W. Stroock. *Probability Theory*. Cambridge University Press, Cambridge, second edition, 2011.

[50] A. M. Stuart. Inverse problems: A Bayesian perspective. *Acta Numer.*, **19**:451–559, 2010.

[51] D. Talay and L. Tubaro. Expansion of the global error for numerical schemes solving stochastic differential equations. *Stoch. Proc. Appl.*, **8**(4):483–509, 1990.