Ergodic SDEs on submanifolds and related numerical sampling schemes

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Abstract

In many applications, it is often necessary to sample the mean value of certain quantity with respect to a probability measure $\mu$ on the level set of a smooth function $\xi : \mathbb{R}^d \to \mathbb{R}^k$, $1 \leq k < d$. A specially interesting case is the so-called conditional probability measure, which is useful in the study of free energy calculation and model reduction of diffusion processes. By Birkhoff’s ergodic theorem, one approach to estimate the mean value is to compute the time average along an infinitely long trajectory of an ergodic diffusion process on the level set whose invariant measure is $\mu$. Motivated by the previous work of Ciccotti, Lelièvre, and Vanden-Eijnden [11], as well as the work of Lelièvre, Roussel, and Stoltz [33], in this paper we construct a family of ergodic diffusion processes on the level set of $\xi$ whose invariant measures coincide with the given one. For the conditional measure, in particular, we show that the corresponding SDEs of the constructed ergodic processes have relatively simple forms, and, moreover, we propose a consistent numerical scheme which samples the conditional measure asymptotically. The numerical scheme doesn’t require computing the second derivatives of $\xi$ and the error estimates of its long time sampling efficiency are obtained.

Keywords ergodic diffusion process, reaction coordinate, level set, conditional probability measure

1 Introduction

Many stochastic dynamical systems in real-world applications in physics, chemistry, and biology often involve a large number of degrees of freedom which evolve on vastly different time scales. Understanding the behavior of these systems can be highly challenging due to the high dimensionality and the existence of multiple time scales. To tackle these difficulties, the terminology reaction coordinate, or collective variable, is often introduced to help describe the essential dynamical behavior of complex systems [19, 20, 28, 36, 39].

In various research topics, in particular those related to molecular dynamics, such as free energy calculation [32, 33] and model reduction of stochastic processes along reaction coordinates [26, 16, 28, 46], one often encounters the problem to compute the mean value

$$\mathcal{F} = \int_{\Sigma} f(x) \, d\mu_1(x)$$

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constructed a diffusion process $Y$ on the level set $\Sigma = \xi^{-1}(0) = \{x \in \mathbb{R}^d \mid \xi(x) = 0 \in \mathbb{R}^k\}$ (2)
of a reaction coordinate function $\xi : \mathbb{R}^d \to \mathbb{R}^k$, $1 \leq k < d$, where $\mu_1$ is the so-called conditional probability measure on $\Sigma$, defined by

$$d\mu_1 = \frac{1}{Z} e^{-\beta U} [\det(\nabla \xi^T \nabla \xi)]^{-1} d\nu. \tag{3}$$

In [3], the parameter $\beta > 0$, $U : \mathbb{R}^d \to \mathbb{R}$ is a smooth function, $Z$ is the normalization constant, $\nabla \xi$ denotes the $d \times k$ Jacobian matrix of the mapping $\xi$, and $\nu$ is the surface measure on $\Sigma$ induced from the Lebesgue measure on $\mathbb{R}^d$. Applying Birkhoff’s ergodic theorem, the mean value $\overline{f}$ can be approximated by the time average $\frac{1}{T} \int_0^T f(X_s) ds$ along a long trajectory of the process $X_s$ which evolves on the level set $\Sigma$ and has the invariant measure $\mu_1$. For this purpose, it is helpful to construct a diffusion process on the level set with the correct invariant measure $\mu_1$, i.e., to write down the stochastic differential equation (SDE) of $X_s$ in $\mathbb{R}^d$. While finding such an SDE is trivial in the linear reaction coordinate case [44], it is not obvious when the reaction coordinate $\xi$ is a nonlinear function of system’s state.

In the literature, the aforementioned problem has been considered in the study of free energy calculations [10, 32, 11, 33]. Given a smooth function $U : \mathbb{R}^d \to \mathbb{R}$ and its effective dynamics have been considered in [11], where the matrix-valued coefficients $\sigma, \alpha : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ are related by $a = \sigma \sigma^T$, such that $a$ is uniformly positive definite. Notice that,

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In the literature, the aforementioned problem has been considered in the study of free energy calculations [10, 32, 11, 33]. Given a smooth function $U : \mathbb{R}^d \to \mathbb{R}$, the authors in [11] constructed a diffusion process $Y_s$ on $\Sigma$ whose unique invariant measure is $\mu_2$, given by

$$d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu. \tag{4}$$

It is also shown in [11] that this process $Y_s$ can be obtained by projecting the dynamics

$$d\tilde{Y}_s = -\nabla U(\tilde{Y}_s) ds + \sqrt{2\beta^{-1}} dW_s \tag{5}$$

from $\mathbb{R}^d$ onto the level set $\Sigma$, where $W_s = (W_{s,1}^1, \cdots, W_{s,d}^d)^T$ is a $d$-dimensional Brownian motion. The dynamics $Y_s$ can be used to sample $\mu_2$, and therefore to sample the conditional measure $\mu_1$ in [3] as well, by either modifying the potential $U$ or reweighting the function $f$ according to the factor $[\det(\nabla \xi^T \nabla \xi)]^{-\frac{1}{2}}$. In the more recent work [33], the authors studied the constrained Langevin dynamics, which evolves on the submanifold of the entire phase space including both position and momentum. It is shown in [33] that the position components of the constrained Langevin dynamics have the marginal invariant measure which coincides with $\mu_2$. Therefore, it can also be used to compute the average $\overline{f}$ with respect to the conditional measure $\mu_1$ (by either modifying the potential or reweighting $f$ according to $[\det(\nabla \xi^T \nabla \xi)]^{-\frac{1}{2}}$). Comprehensive studies on the numerical schemes as well as the applications of the constrained Langevin dynamics in free energy calculations have been carried out in [33].

The same conditional probability measure $\mu_1$ in [3], as well as the average $\overline{f}$ in [11], also plays an important role in the study of the effective dynamics of diffusion processes [24, 16, 28, 46]. As a generalization of the dynamics [5], the diffusion process

$$d\tilde{Y}_s^i = -\left(\frac{\partial U}{\partial x_j}(\tilde{Y}_s) + \frac{1}{\beta} \frac{\partial^2 U}{\partial x_j^2}(\tilde{Y}_s) + \sqrt{2\beta^{-1}} \sigma_{ij}(\tilde{Y}_s)\right) ds + \sqrt{2\beta^{-1}} \sigma_{ij}(\tilde{Y}_s) dW_s^j, \quad 1 \leq i \leq d, \tag{6}$$

and its effective dynamics have been considered in [46], where the matrix-valued coefficients $\sigma, \alpha : \mathbb{R}^d \to \mathbb{R}^{d \times d}$ are related by $a = \sigma \sigma^T$, such that $a$ is uniformly positive definite. Notice that,
is written in component-wise form with Einstein’s summation convention, and it reduces to (5) when \( \sigma = a = \text{id} \). The infinitesimal generator of (6) can be written as

\[
\mathcal{L} = \frac{e^{\beta U}}{\beta} \frac{\partial}{\partial x_i} \left( e^{-\beta U} a_{ij} \frac{\partial}{\partial x_j} \right). \tag{7}
\]

Under mild conditions on \( U \), it is known that, for any (smooth, uniformly positive definite) coefficient \( a \), the dynamics (6) has the common unique invariant measure whose probability density is \( \frac{1}{Z} e^{-\beta U} \) with respect to the Lebesgue measure on \( \mathbb{R}^d \).

Motivated by these previous work, in this paper we try to answer the following questions.

(Q1) Besides the process constructed in [11] that is closely related to (5), can we obtain other diffusion processes on \( \Sigma \), which are probably related to (6) involving the coefficients \( \sigma, a \), and have the same invariant measure? In particular, since the conditional probability measure \( \mu_1 \) is relevant in applications, can we construct SDE on \( \Sigma \) whose invariant measure is \( \mu_1 \)?

(Q2) On \( \mathbb{R}^d \), it is well known that the overdamped dynamics (5) can be derived from the Langevin dynamics in the large friction limit, together with a rescaling of time [32]. Are there similar relations for processes on the level set \( \Sigma \)? In another word, what is the relation between the processes considered in [11] and [33]?

(Q3) Numerically, sampling tasks involving \( \mu_1 \) are often solved in the literature by relating the problems to the measure \( \mu_2 \). Besides this approach, can we estimate the mean value in (1) with respect to the conditional measure \( \mu_1 \) directly, preferably with a numerical algorithm that is easy to implement?

In the following, let us summarize the main contributions of the current work related to the above questions. Firstly, for Question (Q1), in Theorem 1 of Section 3, we will construct a family of diffusion processes on \( \Sigma \) which sample either \( \mu_1 \) or \( \mu_2 \). In particular, we show that the diffusion process

\[
dX_i = - (Pa)_{ij} \frac{\partial U}{\partial x_j} ds + \frac{1}{\beta} \frac{\partial (Pa)_{ij}}{\partial x_j} ds + \sqrt{2 \beta^{-1} P_{ji}} dW_j, \quad 1 \leq i \leq d, \tag{8}
\]
evolves on \( \Sigma \) and the invariant measure is the conditional probability measure \( \mu_1 \) in (3). (The matrices \( P \) and \( P_{ji} \) are related to the projection operator on \( \Sigma \) and their definitions will be given in Section 2.) Correspondingly, the infinitesimal generator of (8) is

\[
\mathcal{L} = \frac{e^{\beta U}}{\beta} \frac{\partial}{\partial x_i} \left( e^{-\beta U} (Pa)_{ij} \frac{\partial}{\partial x_j} \right), \tag{9}
\]

which should be compared to the infinitesimal generator in (7). We emphasize that knowing the SDE (8) and the expression (9) of its infinitesimal generator is helpful for theoretical analysis. For instance, in Section 4, the Poisson equation on \( \Sigma \) related to (9) will be used to study the long time sampling efficiency of numerical schemes. Furthermore, the infinitesimal generator (9) plays a role in the subsequent work [31] in analyzing the approximation quality of the effective dynamics for the diffusion process (6), while the dynamics (8) has been used in [21] to study the fluctuation relations and Jarzynski’s equality for nonequilibrium systems in the reaction coordinate case.

Secondly, for Question (Q2), in Subsection 3.2, we study the constrained Langevin dynamics in [32], where we introduce a parameter \( \epsilon > 0 \) and we modify the potential function \( U \) properly
such that its marginal invariant measure is $\mu_1$. Using asymptotic expansion argument \cite{39,32}, we formally show that, as $\epsilon \to 0$, the constrained Langevin dynamics converges to a dynamics whose SDE has the same form as in \cite{5}. Based on this fact, we can view the process \cite{5} constructed in the current work as the overdamped limit of the constrained Langevin dynamics in \cite{33} (with modified potential).

Thirdly, for Question (Q3), in Section \ref{4} we study a numerical algorithm which estimates the mean value $\bar{f}$ in (1). Specifically, we propose to use the numerical scheme

$$
\begin{align*}
x^{(l+1)}_i &= x^{(l)}_i + \left( -a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right) (x^{(l)}) h + \sqrt{2\beta^{-1}} h \sigma_{ij}(x^{(l)}) \eta^{(l)}_j, \quad 1 \leq i \leq d, \\
x^{(l+1)} &= \Theta(x^{(l+\bullet)}),
\end{align*}
$$

with $x^{(0)} \in \Sigma$, and to approximate $\bar{f}$ by $\tilde{f}_n = \frac{1}{n} \sum_{l=0}^{n-1} f(x^{(l)})$. In (10), $h$ is the step-size, $\eta^{(l)} = (\eta_1^{(l)}, \eta_2^{(l)}, \ldots, \eta_d^{(l)})^T$ are independent $d$-dimensional standard Gaussian random variables, and $\Theta(x) = \lim_{s \to +\infty} \varphi(x, s)$ is the limit of the flow

$$
\frac{d\varphi(x, s)}{ds} = -(a \nabla F)(\varphi(x, s)), \quad \varphi(x, 0) = x, \quad \forall x \in \mathbb{R}^d,
$$

with the function $F(x) = \frac{1}{2} \xi(x)^2 = \frac{1}{2} \sum_{i=1}^{k} \xi_i^2(x)$. Following the approach developed in \cite{28}, in Theorem \ref{2} we obtain the estimates of the approximation error between $\tilde{f}_n$ and $\bar{f}$, quantified in term of $h$ and $T = nh$. While different constraint approaches have been proposed in the literature \cite{29,33,45}, to the best of the author’s knowledge, constraint using the flow map $\varphi$ has not been studied yet. We point out that both the properties of the map $\Theta$ and the infinitesimal generator (\ref{6}) of the SDE (\ref{5}) play important roles in proving the estimates of Theorem \ref{2}.

Let us emphasize that $\Theta(x)$ in the scheme (10) can be evaluated by solving the ODE (11) starting from $x$. Although $\Theta$ is defined as the limit when $s \to +\infty$, in many cases the computational cost is not large, due to the exponential convergence of the (gradient) flow (11) to its limit, particularly for the initial state $x = x^{(l+\frac{1}{2})}$ that is close to $\Sigma$. Furthermore, comparing to the direct (Euler-Maruyama) discretization of SDE (\ref{5}) which may deviate from $\Sigma$, the scheme (10) satisfies $x^{(l)} \in \Sigma$ for all $l \geq 0$, and it doesn’t require computing the second order derivatives of the reaction coordinate $\xi$. Therefore, we expect the numerical scheme (10)–(11) is both stable and relatively easy to implement. Readers are referred to Remark \ref{4} in Section \ref{3} and the third example in Section \ref{5} for further algorithmic discussions.

In the following, we briefly explain the approach that we will use to study Question (Q1), as well as the idea behind the numerical scheme (10)–(11). Concerning Question (Q1), i.e., the construction of ergodic SDEs on $\Sigma$, an important observation for us is the similarity between the expressions of the infinitesimal generator of the dynamics \cite{5} and the expressions of differential operators on Riemannian manifold. Assuming the matrix $a$ is positive definite, we can define $g = a^{-1}$ and let $G = \text{det}g$. $g_{ij}$, $g^{ij}$ denote the components of the matrices $g$ and $g^{-1}$, respectively. Clearly, we have $g^{ij} = (g^{-1})_{ij} = a_{ij}, \ 1 \leq i, j \leq d$. For smooth functions $f : \mathbb{R}^d \to \mathbb{R}$, using (7) we can compute

$$
\mathcal{L}f = \frac{e^{\delta U}}{\beta} \frac{\partial}{\partial x_i} \left( \frac{e^{-\beta U}}{\sqrt{G}} \sqrt{G} g^{ij} \frac{\partial f}{\partial x_j} \right).
$$
\[
\begin{align*}
\frac{1}{\beta} \frac{\partial}{\partial x_i} \left( \ln \frac{e^{-\beta U}}{\sqrt{G}} \right) g^{ij} \frac{\partial f}{\partial x_j} + \frac{1}{\beta \sqrt{G}} \frac{\partial}{\partial x_i} \left( \sqrt{G} g^{ij} \frac{\partial f}{\partial x_j} \right) \\
= - \left( \nabla^\mathcal{M} (U + \frac{1}{2\beta} \ln G), \nabla^\mathcal{M} f \right)_g + \frac{1}{\beta} \Delta^\mathcal{M} f \\
= \left[ - \nabla^\mathcal{M} \left( U + \frac{1}{2\beta} \ln G \right) + \frac{1}{\beta} \Delta^\mathcal{M} \right] f.
\end{align*}
\]

In the last two equalities above, we have viewed \( \mathcal{M} = (\mathbb{R}^d, g) \) as a Riemannian manifold with the tensor metric \( g \), defined by
\[
g(u, v) = \langle u, v \rangle_g = u_i (a^{-1})_{ij} v_j, \quad \forall \ u, v \in \mathbb{R}^d,
\]
and \( \nabla^\mathcal{M}, \Delta^\mathcal{M} \) denote the gradient and the Laplacian operator on \( \mathcal{M} \), respectively. Accordingly, (6) can be written as a SDE on the manifold \( \mathcal{M} \) as
\[
d\tilde{Y}_s = - \nabla^\mathcal{M} \left( U + \frac{1}{2\beta} \ln G \right) ds + \sqrt{2 \beta^{-1}} dB_s,
\]
where \( \tilde{B}_s \) is the Brownian motion on \( \mathcal{M} \). Conversely, SDE (6) can be seen as the equation of (13) under the (global) coordinate chart of the manifold \( \mathcal{M} \). This equivalence allows us to study the SDE (6) on \( \mathbb{R}^d \) by the corresponding SDE (13) on manifold \( \mathcal{M} \). Comparing to (6), one advantage of working with the abstract equation (13) is that the invariant measure of (13) can be recognized as easily as in (5), provided that we apply integration by parts formula on manifold.

This manifold point of view is also useful when we study diffusion processes on \( \Sigma \), i.e., to answer Question (Q1). Specifically, \( \Sigma \) can be considered as a submanifold of \( \mathcal{M} \) and we denote by \( \nabla^\Sigma, \Delta^\Sigma, B_s \) the gradient operator, the Laplacian and the Brownian motion on \( \Sigma \), respectively. Since the infinitesimal generator of \( B_s \) is \( \frac{1}{2} \Delta^\Sigma \), we know the infinitesimal generator of the SDE
\[
dY_s = - \nabla^\Sigma U ds + \sqrt{2 \beta^{-1}} dB_s,
\]
is given by \( L = - \nabla^\Sigma U + \frac{1}{2} \Delta^\Sigma \). Under mild assumptions on \( U \), it is straightforward to verify that dynamics (14) evolves on \( \Sigma \) and has the unique invariant measure \( \frac{1}{2} \beta^{-1} \nu_g \), where \( \nu_g \) is the surface measure on \( \Sigma \) induced from the metric \( g = a^{-1} \) on the manifold \( \mathcal{M} = (\mathbb{R}^d, g) \). Therefore, answering Question (Q1) boils down to calculating the expression of (14) under the coordinate chart of the manifold \( \mathcal{M} \) (not \( \Sigma \)). This can be achieved by calculating the expressions of \( \nabla^\Sigma \), \( \Delta^\Sigma \) under the coordinate chart of \( \mathcal{M} \) and then figuring out the relation between the two measures \( \nu \) and \( \nu_g \).

Concerning the idea behind the numerical scheme (10)–(11), we recall that one way to sample \( \mu_1 \) on the level set \( \Sigma \) (approximately) is to constrain the dynamics (8) in the neighborhood of \( \Sigma \) by adding an extra potential to it. This is often termed as softly constrained dynamics [11, 37] and has been widely explored in the literature. Specifically, in this context, one consider the dynamics
\[
dX_s^{i} = \left[ - a_{ij} \frac{\partial U}{\partial x_j} - \frac{1}{\epsilon} a_{ij} \frac{\partial}{\partial x_j} \left( \frac{1}{2} \sum_{\alpha=1}^{k} \xi_{a}^{2} \right) + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right] ds + \sqrt{2 \beta^{-1}} \sigma_{ij} dW_s^{j},
\]
where \( \epsilon > 0, 1 \leq i \leq d \). It is known that the invariant measure of (15) converges weakly to the conditional measure \( \mu_1 \), as \( \epsilon \to 0 \). The dynamics (15) stays close to \( \Sigma \) all the time, thanks to
the existence of the extra constraint force. Furthermore, only the first order derivatives of $\xi$ are involved. In spite of these nice properties, however, direct simulation of (15) is inefficient when $\epsilon$ is small, because the time step-size in numerical simulations becomes severely limited due to the strong stiffness in the dynamics. Indeed, our numerical scheme is motivated in order to overcome the aforementioned drawback of the softly constrained dynamics (15), and (10)–(11) can be viewed as a multiscale numerical method for (15), where the stiff and non-stiff terms in (15) are handled separately [44]. In contrast to the previous work [24, 15, 11], where the convergence of the SDE (15) was studied on a finite time interval, our result is new in that it concerns the long time sampling efficiency of the discretized numerical scheme.

In principle, one might consider to discretize the SDE (8) and use it to sample the mean value $\bar{f}$ in (1) numerically. However, in practice this approach may be numerically infeasible for two reasons. First, although the dynamics (8) stays on the level set $\Sigma$ all the time, the dynamics after discretization may violate this property. In particular, for long time simulation that is needed to approximate the average value $\bar{f}$, the discretized dynamics may become far away from the level set $\Sigma$, in which case the estimated average will no longer be reliable. Second, although the SDE (8) and its infinitesimal generator in (9) have relatively simple structures, simulating the SDE (8) requires computing the second order derivatives of the reaction coordinate $\xi$. In fact, the dependence on the second order derivatives can make the numerical implementation complicate, particularly in molecular dynamics applications. We refer to the third example in Section 5 for numerical tests of this approach on a simple example.

Before concluding this introduction, we would like to compare the current work with several previous ones. Generally speaking, Monte Carlo samplers (based on ergodicity) for mean values of functions either on $\mathbb{R}^d$ or on its submanifolds can be classified into Metropolis-adjusted samplers and unadjusted samplers. For the Metropolis-adjusted method, probably the best known one is the Markov Chain Monte Carlo (MCMC) method, which has been well studied in statistics community [35]. In particular, the idea of exploiting Riemannian geometry structure of the space to develop MCMC methods has been considered in [18]. The authors there studied a number of interesting applications and demonstrated that incorporating the geometry of the space into numerical methods can lead to significant improvement of the sampling efficiency. We argue that this is also true in our case. In Section 5 we will consider a concrete example where a non-identity matrix $a$ can help remove the stiffness both in the dynamics and in numerical algorithms. On the other hand, despite of the common Riemannian manifold point of view in the current work and in [18], the main difference is that the work [18] considered sampling on the entire space $\mathbb{R}^d$ (or a domain of it), while the current work deals with sampling on its submanifold $\Sigma$. The computations in the current work are more involved mainly due to this difference. Besides of sampling on the entire space, the Metropolis-adjusted samplers on submanifolds, using either MCMC or Hybrid Monte Carlo, have been considered in several recent work [8, 33, 45, 34]. Reversible Metropolis random walk on submanifolds has been constructed in [45], which is then extended in [34] to develop Hybrid Monte Carlo algorithms by allowing non-zero gradient forces in the proposal move. The numerical schemes in these work are unbiased and therefore large time step-sizes can be used in numerical estimations.

In contrast to these work, the numerical scheme (10)–(11) proposed in the current work is unadjusted and samples the conditional probability measure $\mu_1$ only when the step-size $h \to 0$. This means that, in practice, the step-size $h$ should be chosen properly such that the discretiza-
tion error is tolerable. In this direction, we point out that the unadjusted samplers on the entire space \( \mathbb{R}^d \), which naturally arise from discretizing SDEs, have been well studied in the literature \([43, 31, 12, 3, 38]\). The current work can be thought as a further step along this direction for sampling schemes on submanifolds, by applying the machinery developed in \([38]\).

One feature of the current work is that we will go beyond reversibility and will also characterize non-reversible SDEs on submanifolds. The idea of developing (unadjusted) sampling schemes based on non-reversible dynamics will be discussed as well (Remark 5 and Section 5). We refer to \([30]\) for discussions on the comparison between Metropolis-adjusted and unadjusted samplers.

The rest of the paper is organized as follows. In Section 2, we introduce notations and summarize some useful results related to both the Riemannian manifold \( \mathcal{M} = (\mathbb{R}^d, g) \) and its submanifold \( \Sigma \). In particular, the expression of the Laplacian \( \Delta^\Sigma \) on \( \Sigma \) will be stated. In Section 3, we construct ergodic SDEs on \( \Sigma \) which sample either \( \mu_1 \) or \( \mu_2 \) by applying the manifold point of view. The overdamped limit of the constrained Langevin dynamics will be studied as well. In Section 4, we study the numerical scheme (10)–(11) and quantify its approximation error in estimating the mean value in (1). In Section 5, we demonstrate our results through some concrete examples. Conclusions and further discussions are made in Section 6. Further details related to the Riemannian manifold \( \mathcal{M} \) in Section 2 are included in Appendix A. The properties of the limiting flow map \( \Theta \) and the projection map \( \Pi \) along geodesic curves on \( \mathcal{M} \) are studied in Appendix B and Appendix C respectively.

Finally, let us mention that, although the manifold point of view plays an important role, the Riemannian manifold setting in Section 2 is only used in Section 3 and in the end of Section 4. Once having a general idea of the approach explained in the Introduction, readers who are not interested in the Riemannian manifold discussions can directly read Proposition 1 in Section 2 and skip the rest discussions there.

## 2 Notations and preparations

In this section, we fix notations and summarize results which will be used in the subsequent sections.

Suppose that the \( d \times d \) matrix-valued smooth function \( \sigma : \mathbb{R}^d \to \mathbb{R}^{d \times d} \) is invertible at each \( x \in \mathbb{R}^d \) and therefore the matrix \( a = \sigma \sigma^T \) is both smooth and positive definite. Given two vectors \( \mathbf{u} = (u_1, u_2, \ldots, u_d)^T \), \( \mathbf{v} = (v_1, v_2, \ldots, v_d)^T \), we consider the space \( \mathbb{R}^d \) with the weighted inner product

\[
g(\mathbf{u}, \mathbf{v}) = \langle \mathbf{u}, \mathbf{v} \rangle_g = u_i (a^{-1})_{ij} v_j.
\]

In the above, the repeated indices \( i, j \) are summed up for \( 1 \leq i, j \leq d \), and the same Einstein’s summation convention will be used throughout this paper, whenever no ambiguity will arise. The inner product in (16) defines a Riemannian metric \( g \) on \( \mathbb{R}^d \) and we denote by \( \mathcal{M} = (\mathbb{R}^d, g) \) the Riemannian manifold \( \mathbb{R}^d \) endowed with this metric.

The main result of this section is Proposition 1 where we give the expression of the Laplacian operator \( \Delta^\Sigma \) on the level set \( \Sigma \) in (2), viewed as a submanifold of \( \mathcal{M} \). Before that, we need to introduce some notations and quantities related to \( \mathcal{M} \) and \( \Sigma \). To keep the discussions transparent, we will only state results that are useful in the following sections and will leave the
derivations and further details in Appendix \( \Xi \). Readers are referred to \( \Xi \) for related discussions on general Riemannian manifolds.

First of all, notice that \( \mathcal{M} \) as a manifold is quite special (simple), in that it has a natural global coordinate chart which is given by the usual Euclidean coordinate. Since we will always work with this coordinate, we will not distinguish between tangent vectors (operators acting on functions) and their coordinate representations (\( d \)-dimensional vectors). In particular, \( e_i \) denotes the vector whose \( i \)th component equals 1 while all the other \( d - 1 \) components equal to 0, where \( 1 \leq i \leq d \). At each point \( x \in \mathcal{M} \), vectors \( e_1, e_2, \cdots, e_d \) form a basis of the tangent space \( T_x \mathcal{M} \) and under this basis we have \( g = a^{-1} \), as can be seen from \( \Xi \).

Denote by \( \text{grad}^\mathcal{M} \), \( \text{div}^\mathcal{M} \) the gradient and the divergence operator on \( \mathcal{M} \), respectively. For any smooth function \( f : \mathcal{M} \to \mathbb{R} \), it is direct to verify that
\[
\text{grad}^\mathcal{M} f = g^{ij} \frac{\partial f}{\partial x_j} e_i = (a \nabla f)_i e_i, \tag{17}
\]
where \( g^{ij} = (g^{-1})_{ij} = a_{ij} \), and \( \nabla f \) denotes the ordinary gradient operator for functions on the Euclidean space \( \mathbb{R}^d \). For simplicity, we will also write \( \partial_i f \) for the partial derivative with respect to \( x_i \), and \( (a \nabla f)_i \) to denote the \( i \)th component of the vector \( a \nabla f \), i.e., \( \partial_i f = \frac{\partial f}{\partial x_i} \), and \( (a \nabla f)_i = a_{ij} \frac{\partial f}{\partial x_j} = a_{ij} \partial_j f \).

The Laplace-Beltrami operator on \( \mathcal{M} \) is defined by \( \Delta^\mathcal{M} f = \text{div}^\mathcal{M} (\text{grad}^\mathcal{M} f) \). Equivalently, we have \( \Delta^\mathcal{M} f = \text{tr}(\text{Hess}^\mathcal{M} f) \), where \( \text{Hess}^\mathcal{M} \) is the Hessian operator on \( \mathcal{M} \) and “tr” is the trace operator. The integration by parts formula on \( \mathcal{M} \) has the form
\[
\int_{\mathcal{M}} (\Delta^\mathcal{M} f_1) f_2 \, dm = - \int_{\mathcal{M}} (\text{grad}^\mathcal{M} f_1, \text{grad}^\mathcal{M} f_2)_g \, dm = \int_{\mathcal{M}} (\Delta^\mathcal{M} f_2) f_1 \, dm, \tag{18}
\]
for \( \forall f_1, f_2 \in C_c^\infty(\mathcal{M}) \), where \( dm = (\det g)^{\frac{1}{2}} dx = (\det a)^{-\frac{1}{2}} dx \) is the volume form, and \( C_c^\infty(\mathcal{M}) \) consists of all smooth functions on \( \mathcal{M} \) with compact support.

Besides the vector basis \( e_1, e_2, \cdots, e_d \), the vectors
\[
\sigma_i = (\sigma_{i1}, \sigma_{i2}, \cdots, \sigma_{id})^T, \quad 1 \leq i \leq d, \tag{19}
\]
will also be useful. From the fact \( a = \sigma \sigma^T = g^{-1} \), we have \( \langle \sigma_i, \sigma_j \rangle_g = (a^{-1})_{ij} \sigma_i \sigma_j = \delta_{ij} \). In another word, \( \sigma_1, \sigma_2, \cdots, \sigma_d \) form an orthonormal basis of \( T_x \mathcal{M} \) at each \( x \in \mathcal{M} \).

Now let us consider a \( C^2 \) function \( \xi : \mathbb{R}^d \to \mathbb{R}^k \) with \( \xi = (\xi_1, \xi_2, \cdots, \xi_k)^T, 1 \leq k < d \). The level set of \( \xi \) corresponding to the value \( 0 \in \text{Im} \xi \subseteq \mathbb{R}^k \) is defined as the pre-image
\[
\Sigma = \xi^{-1}(0) = \left\{ x \in \mathcal{M} = \mathbb{R}^d \mid \xi(x) = 0 \in \mathbb{R}^k \right\}. \tag{20}
\]
Applying the regular value theorem \( \Xi \), we know that \( \Sigma \) is a \((d - k)\)-dimensional submanifold of \( \mathcal{M} \), under the Assumption \( \Xi \) below.

Given \( x \in \Sigma \) and a vector \( v \in T_x \mathcal{M} \), the orthogonal projection operator \((d \times d \text{ matrix}) \)
\[
P : \mathbb{R}^d \to T_x \Sigma \text{ is defined such that } (v - P_x v, u)_g = 0, \forall u \in T_x \Sigma. \] It is straightforward to verify that \( P = \text{id} - a \nabla \xi \Psi^{-1} \nabla \xi^T \), or entrywise,
\[
P_{ij} = \delta_{ij} - (\Psi^{-1})_{\alpha\gamma}(a \nabla \xi_\alpha) \partial_j \xi_\gamma, \quad 1 \leq i, j \leq d, \tag{21}
\]
where \( \Psi \) is the invertible \( k \times k \) symmetric matrix at each point \( x \in \Sigma \), given by
\[
\Psi_{\alpha\gamma} = (\text{grad}^\mathcal{M} \xi_\alpha, \text{grad}^\mathcal{M} \xi_\gamma)_g = (\nabla \xi^T a \nabla \xi)_{\alpha\gamma}, \quad 1 \leq \alpha, \gamma \leq k. \tag{22}
\]
In the above, \( \nabla \xi \) denotes the \( d \times k \) matrix with entries \( (\nabla \xi)_{\alpha i} = \partial_i \xi_\alpha \), for \( 1 \leq \alpha \leq k, 1 \leq i \leq d \).

We can verify that the matrix \( P \) satisfies
\[
aP^T = Pa, \quad P^2 = P, \quad P^T \nabla \xi_\alpha = 0, \quad 1 \leq \alpha \leq k. \tag{23}
\]

Let us further assume that \( v \in T_x \Sigma \) is a tangent vector of \( \Sigma \) at \( x \). Since \( \{\sigma_i\}_{1 \leq i \leq d} \) forms an orthonormal basis of the tangent space \( T_x \mathcal{M} \), we have \( v = \langle v, \sigma_i \rangle g \sigma_i \). Using the fact that \( P \nu = v \), we obtain \( v = \langle v, P \sigma_i \rangle g \sigma_i \), where \( P \sigma_i \in T_x \Sigma \). If we denote \( P_i = P_i e_i \), then it follows from (21) and (23) that
\[
P_{i,j} = (P \sigma)_{ji} = \sigma_{ji} - (\Psi^{-1})_{\alpha \gamma} (a \nabla \xi_\alpha)_j (\sigma^T \nabla \xi_\gamma)_i, \quad P_{i,j}P_{j,i} = (aP^T)_{ij} = a_{ij} - (\Psi^{-1})_{\alpha \gamma} (a \nabla \xi_\alpha)_i (a \nabla \xi_\gamma)_j, \tag{24}
\]
for \( 1 \leq i, j \leq d \).

Let \( \text{grad}^\Sigma, \text{div}^\Sigma, \Delta^\Sigma, \text{Hess}^\Sigma \) denote the gradient operator, the divergence operator, the Laplace-Beltrami operator and the Hessian operator on \( \Sigma \), respectively. It is direct to check that \( \text{grad}^\Sigma = P \text{grad}^\mathcal{M} \). That is, for \( f \in C^\infty(\Sigma) \) and let \( \tilde{f} \) be its extension to \( \mathcal{M} \) such that \( \tilde{f} \in C^\infty(\mathcal{M}) \) and \( f|_\Sigma = f \), we have
\[
\text{grad}^\Sigma f = P \text{grad}^\mathcal{M} \tilde{f} = Pa \nabla \tilde{f}. \tag{25}
\]

Let \( \nu_g \) be the surface measure on \( \Sigma \) induced from the metric \( g \) on \( \mathcal{M} \). We recall that the mean curvature vector \( H \) on \( \Sigma \) is defined such that \([2,11]\)
\[
\int_\Sigma \text{div}^\Sigma v \, d\nu_g = - \int_\Sigma \langle H, v \rangle_g \, d\nu_g, \tag{26}
\]
for all vector fields \( v \) on \( \mathcal{M} \).

Next, we discuss the Laplace-Beltrami operator \( \Delta^\Sigma \) on the submanifold \( \Sigma \). Clearly, \( \Delta^\Sigma \) is self-adjoint and, similar to [18], we have the integration by parts formula on \( \Sigma \) with respect to the measure \( \nu_g \), as
\[
\int_\Sigma (\Delta^\Sigma f_1) f_2 \, d\nu_g = - \int_\Sigma \langle \text{grad}^\Sigma f_1, \text{grad}^\Sigma f_2 \rangle_g \, d\nu_g = \int_\Sigma (\text{grad}^\Sigma f_2) f_1 \, d\nu_g, \tag{27}
\]
for \( \forall f_1, f_2 \in C^\infty(\Sigma) \). The expression of \( \Delta^\Sigma \) can be computed explicitly and this is the content of the following proposition. Its proof requires tedious calculations and therefore is presented in Appendix [A].

**Proposition 1.** Let \( \Sigma \) be the submanifold of \( \mathcal{M} \) defined in (20), \( P \) be the projection matrix in (21), and \( \Delta^\Sigma \) be the Laplace-Beltrami operator on \( \Sigma \). We have
\[
\Delta^\Sigma = (Pa)_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + [\partial(Pa)_{ij} \frac{1}{2} (Pa)_{ij} \frac{\partial}{\partial x_j} \ln \left( \det a \right)^{-1} \det (\nabla \xi^T a \nabla \xi) \frac{\partial}{\partial x_i}]. \tag{28}
\]
In the special case when \( a = e_i \) is id, we have
\[
\Delta^\Sigma = \sum_{i=1}^{d} P_i \frac{\partial^2}{\partial x_i \partial x_i} + P_{ij} \frac{\partial P_{ij}}{\partial x_j} \frac{\partial}{\partial x_i} + H_i \frac{\partial}{\partial x_i} \tag{29}
\]
where \( H = H_i e_i \) is the mean curvature vector of the submanifold \( \Sigma \).
We point out that the proof of Proposition 1 in Appendix A is indeed valid for a general Riemannian manifold \( \mathcal{M} \) and its level set \( \Sigma \) as well. In this case, (28) holds true on a local coordinate of the manifold \( \mathcal{M} \).

Finally, we conclude this section by summarizing the assumptions which will be made (implicitly) throughout this paper.

**Assumption 1.** The matrix \( \sigma : \mathbb{R}^d \to \mathbb{R}^{d \times d} \) is both smooth and invertible at each \( x \in \mathbb{R}^d \). The matrix \( a = \sigma \sigma^T \) is uniformly positive definite with uniformly bounded inverse \( a^{-1} \).

**Assumption 2.** The function \( \xi : \mathbb{R}^d \to \mathbb{R}^k \) is \( C^2 \) smooth and the level set \( \Sigma \) is both connected and compact, such that \( \text{rank}(\nabla \xi) = k \) at each \( x \in \Sigma \).

**Remark 1.** Under the above assumptions, we can find a neighborhood \( \mathcal{O} \) of \( \Sigma \), such that the matrices \( P \) and \( \Psi \), defined in (21) and (22) respectively, can be extended to \( \mathcal{O} \). Furthermore, the relations in (23) are still satisfied in \( \mathcal{O} \). Due to this fact, we can talk about the derivatives of \( P \) at states \( x \in \Sigma \). Notice that the derivatives of \( P \) have appeared in the SDE (3) and in the expression (28) of the operator \( \Delta^\Sigma \).

### 3 Ergodic diffusion processes on the submanifold of \( \mathbb{R}^d \)

In this section, we study ergodic diffusion processes on \( \Sigma \) which sample the given invariant probability distributions. Recall that the coefficients \( \sigma, a \) are given such that \( a = \sigma \sigma^T \) is uniformly positive definite. In Subsection 3.1 SDEs of ergodic processes on the submanifold \( \Sigma \) will be constructed by applying Proposition 1 in Section 2. In Subsection 3.2 we show that the processes constructed in Subsection 3.1 are related to the overdamped limit of the constrained Langevin dynamics [33].

#### 3.1 SDEs of ergodic diffusion processes on \( \Sigma \)

First of all, let us point out that, the semigroup approach based on functional inequalities on Riemannian manifolds is well developed to study the solution of Fokker-Planck equation towards equilibrium. One sufficient condition for the exponential convergence of the Fokker-Planck equation (and therefore the ergodicity of the corresponding dynamics) is the famous Bakry-Emery criterion [4]. In particular, concrete conditions are given in [42] which guarantee the exponential convergence to the unique invariant measure. In the following, we will always assume that the potential \( U \in C^\infty(\Sigma) \) and the Bakry-Emery condition in [42] is satisfied.

Recall that \( g = a^{-1} \) and \( \nu_g \) is the surface measure on \( \Sigma \) induced from the metric \( g \) on \( \mathcal{M} \). Let us first consider the probability measure \( \mu \) on \( \Sigma \) given by \( d\mu = \frac{1}{Z} e^{-\beta U} d\nu_g \), where \( \beta > 0 \) and \( Z \) is a normalization constant. The following proposition is a direct application of Proposition 1.

**Proposition 2.** Consider the dynamics on \( \mathbb{R}^d \) which satisfies the Ito SDE

\[
\frac{dY^i_s}{ds} = -(Pa)_{ij} \frac{\partial [U - \frac{1}{2\beta} \ln ((\det a)^{-1} \det(\nabla \xi^T a \nabla \xi))]}{\partial x_j} ds + \frac{1}{\beta} \frac{\partial (Pa)_{ij}}{\partial x_j} ds + \sqrt{2\beta^{-1} P_{ji}} dW^j_s
\]

(30)
for $1 \leq i \leq d$, where $W_s = (W^i_s, W^j_s, \cdots, W^d_s)^T$ is a $d$-dimensional Brownian motion. Suppose $Y_0 \in \Sigma$, then $Y_s \in \Sigma$ almost surely for $s \geq 0$. Furthermore, it has a unique invariant measure $\mu$ given by $d\mu = \frac{1}{Z} e^{-\beta U} d\nu$.

**Proof.** Using (31) and applying Proposition H we know that the infinitesimal generator of SDE (30) is

$$L f = -\langle \text{grad}^\Sigma \mu, \text{grad}^\Sigma f \rangle \mu + \frac{1}{\beta} \Delta^\Sigma f, \quad \forall f : \Sigma \to \mathbb{R}. \tag{31}$$

Applying Ito’s formula to $\xi_\alpha(Y_s)$, we have

$$d\xi_\alpha(Y_s) = L\xi_\alpha(Y_s) \, ds + \sqrt{2 \beta^{-1} \frac{\partial \xi_\alpha(Y_s)}{\partial x_i}} \, P_{ij} \, dW^j_s, \quad 1 \leq \alpha \leq k.$$

Using (31) and the fact that $\text{grad}^\Sigma \mu = P \text{grad}^\Sigma^\mu \xi_\alpha = 0$, it is straightforward to verify that

$$L\xi_\alpha = -\langle \text{grad}^\Sigma \mu, \text{grad}^\Sigma \xi_\alpha \rangle \mu + \frac{1}{\beta} \text{div}^\Sigma (\text{grad}^\Sigma \xi_\alpha) = 0,$$

$$\frac{\partial \xi_\alpha}{\partial x_i} P_{ij} = P_j \xi_\alpha = (P \sigma^\mu, \text{grad}^\Sigma \xi_\alpha) \mu = 0, \quad 1 \leq j \leq d,$$

on $\Sigma$, which implies $\xi_\alpha(Y_s) = 0$, $\forall s \geq 0$. Since $Y_0 \in \Sigma$, we conclude that $\xi_\alpha(Y_s) = \xi_\alpha(Y_0) = 0$ a.s. $s \geq 0$, for $1 \leq \alpha \leq k$, and therefore $Y_s \in \Sigma$ for $s \geq 0$, almost surely.

Using the expression (31) of $L$ and the integration by parts formula (27), it is easy to see that $\mu$ is an invariant measure of the dynamics (30). The uniqueness is implied by the exponential convergence result established in [42, Remark 1.1 and Corollary 1.5], since we assume Bakry-Emery condition is satisfied. \hfill \box

Until now, we have considered the level set $\Sigma$ as a submanifold of $\mathcal{M} = (\mathbb{R}^d, g)$ and introduced the surface measure $\nu$ for technical reasons. In applications, on the other hand, it is natural to view $\Sigma$ as a submanifold of the standard Euclidean space $\mathbb{R}^d$, with the surface measure $\nu$ on $\Sigma$ that is induced from the Euclidean metric on $\mathbb{R}^d$. In particular, as already mentioned in the Introduction, the following two probability measures

$$d\mu_1 = \frac{1}{Z} e^{-\beta U} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu, \quad d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu, \tag{32}$$

where $Z$ denotes possibly different normalization constants, are often interesting and arise in many situations. In order to construct processes which sample $\mu_1$ or $\mu_2$, we need to figure out the relations between the two surface measures $\nu_\gamma$ and $\nu$ on $\Sigma$.

**Lemma 1.** Let $\nu_\gamma$, $\nu$ be the surface measures on $\Sigma$ induced from the metric $g = a^{-1}$ and the Euclidean metric on $\mathbb{R}^d$, respectively. We have

$$d\nu_\gamma = (\det a)^{-\frac{1}{2}} \left[ \frac{\det(\nabla \xi^T a \nabla \xi)}{\det(\nabla \xi^T \nabla \xi)} \right]^{\frac{1}{2}} d\nu. \tag{33}$$

**Proof.** Let $x \in \Sigma$ and $v_1, v_2, \cdots, v_{d-k}$ be a basis of $T_x \Sigma$. Assume that $v_i = c_{ij} e_j$, where $c = (c_{ij})$ is a $(d-k) \times d$ matrix whose rank is $d-k$. Using the fact $\langle v_i, \text{grad}^\Sigma \xi_\alpha \rangle = 0$ for $1 \leq i \leq d-k$,
1 \leq \alpha \leq k$, we can deduce that $c \nabla \xi = 0$. Calculating the surface measures $\nu_g$ and $\nu$ under this basis, we obtain
\[
d\nu_g = \left[ \frac{\det((ca^{-1}c^T)^T)}{\det(cc^T)} \right]^{\frac{1}{2}} d\nu.
\] (34)
To simplify the right hand side of (34), we use the following equality
\[
\left( \begin{array}{c} c \\ \nabla \xi^T a \end{array} \right) \left( \begin{array}{c} c^T \\ \nabla \xi \end{array} \right) = \left( \begin{array}{cc} cc^T & 0 \\ \nabla \xi^T ac^T & \nabla \xi^T a \nabla \xi \end{array} \right) = \left( \begin{array}{cc} ca^{-1} \\ \nabla \xi \end{array} \right) \left( \begin{array}{c} c^T \\ \nabla \xi \end{array} \right).
\] (35)
After computing the determinants of the last two matrices above, we obtain
\[
\det(cc^T) \det(\nabla \xi^T a \nabla \xi) = (\det a) \det \left[ \begin{array}{cc} ca^{-1} \\ \nabla \xi \end{array} \right] \left( \begin{array}{c} c^T \\ \nabla \xi \end{array} \right) = (\det a) \det \left[ \begin{array}{cc} ca^{-1}c^T \\ 0 \\ ca^{-1} \nabla \xi \end{array} \right] \left( \begin{array}{c} c^T \\ \nabla \xi \end{array} \right).
\]
The conclusion follows after we substitute the above relation into (34).

Applying Lemma 1 and Proposition 2, we can obtain ergodic processes whose invariant measures are given in (32).

**Theorem 1.** Let $\mu_1, \mu_2$ be the two probability measures on $\Sigma$ defined in (32). Consider the dynamics $X_s, Y_s$ on $\mathbb{R}^d$ which satisfy the Itô SDEs
\[
dX^i_s = -(Pa)_{ij} \frac{\partial U}{\partial x_j} ds + \frac{1}{\beta} \frac{\partial (Pa)_{ij}}{\partial x_j} ds + \sqrt{2\beta^{-1}} P_{s,i} dW^j_s,
\] (36)
and
\[
dY^i_s = -(Pa)_{ij} \frac{\partial [U - \frac{1}{2\beta} \ln \det(\nabla \xi^T \nabla \xi)]}{\partial x_j} ds + \frac{1}{\beta} \frac{\partial (Pa)_{ij}}{\partial x_j} ds + \sqrt{2\beta^{-1}} P_{s,i} dW^j_s,
\] (37)
for $1 \leq i \leq d$, where $\beta > 0$ and $W_s = (W_s^1, W_s^2, \cdots, W_s^d)^T$ is a $d$-dimensional Brownian motion. Suppose that $X_0, Y_0 \in \Sigma$, then $X_s, Y_s \in \Sigma$ almost surely for $s \geq 0$. Furthermore, the unique invariant probability measures of the dynamics $X_s$ and $Y_s$ are $\mu_1$ and $\mu_2$, respectively.

**Proof.** Applying Lemma 1 we can rewrite the probability measures $\mu_1, \mu_2$ as
\[
d\mu_1 = \frac{1}{Z} e^{-\beta U} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{\beta}{2}} d\nu_g = \frac{1}{Z} \exp \left[ -\beta \left( U + \frac{1}{2\beta} \ln \frac{\det(\nabla \xi^T a \nabla \xi)}{\det a} \right) \right] d\nu_g,
\] (38)
\[
d\mu_2 = \frac{1}{Z} e^{-\beta U} d\nu = \frac{1}{Z} \exp \left[ -\beta \left( U + \frac{1}{2\beta} \ln \frac{1}{\det a} \det(\nabla \xi^T \nabla \xi) \right) \right] d\nu_g,
\]
where again $Z$ denotes different normalization constants. Applying Proposition 2 to the two probability measures expressed in (38), we can conclude that both the dynamics $X_s$ in (36) and $Y_s$ in (37) evolve on the submanifold $\Sigma$, and their invariant probability measures are given by $\mu_1$ and $\mu_2$, respectively.

**Remark 2.** 1. Notice that, similar to (4), the infinitesimal generator of $X_s$ in (36) can be written as
\[
\mathcal{L} = \frac{e^{\beta U}}{\beta} \frac{\partial}{\partial x_i} \left( e^{-\beta U} (Pa)_{ij} \frac{\partial}{\partial x_j} \right).
\] (39)
2. Using Jacobi’s formula \[ \frac{\partial \ln \det (\nabla^T \nabla \xi)}{\partial x_j} = (\nabla^T \nabla \xi)^{-1} \frac{\partial (\nabla^T \nabla \xi)}{\partial x_j} \] and the relation \((Pa)_{ij} \partial_j \xi_\alpha = 0\), the equation (37) can be simplified as

\[
dY^i_s = -(Pa)_i \frac{\partial U}{\partial x_j} \, ds + \frac{1}{\beta} \left( P_{ji} \frac{\partial (Pa)_j}{\partial x_i} \right) \, ds + \sqrt{2\beta^{-1}} P_{ji} \, dW^j_s, \tag{40}
\]

where the matrix \(Q = \text{id} - \nabla \xi (\nabla^T \nabla \xi)^{-1} \nabla^T \xi\). In the special case when \(g = a = \text{id}\), we have \(\nu_g = \nu\) and \(P_{ji} = Q_{ji}\) from (39). Accordingly, we can write the dynamics (37) as

\[
dY^i_s = -P_{ij} \frac{\partial U}{\partial x_j} \, ds + \frac{1}{\beta} P_{ij} \frac{\partial P_{ji}}{\partial x_j} \, ds + \sqrt{2\beta^{-1}} P_{ji} \, dW^j_s, \tag{41}
\]

for \(1 \leq i \leq d\), where \(H = H(e_i)\) is the mean curvature vector of \(\Sigma\) (see Proposition 2 in Appendix A). In Stratonovich form, (40) can be written as

\[
dY^i_s = -P_{ij} \frac{\partial U}{\partial x_j} \, ds + \sqrt{2\beta^{-1}} P_{ji} \, dW^j_s, \quad 1 \leq i \leq d. \tag{42}
\]

In this case, our results are accordant with those in [11].

The dynamics constructed in Proposition 2 and Theorem 4 are reversible on \(\Sigma\), in the sense that their infinitesimal generators are self-adjoint with respect to their invariant measures. In fact, using the same idea, we can construct non-reversible ergodic SDEs on \(\Sigma\) as well. We will only consider the conditional probability measure \(\mu_1\), since it is more relevant in applications and the result is also simpler.

**Corollary 1.** Let \(\mu_1\) be the conditional probability measure on \(\Sigma\) defined in (32). The vector field \(J = (J_1, J_2, \cdots, J_d)^T = J_i e_i\), defined on \(x \in \Sigma\), satisfies

\[
J(x) \in T_x \Sigma, \quad \forall x \in \Sigma, \quad P_{ij} \frac{\partial J_i}{\partial x_j} + J_i \frac{\partial P_{ji}}{\partial x_i} - \beta J_i \frac{\partial U}{\partial x_i} = 0. \tag{43}
\]

Consider the dynamics \(X_s\) on \(\mathbb{R}^d\) which satisfies the Ito SDE

\[
dX^i_s = J_i \, ds - (Pa)_{ij} \frac{\partial U}{\partial x_j} \, ds + \frac{1}{\beta} \left( P_{ji} \frac{\partial (Pa)_j}{\partial x_i} \right) \, ds + \sqrt{2\beta^{-1}} P_{ji} \, dW^j_s, \tag{44}
\]

for \(1 \leq i \leq d\), where \(\beta > 0\) and \(W_s = (W^1_s, W^2_s, \cdots, W^d_s)^T\) is a \(d\)-dimensional Brownian motion. Suppose that \(X_0 \in \Sigma\), then \(X_s \in \Sigma\) almost surely for \(s \geq 0\). Furthermore, the unique invariant probability measure of \(X_s\) is \(\mu_1\).

**Proof.** Notice that the infinitesimal generator of (44) can be written as

\[
\mathcal{L}J = J_i \frac{\partial}{\partial x_i} + \mathcal{L}, \tag{45}
\]
where $\mathcal{L}$ is the infinitesimal generator of (30). Using the fact $J \in T_x \Sigma$, the same argument of Proposition 2 implies that (46) evolves on $\Sigma$ as well. Since $\mu_1$ is invariant with respect to $\mathcal{L}$, to show the SDE (44) has the same invariant measure, it is enough to verify that

$$\text{div}^\Sigma \left\{ J \exp \left[ -\beta \left( U + \frac{1}{2\beta} \ln \frac{\det (\nabla \xi^T a \nabla \xi)}{\det a} \right) \right] \right\} = 0, \quad \forall \ x \in \Sigma, \quad (46)$$

where we have used the expression of $\mu_1$ in (38). Applying the formula of $\text{div}^\Sigma$ in Lemma 2 of Appendix A, we can compute the right hand side of (46), as

$$\text{div}^\Sigma \left\{ J \exp \left[ -\beta \left( U + \frac{1}{2\beta} \ln \frac{\det (\nabla \xi^T a \nabla \xi)}{\det a} \right) \right] \right\} = \left( \nabla_{\xi^T}^M \left\{ \exp \left[ -\beta \left( U + \frac{1}{2\beta} \ln \frac{\det (\nabla \xi^T a \nabla \xi)}{\det a} \right) \right] \right\} J, e_i \right\} J, e_i), \quad (47)$$

which implies that (46) is equivalent to

$$0 = (Pa)_{ir} \frac{\partial J_i}{\partial x_l} (a^{-1})_{lr} + (Pa)_{ir} J_i \Gamma_i^r (a^{-1})_{r'} e_r - \beta (Pa)_{ir} J_i (a^{-1})_{ir} \frac{\partial U}{\partial x_l}$$

$$= P_{i r} \frac{\partial J_i}{\partial x_l} + P_{ir} J_i \Gamma_i^r - \beta P_{ir} J_i \frac{\partial U}{\partial x_l} - \frac{1}{2} P_{ir} J_i \frac{\partial}{\partial x_i} \ln \frac{\det (\nabla \xi^T a \nabla \xi)}{\det a} \right]$$

where $\Gamma_i^r$ are the Christoffel’s symbols satisfying $\nabla_{\xi^T}^M e_i = \Gamma_i^r e_r$. Using the expression (140) of $\Gamma_i^r$, the fact $J_i = P_{ij} J_j$, and Lemma 3 in Appendix A, we can further simplify the above equation and obtain

$$P_{ir} J_i \Gamma_i^r = \frac{1}{2} P_{i r} J_i \frac{\partial}{\partial x_i} \ln \frac{\det (\nabla \xi^T a \nabla \xi)}{\det a} \right]$$

Therefore, we see that (46) is equivalent to the condition (43). \hfill \Box

**Remark 3.** We make two remarks regarding the non-reversible vector $J$.

1. Notice that, as tangent vectors acting on functions, we have $Pe_j = P_{ij} \frac{\partial}{\partial x_i} \in T_x \Sigma$. Therefore, the condition (43) indeed only depends on the value of $J$ on $\Sigma$. Supposing that $J$ and $U$ are defined in a neighborhood $O$ of $\Sigma$ (see Remark 1), the condition (43) can be written equivalently as

$$J(x) \in T_x \Sigma, \quad \forall \ x \in \Sigma,$$

$$\frac{\partial}{\partial x_i} \left[ (P_{ij} J_j) e^{-\beta U} \right] = 0, \quad \forall \ x \in \Sigma. \quad (48)$$

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3.2 Overdamped limit of constrained Langevin processes

The associated phase space of (51) is

\[ \mathbb{R}^k \times \mathbb{R}^d \]

where \( \Lambda > 0 \), and we assume that (51) satisfies (50).

Let \( \Lambda = \text{diag}\{m_1, m_2, \ldots, m_d\} \in \mathbb{R}^{d \times d} \) be a diagonal matrix where the constants \( m_i > 0 \), \( 1 \leq i \leq d \). Consider the constrained Langevin dynamics

\[
\begin{align*}
\frac{dq^i_s}{dt} &= -\Lambda^{-1}p^i_s \, ds \\
\frac{dp^i_s}{dt} &= \Lambda^{-1}p^i_s + \frac{1}{\epsilon} \nabla_q (U + \frac{1}{2\beta} \ln \det G_\Lambda) - \frac{1}{\epsilon^2} a \Lambda^{-1} p^i_s \, ds \\
&\quad - \frac{1}{\epsilon} \nabla_G \xi \Lambda^{-1} \frac{\partial}{\partial x_k} - \frac{1}{\epsilon} \nabla_G \xi \Lambda^{-1} \frac{\partial}{\partial p_k} \, ds \\
&\quad + \frac{\sqrt{2\beta}}{\epsilon^2} P_\Lambda \frac{\partial}{\partial p_k} \sigma \, dW_s,
\end{align*}
\]

(51)

where \( \epsilon > 0 \), \( (q^i_s, p^i_s) \in \mathbb{R}^d \times \mathbb{R}^d \), \( \nabla \xi \) is the gradient of the potentials \( \xi(q, \sigma, \Lambda, p) \) with respect to the components \( q \) and \( p \), respectively. The matrices in (51) are defined as

\[ G_\Lambda = \nabla \xi \Lambda^{-1} \nabla \xi \in \mathbb{R}^{k \times k}, \quad a = \sigma \sigma^T \in \mathbb{R}^{d \times d}, \quad P_\Lambda = \text{id} - \nabla \xi G_\Lambda^{-1} \nabla \xi \Lambda^{-1} \in \mathbb{R}^{d \times d}, \]

(52)

and satisfy \( P_\Lambda^T \Lambda^{-1} = \Lambda^{-1} P_\Lambda \). Hence \( \xi \), matrices \( G_\Lambda, a, \sigma, P_\Lambda \) are all functions on \( \mathbb{R}^d \) and depend on the state \( (q^i_s, p^i_s) \in \mathbb{R}^d \) of the dynamics (51). Notice that, (51) is the rescaled version of the constrained Langevin dynamics in (33), and here we also have modified the potential \( U \) by adding the term \( \frac{\epsilon}{2\beta} \ln \det G_\Lambda \). Recall the submanifold \( \Sigma \) defined in (33) and the probability measure \( \mu_1 \) in (34). The associated phase space of (51) is

\[ T^* \Sigma = \left\{ (q, p) \in \mathbb{R}^d \times \mathbb{R}^d \bigg| q \in \Sigma, (\nabla \xi(q))^T \Lambda^{-1} p = 0 \in \mathbb{R}^k \right\}, \]

(53)

and we assume that \( (q^i_0, p^i_0) \in T^* \Sigma \) at time \( s = 0 \). It has been shown in (33) that the dynamics (51) satisfies \( (q^i_s, p^i_s) \in T^* \Sigma \) for \( s \geq 0 \) and is ergodic. In particular, \( q^i_s \) evolves on the submanifold...
Σ and the invariant measure of dynamics (51) has the marginal distribution \((q^*_{\epsilon})\) that is equal to \(\mu_1\).

For the standard Langevin dynamics on \(\mathbb{R}^d\) (without constraint), the limit \(\epsilon \to 0\) corresponds to the overdamped limit and the convergence is well known [32, 39]. In the following, we study the same limit of the constrained Langevin dynamics (51) when \(\epsilon \to 0\). We will use a formal argument for simplicity and the main purpose is to show its connection with the dynamics (36) obtained in Subsection 3.1. To this end, let us consider the Kolmogorov equation

\[
\frac{\partial \epsilon^s}{\partial s} = \mathcal{L}^s
\]  

on the time interval \([0,T]\) with proper initial condition at time \(s = 0\), where the solution \(u^\epsilon : [0,T] \times T^*\Sigma \to \mathbb{R}\), and \(\mathcal{L} = \frac{1}{\epsilon^2} \mathcal{L}_2 + \frac{1}{\epsilon} \mathcal{L}_1\) is the infinitesimal generator of (51) given by

\[
\mathcal{L}_1 = \Lambda^{-1} p \cdot \nabla_q - \left( \nabla \xi G^{-1}_\Lambda \text{Hess} \xi (\Lambda^{-1} p, \Lambda^{-1} p) \right) \cdot \nabla_p - \Lambda \nabla_q \left( U + \frac{1}{2\beta} \ln \det G_\Lambda \right) \cdot \nabla_p
\]

\[
\mathcal{L}_2 = -(\Lambda a \Lambda^{-1} p) \cdot \nabla_p + \frac{\Lambda a P^T \beta}{\beta} : \nabla^2_p.
\]  

(55)

Assume that the solution \(u^\epsilon\) can be expanded as \(u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \cdots\), where the functions \(u_i, i = 0, 1, 2, \cdots\), are defined on \([0,T] \times T^*\Sigma\) and are independent of \(\epsilon\). Substituting this expansion into the equation (54) and matching the terms of different orders of \(\epsilon\) on both sides of the equation, we obtain the following equations

\[
\mathcal{L}_2 u_0 = 0,
\]

\[
\mathcal{L}_2 u_1 = - \mathcal{L}_1 u_0,
\]

\[
\frac{\partial u_0}{\partial s} = \mathcal{L}_2 u_2 + \mathcal{L}_1 u_1.
\]  

(56)

In the current setting, it is helpful to notice that, for given \(q \in \Sigma\), the generator \(\mathcal{L}_2\) acts on functions which are defined on the \((d - k)\)-dimensional linear subspace

\[
T_\Sigma^* = \left\{ p \in \mathbb{R}^d \mid (\nabla \xi(q))^T \Lambda^{-1} p = 0 \in \mathbb{R}^k \right\}.
\]  

(57)

The computations become more transparent if we consider the linear coordinate transformation

\[
p = V x \in \mathbb{R}^d, \quad x \in \mathbb{R}^{d-k} \text{ and the matrix } V = V(q) \in \mathbb{R}^{d \times (d-k)} \text{ satisfies}
\]

\[
V^T \Lambda^{-1} V = \text{id} \in \mathbb{R}^{(d-k) \times (d-k)}, \quad \nabla \xi^T \Lambda^{-1} V = 0.
\]  

(58)

One can also check that \(P_\Lambda = V V^T \Lambda^{-1}\) and \(P_\Lambda V = V\). With the help of this transformation and taking the first two equations in (56) into account, we can verify the following conclusions.

1. Given \(q \in \Sigma\), the diffusion process corresponding to the infinitesimal generator \(\mathcal{L}_2\) is ergodic on \(T_\Sigma^*\), and the invariant measure is determined by the probability density

\[
\rho_q(p) \propto \exp \left( - \frac{\beta p^T \Lambda^{-1} p}{2} \right), \quad p \in T_\Sigma^*.
\]  

(59)

2. The function \(u_q = u_0(s,q)\) is independent of \(p \in T_\Sigma^*\).
3. The function \( u_1 \) is given by

\[
    u_1(s, q, p) = p^T \Xi \nabla_q u_0 + \overline{u}_1(s, q),
\]

where \( \overline{u}_1 \) is a function independent of \( p \in T_q^* \Sigma \), and we have introduced the matrix \( \Xi = \Lambda^{-1} V (V^T \Lambda^{-1} a \Lambda^{-1} V)^{-1} V^T \Lambda^{-1} \) to simplify the notations.

The derivations are standard and readers are referred to [32, Section 2.2.4], as well as [39, 6] for details. Multiplying by \( \rho_q(p) \) on both sides of the third equation in (56), and integrating with respect to \( p \) over the linear subspace \( T_q^* \Sigma \), we obtain that the leading term \( u_0 \) satisfies the PDE

\[
    \frac{\partial u_0}{\partial s} = - \left[ \Xi \nabla_q \left( U + \frac{1}{2 \beta} \ln \det G_\lambda \right) \right] \cdot \nabla_q u_0 + \frac{1}{\beta} (VV^T \Lambda^{-1})_2 (\partial_{\eta} \Xi, \partial_{\eta} u_0) + \frac{1}{\beta} \Xi : \nabla^2 u_0. \tag{61}
\]

where the relations \( \Xi \nabla \xi = 0 \), \( \Xi P_\lambda = \Xi \) have been used. Using (52), the relations

\[
    \partial_{\eta} (\ln \det G_\lambda) = (G_\lambda^{-1})_{\alpha \eta} \partial_{\eta} (G_\lambda)_{\alpha \eta}, \quad VV^T \Lambda^{-1} = P_\lambda, \quad \Xi_{ij} \partial_{\eta} \xi_\alpha = 0, \quad \text{and integrating by parts, we can further deduce from (61) that}
\]

\[
    \frac{\partial u_0}{\partial s} = - \Xi \nabla_q U \cdot \nabla_q u_0 + \frac{1}{\beta} (\partial_\eta \Xi, ij (G_\lambda^{-1})_{\alpha \eta} \partial_{\eta} (\partial_{\eta} u_0) m_i - \partial_{\eta} \Xi_\eta \partial_{\eta} u_0 + \frac{1}{\beta} G_\lambda_{ij} \partial_{\eta} \Xi_\eta \partial_{\eta} u_0 + \frac{1}{\beta} \Xi : \nabla^2 u_0.
\]

The final equation above implies that when \( \epsilon \to 0 \), the constrained Langevin dynamics (61) converges to the dynamics

\[
    d\delta_{\xi, \eta} = - \Xi \delta_{\eta} \partial_{\eta} U ds + \frac{1}{\beta} \delta_{\eta} \Xi_{ij} ds + \sqrt{2 \beta^{-1} \Xi} dW_\eta^j, \quad 1 \leq i \leq d, \tag{62}
\]

where \( \Xi^{\frac{1}{2}} \) is a matrix satisfying \( \Xi = \Xi^{\frac{1}{2}} (\Xi^{\frac{1}{2}})^T \). Notice that the matrix \( \Xi \) has similar properties as the matrix \( P \alpha \) in Subsection 3.1. Therefore, we can conclude that the dynamics (62) has the same form as the dynamics (59) constructed in Theorem 4.

4 Numerical schemes sampling on \( \Sigma \)

Given a smooth function \( f : \Sigma \to \mathbb{R} \) on the level set \( \Sigma \), in this section we study the numerical scheme (10)–(11) in the Introduction, which allows us to numerically compute the average

\[
    \overline{f} = \int_{\Sigma} f(x) d\mu_1(x) \tag{63}
\]

with respect to the conditional probability measure \( \mu_1 \) in (32).

Since the numerical scheme can be considered as a multiscale method of the dynamics with soft constraint, let us first introduce the softly constrained dynamics, which satisfies the SDE

\[
    dX^\epsilon_s = \left[ - a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\epsilon} a_{ij} \frac{\partial}{\partial x_j} \left( \frac{1}{2} \sum_{\alpha=1}^k \xi_{ij}^\alpha \right) + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} (X^\epsilon_s) ds + \sqrt{2 \beta^{-1} \epsilon \sigma_{ij} (X^\epsilon_s)} dW^j_s, \tag{64}
\]

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where $\epsilon > 0$, $1 \leq i \leq d$. It is straightforward to verify that the dynamics (64) has a unique invariant measure
\[
d\mu^\epsilon(x) = \frac{1}{Z^\epsilon} \exp \left[ -\beta \left( U(x) + \frac{1}{2\epsilon} \sum_{\alpha=1}^{k} \xi_{\alpha}^2(x) \right) \right] dx, \quad \forall x \in \mathbb{R}^d,
\]
where $Z^\epsilon$ is the normalization constant. As $\epsilon \to 0$, the authors in [11] studied the convergence of the dynamics (64) itself on a finite time horizon in the case when $a = \sigma = \text{id}$ and $k = 1$. Closely related problems have also been studied in [13, 24, 17]. Since we are mainly interested in sampling the invariant measure, let us record the following known convergence result of the measure $\mu^\epsilon$ to $\mu_1$.

**Proposition 3.** Let $f : \mathbb{R}^d \to \mathbb{R}$ be a bounded smooth function. $\mu_\epsilon$ is the probability measure in (65) and $\mu_1$ is the conditional probability measures on $\Sigma$ defined in (62). We have
\[
\lim_{\epsilon \to 0} \int_{\mathbb{R}^d} f(x) d\mu^\epsilon(x) = \frac{1}{Z} \int_{\mathbb{R}^d} f(x) e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu (x) = \int_{\Sigma} f(x) d\mu_1(x),
\]
where $Z$ is the normalization constant given by
\[
Z = \int_{\Sigma} e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu (x).
\]

**Proof.** For any bounded smooth function $f$, using (65) and applying co-area formula, we can compute
\[
\int_{\mathbb{R}^d} f(x) d\mu^\epsilon(x) = \frac{1}{Z^\epsilon} \int_{\mathbb{R}^d} f(x) \exp \left[ -\beta \left( U(x) + \frac{1}{2\epsilon} \sum_{\alpha=1}^{k} \xi_{\alpha}^2(x) \right) \right] dx
\]
\[
= \frac{1}{Z^\epsilon} \int_{\mathbb{R}^d} \int_{\{x : \xi(x) = y\}} f(x) \exp \left[ -\beta \left( U(x) + \frac{1}{2\epsilon} \sum_{\alpha=1}^{k} \xi_{\alpha}^2(x) \right) \right] \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu dy
\]
\[
= \frac{1}{Z^\epsilon} \left( \frac{\beta}{2\pi\epsilon} \right)^{\frac{1}{2}} \left( \frac{\beta}{2\pi\epsilon} \right)^{\frac{1}{2}} \int_{\mathbb{R}^k} \exp \left[ -\beta \frac{1}{2\epsilon} \sum_{i=1}^{k} y_i^2 \right] \left\{ \int_{\{x : \xi(x) = y\}} f(x) e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu \right\} dy.
\]
Taking $f \equiv 1$, we obtain
\[
Z^\epsilon \left( \frac{\beta}{2\pi\epsilon} \right)^{\frac{1}{2}} = \left( \frac{\beta}{2\pi\epsilon} \right)^{\frac{1}{2}} \int_{\mathbb{R}^k} \exp \left[ -\beta \frac{1}{2\epsilon} \sum_{i=1}^{k} y_i^2 \right] \left\{ \int_{\{x : \xi(x) = y\}} e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu \right\} dy
\]
\[
\xrightarrow{\epsilon \to 0} \int_{\Sigma} e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu = Z > 0.
\]
Similarly, for a general bounded smooth function $f$,
\[
\left( \frac{\beta}{2\pi\epsilon} \right)^{\frac{1}{2}} \int_{\mathbb{R}^k} \exp \left[ -\beta \frac{1}{2\epsilon} \sum_{i=1}^{k} y_i^2 \right] \left\{ \int_{\{x : \xi(x) = y\}} f(x) e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu \right\} dy
\]
\[
\xrightarrow{\epsilon \to 0} \int_{\Sigma} f(x) e^{-\beta U(x)} \left[ \det(\nabla \xi^T \nabla \xi) \right]^{-\frac{1}{2}} d\nu.
\]
Therefore, from (67) we conclude that
\[
\int_{\mathbb{R}^d} f(x) \, d\mu(x) \xrightarrow{\epsilon \to 0} \frac{1}{Z} \int_{\Sigma} f(x) e^{-\beta U(x)} \det(\nabla \xi^T \nabla \xi)(x) \frac{1}{2} \, d\nu(x) = \int_{\Sigma} f(x) \, d\mu_1(x).
\]

Proposition 3 suggests that the softly constrained dynamics (64) with a small \(\epsilon\) is a good candidate to sample the probability measure \(\mu_1\) on \(\Sigma\). However, direct simulation of (64) is probably inefficient when \(\epsilon\) is small, because the time step-size in numerical simulations becomes limited due to the strong stiffness in the dynamics. The numerical scheme we will study below can be viewed as a multiscale numerical method for the dynamics (64). To explain the method, let us introduce the flow map \(\varphi: \mathbb{R}^d \times [0, +\infty) \to \mathbb{R}^d\), defined by

\[
d\varphi(x,s) = - (a \nabla F)(\varphi(x,s)) , \quad \varphi(x,0) = x, \quad \forall x \in \mathbb{R}^d,
\]

where the function \(F\) is
\[
F(x) = \frac{1}{2} |\xi(x)|^2 = \frac{1}{2} \sum_{\alpha=1}^{k} \xi^2_\alpha(x).
\]

Under proper conditions \([24, 15]\), one can define the limiting map of \(\varphi\) as
\[
\Theta(x) = \lim_{s \to +\infty} \varphi(x,s), \quad \forall x \in \mathbb{R}^d.
\]

Since \(\nabla F|_{\Sigma} = 0\) and \(\Sigma\) is the set consisting of all global minima of \(F\), it is clear that \(\Theta: \mathbb{R}^d \to \Sigma\) and \(\Theta(x) = x\), for \(\forall x \in \Sigma\).

With the mapping \(\Theta\), we propose to approximate the average \(\bar{f}\) in (63) by
\[
\hat{f}_n = \frac{1}{n} \sum_{l=0}^{n-1} f(x^{(l)}) ,
\]

where \(n\) is a large number and the states \(x^{(l)}\) are sampled from the numerical scheme
\[
x^{(l+\frac{1}{2})}_i = x^{(l)}_i + \left( -a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right) h + \sqrt{2\beta^{-1} h} \sigma_j \eta^{(l)}_j, \quad 1 \leq i \leq d, \quad x^{(l+1)} = \Theta(x^{(l+\frac{1}{2})}) ,
\]

starting from \(x^{(0)} \in \Sigma\). In (72), \(h > 0\) is the time step-size, functions \(a, \sigma, U\) are evaluated at \(x^{(l)}\), and \(\eta^{(l)} = (\eta^{(l)}_1, \eta^{(l)}_2, \ldots, \eta^{(l)}_d)^T\) are independent \(d\)-dimensional standard Gaussian random variables, for \(0 \leq l < n - 1\).

**Remark 4.** Several comments on the scheme (71)–(72) are in order.

1. Since the image of \(\Theta\) is on \(\Sigma\), the discrete dynamics \(x^{(l)}\) stays on \(\Sigma\) all the time. As in the case of the softly constrained dynamics (64), the numerical scheme has the advantage that only the 1st order derivatives of \(\xi\) are needed.

2. At each step \(l \geq 0\), one needs to compute \(\Theta(x^{(l+\frac{1}{2})})\). This can be done by solving the ODE (72) starting from \(x^{(l+\frac{1}{2})}\). Exploiting the gradient structure of the ODE (72), we can in fact establish exponential convergence of the dynamics \(\varphi\) to its limit \(\Theta\), at least in the
neighborhood $O$ of $\Sigma$. For instance, we refer to \cite{24} and \cite{3, Chapter 4}. Here, for brevity, we point out that the exponential decay of $F(\phi(x, s))$ can be easily obtained and is therefore a good candidate for the convergence criterion in numerical implementations. Actually, under Assumption 1–2, we can suppose

$$z^T \Psi(x) z \geq c_0 |z|^2, \quad \forall z \in \mathbb{R}^k, \quad \forall x \in O,$$

for some $c_0 > 0$. Direct calculation gives

$$\frac{dF(\phi(x, s))}{ds} = -\left(\xi_\alpha \Psi_\alpha \eta \xi_\eta\right) (\phi(x, s)) \leq -c_0 |\xi(\phi(x, s))|^2 = -2c_0 F(\phi(x, s)), \quad (73)$$

which implies that $|\xi(\phi(x, s))|^2 = 2F(\phi(x, s)) \leq e^{-2c_0 s}|\xi(x)|^2$. In practice, suppose that we choose the condition $|\xi(\phi(x, s))| \leq \epsilon_{\text{tol}}$ as the stop criterion of ODE solvers and set $\Theta(x) = \phi(x, s)$ when the condition is met at time $s$. Then the above analysis indicates that we need to integrate the ODE \((68)\) until the time $s = \max\{\frac{1}{c_0} (\ln |\xi(x(l + \frac{1}{2}))| + \ln \epsilon_{\text{tol}}), 0\}$, which grows logarithmically as $\epsilon_{\text{tol}} \to 0$. Since $x(l + \frac{1}{2})$ is likely to remain close to $\Sigma$ when $h$ is small, we can expect that $\Theta(x(l + \frac{1}{2}))$ can be computed with high precision within only a few iteration steps. We refer to the third example in Section \ref{section} for concrete numerical experiments.

3. Lastly, notice that, when $a = \text{id}$, the numerical scheme \((72)\) becomes

$$x(l + \frac{1}{2}) = x(l) - \nabla U(x(l)) h + \sqrt{2\beta^{-1}h} \eta^{(l)},$$

$$x(l + 1) = \Theta(x(l + \frac{1}{2})). \quad (74)$$

Our main result of this section concerns the approximation quality of the mean value $\overline{f}$ by the running average $\hat{f}_n$ in \((71)\), in the case when $h$ is small and $n$ is large. For this purpose, it is necessary to study the properties of the limiting flow map $\Theta$, since it is involved in the numerical scheme \((72)\). In fact, we have the following important result, which characterizes the derivatives of $\Theta$ by the projection map $P$ in \((21)\).

**Proposition 4.** Let $\Theta$ be the limiting flow map in \((70)\) and $P$ be the projection map in \((21)\). At each $x \in \Sigma$, we have

$$\frac{\partial \Theta_i}{\partial x_j} = P_{ij},$$

$$a_{ir} \frac{\partial^2 \Theta_i}{\partial x_l \partial x_r} = \frac{\partial (P a)_{il}}{\partial x_l} - P_{il} \frac{\partial a_{ir}}{\partial x_r}, \quad (75)$$

for $1 \leq i, j \leq d$.

The proof of Proposition \ref{prop4} can be found in Appendix \ref{appendix}.

Based on the above result, we are ready to quantify the approximation error between the estimator $\hat{f}_n$ and the mean value $\overline{f}$. We will follow the approach developed in \cite{38}, where the Poisson equation (see \((80)\) below) played a crucial role in the analysis. However, let us emphasize that, in contrast to \cite{38}, in the current setting we are working on the submanifold $\Sigma$ and, furthermore, the mapping $\Theta$ is involved in our numerical scheme.

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Theorem 2. Assume that \( f : \Sigma \to \mathbb{R} \) is a smooth function on \( \Sigma \) and \( \mathcal{F} \) is its mean value defined in (63) with respect to the measure \( \mu_1 \). Consider the running average \( \hat{f}_n \) in (71), which is computed by simulating the numerical scheme (72) with time step-size \( h > 0 \). Let \( T = nh \) and \( C \) denote a generic positive constant that is independent of \( h, T \). We have the following approximation results.

1. \( |E\hat{f}_n - \mathcal{F}| \leq C(h + \frac{1}{h}) \).
2. \( E|\hat{f}_n - \mathcal{F}|^2 \leq C(h^2 + \frac{1}{h}) \).
3. For any \( 0 < \epsilon < \frac{1}{2} \), there is an almost surely bounded positive random variable \( \zeta(\omega) \), such that \( |\hat{f}_n - \mathcal{F}| \leq C h + \frac{\zeta(\omega)}{T^{1/2-\epsilon}} \), almost surely.

Proof. Since we follow the approach in [38], we will only sketch the proof and will mainly focus on the differences.

First of all, we introduce some notations. Let \( x^{(l)} \), \( l = 0, 1, \ldots \), be the states generated from the numerical scheme (72) and let \( \psi \) be a function on \( \Sigma \). We will adopt the abbreviations \( \psi^{(l)} = \psi(x^{(l)}) \), \( P^{(l)} = P(x^{(l)}) \), etc. For \( j \geq 1 \), \( D^j\psi[u_1, u_2, \ldots, u_j] \) denotes the \( j \)th order directional derivatives of \( \psi \) along the vectors \( u_1, u_2, \ldots, u_j \), and \( |D^j\psi|_{\infty} \) is the supremum norm of \( D^j\psi \) on \( \Sigma \). Similarly, \( D^j\Theta[u_1, u_2, \ldots, u_j] \) denotes the \( d \)-dimensional vector whose \( \theta \) component is \( D^j\Theta[u_1, u_2, \ldots, u_j] \), for \( 1 \leq i \leq d \).

Define the vector \( b^{(l)} = (b_1^{(l)}, b_2^{(l)}, \ldots, b_d^{(l)})^T \) by

\[
b_i^{(l)} = \left( -a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ji}}{\partial x_j} \right)(x^{(l)}), \quad 1 \leq i \leq d, \tag{76}
\]

for \( l = 0, 1, \ldots \), and set

\[
\delta^{(l)} = b^{(l)} h + \sqrt{2\beta^{-1} h} \sigma^{(l)} \eta^{(l)}. \tag{77}
\]

We have

\[
\delta^{(l)} = x^{(l+\frac{1}{2})} - x^{(l)}, \quad \text{and} \quad x^{(l+1)} = \Theta(x^{(l+\frac{1}{2})}) = \Theta(x^{(l)} + \delta^{(l)}). \tag{78}
\]

Let \( \mathcal{L} \) be the infinitesimal generator of the SDE (80), given by

\[
\mathcal{L} = -(Pa)_{ij} \frac{\partial U}{\partial x_j} \frac{\partial}{\partial x_i} + \frac{1}{\beta} \frac{\partial (Pa)_{ij}}{\partial x_j} \frac{\partial}{\partial x_i} + \frac{1}{\beta} (Pa)_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \tag{79}
\]

in Remark 2. We consider the Poisson equation on \( \Sigma \)

\[
\mathcal{L} \psi = f - \mathcal{F}. \tag{80}
\]

The existence and the regularity of the solution \( \psi \) can be established under Assumption 1 and the Bakry-Emery condition in Section 3. Applying Taylor’s theorem and using the fact that \( \Theta(x^{(l)}) = x^{(l)} \) since \( x^{(l)} \in \Sigma \), we have

\[
\psi^{(l+1)} = (\psi \circ \Theta)(x^{(l)} + \delta^{(l)}) \tag{81}
\]

\[
= \psi^{(l)} + D(\psi \circ \Theta)^{(l)}[\delta^{(l)}] + \frac{1}{2} D^2(\psi \circ \Theta)^{(l)}[\delta^{(l)}, \delta^{(l)}] + \frac{1}{6} D^3(\psi \circ \Theta)^{(l)}[\delta^{(l)}, \delta^{(l)}, \delta^{(l)}] + R^{(l)},
\]

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where the reminder is given by

\[ R^{(l)} = \frac{1}{6} \left( \int_0^1 s^2 D^4(\psi \circ \Theta)(x^{(l)} + (1 - s)\delta^{(l)}) ds \right) [\delta^{(l)}, \delta^{(l)}, \delta^{(l)}, \delta^{(l)}]. \] (82)

Now we apply Proposition 4 to simplify the expression in (81). Using the chain rule, the expressions (77)–(79), we can derive

\[
\psi^{(l+1)} = \psi^{(l)} + D\psi^{(l)} \left[ P^{(l)} \delta^{(l)} + \frac{1}{2} D^2 \Theta^{(l)}[\delta^{(l)}, \delta^{(l)}] \right] + \frac{1}{2} D^2 \psi^{(l)} \left[ P^{(l)} \delta^{(l)}, P^{(l)} \delta^{(l)} \right] \\
+ \frac{1}{6} D^3 (\psi \circ \Theta)^{(l)} [\delta^{(l)}, \delta^{(l)}, \delta^{(l)}] + R^{(l)}
\]

\[
= \psi^{(l)} + (L\psi^{(l)}) h + \sqrt{2\beta^{-1}} h D\psi^{(l)} [(P\sigma)^{(l)} \eta^{(l)}] + \frac{h^2}{2} D\psi^{(l)} \left[ D^2 \Theta^{(l)}[b^{(l)}, b^{(l)}] \right] \\
+ \frac{\sqrt{2\beta^{-1}} h^2}{2} D^2 \psi^{(l)} [(P\sigma)^{(l)} \eta^{(l)}, (P\sigma)^{(l)} \eta^{(l)}] + \frac{h D\psi^{(l)}}{\beta} \left[ D^2 \Theta^{(l)}[\sigma^{(l)} \eta^{(l)}, \sigma^{(l)} \eta^{(l)}] - a^{(l)} : \nabla^2 \Theta^{(l)} \right] \\
+ \frac{h}{\beta} D^2 \psi^{(l)} [(P\sigma)^{(l)} \eta^{(l)}, (P\sigma)^{(l)} \eta^{(l)}] - (P\sigma)^{(l)} \psi^{(l)} + \frac{1}{6} D^3 (\psi \circ \Theta)^{(l)} [\delta^{(l)}, \delta^{(l)}, \delta^{(l)}] + R^{(l)},
\]

where in the last equation we added and subtracted some terms, and we used the identity

\[ D\psi^{(l)} \left[ P^{(l)} b^{(l)} + \frac{1}{\beta} a^{(l)} : \nabla^2 \Theta^{(l)} \right] + \frac{1}{\beta} (P\sigma)^{(l)} : \nabla^2 \psi^{(l)} = (L\psi^{(l)}), \] (84)

which can be verified using Proposition 4 and (70). In (84), \( a : \nabla^2 \Theta \) is the vector whose \( i \)th component is given by \( a_{ji} \partial^2 \Theta/\partial x_j \partial x_i \), and \( (P\sigma)^{\circ} \) : \( \nabla^2 \psi \) is defined in a similar way.

Summing up (83) for \( l = 0, 1, \ldots, n - 1 \), dividing on both sides by \( T \), and using the Poisson equation (80), gives

\[
\hat{f}_n - \hat{T} = \frac{1}{T} \sum_{l=0}^{n-1} f(x^{(l)}) - \hat{T} = \frac{\psi^{(n)} - \psi^{(0)}}{T} + \frac{1}{T} \sum_{i=1}^{5} M_{i,n} + \frac{1}{T} \sum_{i=1}^{4} S_{i,n},
\]

where

\[
M_{1,n} = -\sqrt{2\beta^{-1}} h \sum_{l=0}^{n-1} D\psi^{(l)} [(P\sigma)^{(l)} \eta^{(l)}],
\]

\[
M_{2,n} = -\sqrt{2\beta^{-1}} h^2 \sum_{l=0}^{n-1} D\psi^{(l)} \left[ D^2 \Theta^{(l)}[b^{(l)}, \sigma^{(l)} \eta^{(l)}] \right],
\]

\[
M_{3,n} = -\frac{h}{\beta} \sum_{l=0}^{n-1} D\psi^{(l)} \left[ D^2 \Theta^{(l)}[\sigma^{(l)} \eta^{(l)}, \sigma^{(l)} \eta^{(l)}] - a^{(l)} : \nabla^2 \Theta^{(l)} \right],
\]

\[
M_{4,n} = -\sqrt{2\beta^{-1}} h^2 \sum_{l=0}^{n-1} D^2 \psi^{(l)} \left[ P^{(l)} b^{(l)}, (P\sigma)^{(l)} \eta^{(l)} \right],
\]

\[
M_{5,n} = -\frac{h}{\beta} \sum_{l=0}^{n-1} \left( D^2 \psi^{(l)} \left[ (P\sigma)^{(l)} \eta^{(l)}, (P\sigma)^{(l)} \eta^{(l)} \right] - (P\sigma)^{(l)} : D^2 \psi^{(l)} \right),
\]

\[ 22 \]
Notice that the terms estimates Therefore, since the level set Σ is compact (Assumption 2), the first conclusion follows from the estimates (90) for \( |S_{\infty} M| \) while the second conclusion follows by squaring both sides of (85) and using the estimates

\[
S_{n, n} = -\frac{h^2}{2} \sum_{i=0}^{n-1} D\psi^{(i)} [D^2 \Theta^{(i)}] \left[ b^{(i)}, b^{(i)} \right],
S_{2, n} = -\frac{h^2}{2} \sum_{i=0}^{n-1} 2 D\psi^{(i)} \left[ P^{(i)} b^{(i)}, P^{(i)} b^{(i)} \right],
S_{3, n} = -\frac{1}{6} \sum_{i=0}^{n-1} R^{(i)}, \quad S_{4, n} = -\frac{1}{3} \sum_{i=0}^{n-1} D^3 (\psi \circ \Theta)^{(i)} \left[ \delta^{(i)}, \delta^{(i)}, \delta^{(i)} \right].
\] (87)

Using (77), the last term \( S_{4, n} \) above can be further decomposed as

\[
S_{4, n} = M_{0, n} + S_{0, n},
\] (88)

where

\[
M_{0, n} = -\frac{\sqrt{2} \beta - 1}{6} h^2 \sum_{i=0}^{n-1} \left( \frac{2}{\beta} D^2 (\psi \circ \Theta)^{(i)} \left[ \sigma^{(i)} \eta^{(i)}, \sigma^{(i)} \eta^{(i)}, \sigma^{(i)} \eta^{(i)} \right] + 3 h D^3 (\psi \circ \Theta)^{(i)} \left[ b^{(i)}, b^{(i)}, b^{(i)} \right] \right),
S_{0, n} = -\frac{h^2}{6} \sum_{i=0}^{n-1} \left( \frac{6}{\beta} D^2 (\psi \circ \Theta)^{(i)} \left[ b^{(i)}, \sigma^{(i)} \eta^{(i)}, \sigma^{(i)} \eta^{(i)} \right] + h D^3 (\psi \circ \Theta)^{(i)} \left[ b^{(i)}, b^{(i)}, b^{(i)} \right] \right).
\] (89)

Notice that the terms \( M_{i, n}, 0 \leq i \leq 5 \), are all martingales and in particular we have \( E M_{i, n} = 0 \). Therefore, since the level set \( \Sigma \) is compact (Assumption 2), the first conclusion follows from the estimates

\[
|S_{1, n}| \leq C |D\psi|_\infty h T, \quad |S_{2, n}| \leq C |D^2 \psi|_\infty h T, \quad E|S_{0, n}| \leq C |D^2 \psi|_\infty h T, \quad E|S_{3, n}| \leq C |D^2 \psi|_\infty h T,
\] (90)

while the second conclusion follows by squaring both sides of (85) and using the estimates

\[
E|S_{0, n}|^2 \leq C h^2 T^2 |D^2 \psi|_\infty^2, \quad E|S_{3, n}|^2 \leq C h^2 T^2 |D^2 \psi|_\infty^2,
E|M_{0, n}|^2 \leq C h^2 T |D^2 \psi|_\infty^2, \quad E|M_{1, n}|^2 \leq C T |D^2 \psi|_\infty^2, \quad E|M_{2, n}|^2 \leq C h^2 T |D^2 \psi|_\infty^2,
E|M_{3, n}|^2 \leq C h T |D^2 \psi|_\infty^2, \quad E|M_{4, n}|^2 \leq C h^2 T |D^2 \psi|_\infty^2, \quad E|M_{5, n}|^2 \leq C h T |D^2 \psi|_\infty^2.
\]

As far as the third conclusion (pathwise estimate) is concerned, notice that (85) implies

\[
|\hat{f}_n - \bar{f}| \leq \frac{\psi(n) - \psi(0)}{T} + \frac{1}{T} \sum_{i=0}^{n-1} |M_{i, n}| + \frac{1}{T} \sum_{i=0}^{n-3} |S_{i, n}|
\leq C \left( h + \frac{1}{T} \right) + \frac{5}{T} \sum_{i=0}^{n-1} |M_{i, n}|,
\] (91)

where we have used the estimates (80) for \( |S_{1, n}|, |S_{2, n}| \), and the upper bounds

\[
|S_{0, n}| \leq C h^2 \sum_{i=0}^{n-1} |\eta^{(i)}|^2 + C h^3 n \leq C h T, \quad a.s.
|S_{3, n}| \leq C h^2 \sum_{i=0}^{n-1} |\eta^{(i)}|^4 + C h^4 n \leq C h T, \quad a.s.
\] (92)

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which are implied by the strong law of large numbers for \( \frac{1}{n} \sum_{i=0}^{n-1} |\eta^{(i)}|^4 \), when \( n \to +\infty \). Finally, we estimate the martingale terms \( M_{i,n} \) in (91). Notice that, for any \( r \geq 1 \), we can deduce the following upper bounds (see [38])

\[
\frac{1}{T^{2r}} \mathbb{E} |M_{1,n}|^{2r} \leq \frac{C}{T^r}, \quad \frac{1}{T^{2r}} \mathbb{E} |M_{2,n}|^{2r} \leq \frac{Ch^{2r}}{T^r}, \\
\frac{1}{T^{2r}} \mathbb{E} |M_{3,n}|^{2r} \leq \frac{Ch^r}{T^r}, \quad \frac{1}{T^{2r}} \mathbb{E} |M_{4,n}|^{2r} \leq \frac{Ch^{2r}}{T^r}, \\
\frac{1}{T^{2r}} \mathbb{E} |M_{5,n}|^{2r} \leq \frac{Ch^r}{T^r}, \quad \frac{1}{T^{2r}} \mathbb{E} |M_{6,n}|^{2r} \leq \frac{Ch^{2r}}{T^r},
\]

(93)

which give

\[
\mathbb{E} \left( \frac{1}{T} \sum_{i=0}^{5} |M_{i,n}| \right)^{2r} \leq \frac{C}{T^{2r}} \sum_{i=0}^{5} \mathbb{E} |M_{i,n}|^{2r} \leq \frac{C}{T^r}.
\]

(94)

Now, for any \( 0 < \epsilon < \frac{1}{T} \), the Borel-Cantelli lemma implies that there is an almost surely bounded random variable \( \zeta(\omega) \), such that

\[
\frac{1}{T} \sum_{i=0}^{5} |M_{i,n}| \leq \zeta(\omega) \frac{T^r}{T^r - \epsilon}.
\]

(95)

Therefore, the third conclusion follows readily from (91) and (95).

Remark 5. The idea of using the mapping \( \Theta \) in the constraint step of the numerical scheme (72) is motivated by the softly constrained (reversible) dynamics (64). It is natural to consider whether certain “non-reversible” numerical scheme can be obtained using the same idea. In fact, let \( A \in \mathbb{R}^{d \times d} \) be a constant skew-symmetric matrix such that \( A^T = -A \). The softly constrained (non-reversible) dynamics

\[
dX^x,A,i_s = \left[ A_{ij} \frac{\partial}{\partial x_j} (U + \frac{1}{2\epsilon} \sum_{\alpha=1}^{k} \xi_{\alpha}^2) - a_{ij} \frac{\partial U}{\partial x_j} - \frac{1}{\epsilon} a_{ij} \frac{\partial}{\partial x_j} \left( \frac{1}{\beta} \sum_{\alpha=1}^{k} \xi_{\alpha} \right) + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right] (X^x,A) ds \\
+ \sqrt{2\beta^{-1}} \sigma_{ij} (X_{s_{ij}}^x,A) dW^j_s,
\]

(96)

indeed has the same invariant measure \( \mu^r \) in (65). Based on this fact, a reasonable guess of the “non-reversible” numerical scheme that samples the conditional measure \( \mu^1 \) is the multiscale method of (77), i.e.,

\[
x_{(l+1)} = x_{(l)} + \left( A_{ij} \frac{\partial U}{\partial x_j} - a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right) (x^{(l)}) h + \sqrt{2\beta^{-1}} h \sigma_{ij} (x^{(l)}) \eta^{(l)}_j, \quad 1 \leq i \leq d,
\]

\[
x_{(l+1)} = \Theta^A (x_{(l+1)}),
\]

(97)

where \( \Theta^A(x) = \lim_{s \to +\infty} \varphi^A(x,s) \) is the limit of the (non-gradient) flow map

\[
\frac{d \varphi^A(x,s)}{ds} = -(a - A) \nabla F(\varphi^A(x,s)), \quad \varphi^A(x,0) = x, \quad \forall \ x \in \mathbb{R}^d,
\]

(98)

with the same function \( F \) in (67). We expect that the long time sampling error estimates of the numerical scheme (97) can be studied following the same approach of this section as well. For
this purpose, however, it is necessary to handle the non-gradient term in the ODE (98), which brings difficulties when calculating the derivatives of the map $\Theta^A$ (cf. Proposition 4 as well as its proof in Appendix B). We will postpone the analysis in the future work and readers are referred to the third example in Section 5 for numerical validation of the scheme (97–(98).

Before concluding, let us point out that Theorem 1 in Section 3 and the approach used in the above proof allow us to study other numerical schemes on $\Sigma$ as well. As an example, we consider the projection from $\mathbb{R}^d$ to $\Sigma$ along the geodesic curves defined by the metric $g$ in (16).

Let $d$ be the distance function on $\mathbb{R}^d$ induced by the metric $g$ in (16), i.e., the distance on the Riemannian manifold $M = (\mathbb{R}^d, g)$ in Section 2. We introduce the projection function

$$\Pi(x) = \left\{ y \mid d(x, y) = d(x, \Sigma), y \in \Sigma \right\}, \quad \forall x \in M = \mathbb{R}^d. \quad (99)$$

Clearly, we have $\Pi|_\Sigma = \text{id}|_\Sigma$. Given any $x \in \Sigma$, there is a neighborhood $\Omega \subset \mathbb{R}^d$ of $x$ such that $\Pi|_\Omega$ is a single-valued map. Furthermore, applying inverse function theorem, we can verify that $\Pi$ is smooth on $\Omega$. We have the following result which connects the derivatives of $\Pi$ to the projection map $P$ in (21). Its proof is given in Appendix C.

**Proposition 5.** Let $\Pi = (\Pi_1, \Pi_2, \cdots, \Pi_d)^T : \mathbb{R}^d \to \Sigma$ be the projection function in (99), where $\Pi_i : \mathbb{R}^d \to \mathbb{R}$ are smooth functions, $1 \leq i \leq d$. For $x \in \Sigma \cap \Omega$, we have

$$\frac{\partial \Pi_i}{\partial x_j} = P_{ij}, \quad a_{ij} \frac{\partial^2 \Pi_i}{\partial x_i \partial x_j} = -P_{ij} \frac{\partial a_{ij}}{\partial x_j} + \frac{\partial (Pa)_i}{\partial x_j} + \frac{1}{2} (Pa)_i \frac{\partial \ln \det \Theta}{\partial x_j}, \quad (100)$$

for $1 \leq i, j \leq d$.

Now we are ready to study the numerical scheme

$$x^{(l+\frac{1}{2})}_i = x^{(l)}_i + \left( -a_{ij} \frac{\partial U}{\partial x_j} + \frac{1}{\beta} \frac{\partial a_{ij}}{\partial x_j} \right)(x^{(l)})_j h + \sqrt{2\beta^{-1}h} \sigma_{ij}(x^{(l)})_j \eta^{(l)}_j, \quad 1 \leq i \leq d, \quad (101)$$

where $x^{(0)} \in \Sigma$, and the map $\Pi$ is used in each step to project the states $x^{(l+\frac{1}{2})}$ back to $\Sigma$.

**Theorem 3.** Assume that $f : \Sigma \to \mathbb{R}$ is a smooth function on $\Sigma$ and $\overline{f}$ is its mean value

$$\overline{f} = \int_\Sigma f(x) \, d\mu(x), \quad (102)$$

with respect to the probability measure

$$d\mu = \frac{1}{Z} e^{-\beta U} \sqrt{\frac{\det(\nabla \xi^T \nabla \xi)}{\det(\nabla \xi^T \nabla \xi)}} \, d\nu. \quad (103)$$

Consider the running average $\hat{f}_n$ in (71), which is computed by simulating the numerical scheme (101) with time step-size $h > 0$. Let $T = nh$ and $C$ denote a generic positive constant that is independent of $h, T$. We have the following approximation results.

1. $|E\hat{f}_n - \overline{f}| \leq C(h + \frac{1}{T}).$
2. \( E|\hat{f}_n - \bar{f}|^2 \leq C(h^2 + \frac{1}{h}) \).

3. For any \( 0 < \epsilon < \frac{1}{2} \), there is an almost surely bounded positive random variable \( \zeta(\omega) \), such that \( |\hat{f}_n - \bar{f}| \leq Ch + \frac{\zeta(\omega)}{h^2} \), almost surely.

We omit the proof since it resembles the proof of Theorem 2.

Remark 6. For the projection map \( \Pi \) induced by a general metric \( g = a^{-1} \) or, equivalently, by a general (positive definite) matrix \( a \), implementing the numerical scheme (101) is not as easy as the numerical scheme (72). We decide to omit the algorithmic discussions, due to the fact that the probability measure (103) seems less relevant in applications. However, it is meaningful to point out that, when \( a = \text{id} \), our result is relevant to the one in [11]. In this case, the probability measure in (103) reduces to \( \mu_2 = \frac{1}{2}e^{-\beta U}dv \) in (32) and the numerical scheme (101) can be formulated equivalently using Lagrange multiplier. We refer to [11, 33] for comprehensive numerical details.

5 Some concrete examples

In this section, we study three concrete examples. We start by applying the results in Section 3 to the simple linear reaction coordinate case. After that, in the second example, we show that in some cases it is indeed helpful to consider non-identity matrices \( \sigma \) and \( a \). Finally, in the third example, we numerically investigate the schemes in Section 4. In particular, the sampling performance of the constrained schemes using different maps \( \Theta, \Theta^A, \) and \( \Pi \), as well as the performance of the unconstrained Euler-Maruyama discretization of the SDE (36), will be compared.

Example 1: from \( \mathbb{R}^d \) to \( \mathbb{R}^{d-k} \)

In this example, we consider the linear reaction coordinate function

\[ \xi(x) = \xi(x_1, x_2, \cdots, x_d) = (x_1, x_2, \cdots, x_k)^T, \quad 1 \leq k < d. \]

Accordingly, the level set is given by

\[ \Sigma = \left\{ (x_1, x_2, \cdots, x_d) \in \mathbb{R}^d \mid x_i = 0, \quad 1 \leq i \leq k \right\} = \mathbb{R}^{d-k}. \] (104)

Recalling the expressions in Section 2 we have \( \Psi_{\alpha\gamma} = a_{\alpha\gamma}, \quad 1 \leq \alpha, \gamma \leq k \). It is convenient to write \( a \) as a block matrix

\[ a = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \] (105)

where \( A_{12} = A_{21}^T \), and \( A_{11}, A_{22} \) are square (symmetric) matrices of order \( k \) and \( d-k \), respectively. From [24] we can verify that

\[ Pa = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} - \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}^T = \begin{pmatrix} 0 & 0 \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix}. \]
In this case the two probability measures $\mu_1, \mu_2$ defined in (32) are the same, since we have $\det(\nabla \xi^T \nabla \xi) \equiv 1$. Defining the matrix $\tilde{a} = A_{22} - A_{21} A_{11}^{-1} A_{12} = \tilde{\sigma} \tilde{T} \in \mathbb{R}^{(d-k) \times (d-k)}$ and applying Theorem 1, we conclude that the dynamics

$$
dX^i_s = 0, \quad 1 \leq i \leq k,
$$

$$
dX^{i+k}_s = -\sum_{j=1}^{d-k} \tilde{a}_{ij} \frac{\partial U}{\partial x_{j+k}} ds + \frac{1}{\beta} \sum_{j=1}^{d-k} \tilde{a}_{ij} \frac{\partial U}{\partial x_{j+k}} ds + \sqrt{2(\gamma - 1)} \sum_{j=1}^{d-k} \tilde{\sigma}_{ij} dW^j_s, \quad 1 \leq i \leq d - k,
$$

(106)
evolves on $\Sigma$ and has the invariant measure whose probability density is $\frac{1}{Z} e^{-\beta U}$ with respect to the Lebesgue measure on $\Sigma$.

Notice that, although Assumption 2 is not satisfied due to the non-compactness of the level set $\Sigma$, the computations are still valid. In fact, we expect most of the conclusions in the previous sections can be generalized under proper assumptions on the potential $U$ and the matrix $a$.

**Example 2 : from $\mathbb{R}^d$ to $(d-1)$-dimensional sphere**

In this example, we choose the reaction coordinate function

$$
\xi(x) = \xi(x_1, x_2, \cdots, x_d) = \frac{1}{2} \left(x_1^2 + x_2^2 + \cdots + x_d^2 - 1\right).
$$

(107)

Correspondingly, the level set

$$
\Sigma = \left\{(x_1, x_2, \cdots, x_d) \in \mathbb{R}^d \mid x_1^2 + x_2^2 + \cdots + x_d^2 = 1\right\}
$$

(108)
is the $(d-1)$-dimensional unit sphere, and we have

$$
\nabla \xi = (x_1, x_2, \cdots, x_d)^T, \quad \nabla \xi^T \nabla \xi = \sum_{i=1}^{d} x_i^2.
$$

The two probability measures $\mu_1, \mu_2$ defined in (32) are again the same since $\det(\nabla \xi^T \nabla \xi) \equiv 1$ on $\Sigma$. Recalling the expressions in Section 2 we can verify that

$$
(Pa)_{ij} = a_{ij} - \frac{a_{il} x_i a_{jr} x_r}{a_{lr} x_l x_r}, \quad 1 \leq i, j \leq d.
$$

(109)

Applying Theorem 1 we conclude that the dynamics

$$
dX^i_s = -\left[\frac{a_{ij} - a_{il} x_i a_{jr} x_r}{a_{lr} x_l x_r}\right] \frac{\partial U}{\partial x_{j}} (X_s) ds + \frac{1}{\beta} \frac{\partial}{\partial x_{j}} \left(a_{ij} - \frac{a_{il} x_i a_{jr} x_r}{a_{lr} x_l x_r}\right) (X_s) ds
$$

$$
+ \sqrt{2\beta^{-1}} \left(\frac{\sigma_{ij} - \sigma_{il} x_i a_{lr} x_r}{a_{lr} x_l x_r}\right) (X_s) dW^j_s, \quad 1 \leq i \leq d,
$$

(110)
evolves on $\Sigma$ and its unique invariant measure has the probability density $\frac{1}{Z} e^{-\beta U}$ with respect to the uniform sphere measure on $\Sigma$. In particular, choosing $a = \sigma = \text{id}$, (110) can be simplified as

$$
dX^i_s = -\left(\delta_{ij} - X^i_s X^j_s\right) \frac{\partial U}{\partial x_j} ds + \frac{1 - d}{\beta} X^i_s ds + \sqrt{2\beta^{-1}} (\delta_{ij} - X^i_s X^j_s) dW^j_s.
$$

(111)

In the following, we give an example to show that in some applications it makes sense to consider (110) instead of (111), by choosing a non-identity matrix $a$. Briefly speaking, varying
the matrix \( a \) properly allows to rescale the dynamics along different directions. In particular, it has a preconditioning effect when different time scales (stiffness) exist in the dynamics.

Consider \( d = 3 \) and the spherical coordinate system

\[
x_1 = \rho \cos \theta \cos \phi, \quad x_2 = \rho \cos \theta \sin \phi, \quad x_3 = \rho \sin \theta,
\]

where \( \rho \geq 0, \theta \in [-\frac{\pi}{2}, \frac{\pi}{2}], \) and \( \phi \in [0, 2\pi] \). The potential is given by \( U = \frac{\rho^2}{2\epsilon} \), where \( \epsilon > 0 \) is a small parameter. We can verify that

\[
\nabla \theta = \frac{1}{\rho^2} \left( -\frac{x_1 x_3}{(x_1^2 + x_2^2)^{3/2}}, -\frac{x_2 x_3}{(x_1^2 + x_2^2)^{3/2}}, \frac{x_1^2 + x_2^2}{(x_1^2 + x_2^2)^{3/2}} \right)^T,
\]

and, with the choice of \( \sigma = a = \text{id} \), (113) becomes

\[
\begin{align*}
\frac{dX_1^s}{\epsilon} &= \frac{\theta}{\epsilon} \frac{X_1^1 X_3^3}{((X_1^1)^2 + (X_2^2)^2)^{3/2}} \, ds - \frac{2X_1^1}{\beta} \, ds + \sqrt{2\beta^{-1}} (\delta_{1j} - X_1^1 X_j^1) \, dW_s^j, \\
\frac{dX_2^s}{\epsilon} &= \frac{\theta}{\epsilon} \frac{X_2^1 X_3^3}{((X_1^1)^2 + (X_2^2)^2)^{3/2}} \, ds - \frac{2X_2^2}{\beta} \, ds + \sqrt{2\beta^{-1}} (\delta_{2j} - X_2^2 X_j^1) \, dW_s^j, \\
\frac{dX_3^s}{\epsilon} &= -\frac{\theta}{\epsilon} \frac{(X_1^1)^2 + (X_2^2)^2}{2} \, ds - \frac{2X_3^3}{\beta} \, ds + \sqrt{2\beta^{-1}} (\delta_{3j} - X_3^1 X_j^1) \, dW_s^j
\end{align*}
\]

with \( \theta = \theta(X_s) \). Therefore, applying (117) to sample the invariant measure (115) will be inefficient when \( \epsilon \) is small, since the step-size \( \eta \) is severely limited due to the appearance of \( \epsilon \) in (117).

On the other hand, based on the form of the potential \( U \) and the expression (113), we consider the vectors

\[
\begin{align*}
\sigma_1 &= (x_1, x_2, x_3)^T = \nabla \xi, \\
\sigma_2 &= (x_2, -x_1, 0)^T, \\
\sigma_3 &= \left(-\frac{\sqrt{\epsilon} x_1 x_3}{(x_1^2 + x_2^2)^{3/2}}, -\frac{\sqrt{\epsilon} x_2 x_3}{(x_1^2 + x_2^2)^{3/2}}, \sqrt{\epsilon}(x_1^2 + x_2^2)^{3/2} \right)^T = \sqrt{\epsilon} \rho^2 \nabla \theta,
\end{align*}
\]

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which are orthogonal to each other, and we define the matrix \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \in \mathbb{R}^{3 \times 3} \). Direct calculation shows that

\[
a = \sigma \sigma^T = \begin{pmatrix}
    \frac{1}{x_1^2 + x_2^2 + x_3^2} & \frac{cx_1 x_2}{x_1 + x_2} & \frac{cx_1 x_3}{x_1 + x_3} \\
    \frac{cx_1 x_2}{x_1 + x_2} & \frac{1}{x_1^2 + x_2^2} & \frac{cx_2 x_3}{x_2 + x_3} \\
    \frac{cx_1 x_3}{x_1 + x_3} & \frac{cx_2 x_3}{x_2 + x_3} & \frac{1}{x_3^2 + x_2^2}
\end{pmatrix},
\]

and we have

\[
\begin{align*}
\sigma^T \nabla \xi &= (x_1^2 + x_2^2 + x_3^2, 0, 0)^T, \\
\Psi &= \nabla^T a \nabla \xi = (x_1^2 + x_2^2 + x_3^2)^2, \\
a \nabla U &= (\sigma_1, \sigma_2, \sigma_3)(\sigma_1, \sigma_2, \sigma_3)^T \left( \frac{1}{\epsilon} \nabla \theta \right) \\
&= \theta (x_1^2 + x_2^2 + x_3^2) \nabla \theta.
\end{align*}
\]

With these relations, we can verify that \( P \sigma = (0, \sigma_2, \sigma_3) \) and \((Pa)_{ij} = a_{ij} - x_i x_j \). Therefore,

\[
\begin{align*}
\frac{\partial (Pa)_{ij}}{\partial x_j} &= -(1 + \epsilon) x_1 + \frac{cx_1 x_2^2}{x_1 + x_2}, \\
\frac{\partial (Pa)_{2j}}{\partial x_j} &= -(1 + \epsilon) x_2 + \frac{cx_2 x_3^2}{x_2 + x_3}, \\
\frac{\partial (Pa)_{3j}}{\partial x_j} &= -2cx_3.
\end{align*}
\]

Using the above expressions, we see that, with the matrices \( \sigma \) and \( a \) chosen in (119), dynamics (110) becomes

\[
\begin{align*}
dX_s^1 &= \frac{X_1^4 X_3 \theta}{(X_1^2 + X_2^2)^2} ds + \frac{1}{2} \left[ \frac{\epsilon X_1^2 (X_3^2)}{(X_1^2 + X_2^2)^2} - (1 + \epsilon) X_1^2 \right] ds \\
&\quad + \sqrt{2 \beta^{-1} X_1^2} dW_s^2 - \frac{\sqrt{2 \beta^{-1} X_1^2} X_3^2}{(X_1^2 + X_2^2)^2} dW_s^3, \\
dX_s^2 &= \frac{X_2^4 X_3 \theta}{(X_1^2 + X_2^2)^2} ds + \frac{1}{2} \left[ \frac{\epsilon X_2^2 (X_3^2)}{(X_1^2 + X_2^2)^2} - (1 + \epsilon) X_2^2 \right] ds \\
&\quad - \sqrt{2 \beta^{-1} X_1^2} dW_s^2 - \frac{\sqrt{2 \beta^{-1} X_2^2} X_3^2}{(X_1^2 + X_2^2)^2} dW_s^3, \\
dX_s^3 &= -\left( (X_1^2 + X_2^2) \right)^{\frac{1}{2}} \theta ds - \frac{2X_3}{\beta^2} ds + \sqrt{2 \beta^{-1} \epsilon} \left( (X_1^2 + X_2^2) \right)^{\frac{1}{2}} dW_s^3.
\end{align*}
\]

Again, applying Ito’s formula, after tedious calculations, we obtain the corresponding equation represented using the angles (\( \varphi, \theta \)) as

\[
\begin{align*}
d\varphi &= -\sqrt{2 \beta^{-1}} dW_s^2, \\
\frac{d \theta}{d s} &= -\frac{\theta^2}{2} - \frac{\epsilon \ln \cos \theta}{\beta} ds + \sqrt{2 \beta^{-1} \epsilon} dW_s^3.
\end{align*}
\]

Comparing (123) with (116), we conclude that, while both (122) and (114) have the same invariant measure in (115), the stiffness is no longer present in (122), by choosing the matrix \( a \) in (119).
This choice of matrices $\sigma, a$ also helps improve the efficiency of the numerical scheme (72). In fact, using (119) and (120), the scheme (72) becomes

\[
x^{(l+\frac{1}{2})}_i = x^{(l)}_i + \left[ -\theta \frac{\partial \theta}{\partial x_i} + \frac{1}{2} \sigma_{ij} \right] (x^{(l)})_j h + \sqrt{2} \beta^{-1} h \sigma_{ij} (x^{(l)})_j \eta^{(l)}_j, \quad 1 \leq i \leq 3,
\]

\[
x^{(l+1)} = \Theta(x^{(l+\frac{1}{2})}),
\]

where $\Theta(x)$ is the limit of the ODE flow

\[
y(s) = -\xi(y(s)) \left( 2 \xi(y(s)) + 1 \right) y(s), \quad y(0) = x.
\]

Comparing to the scheme (117) corresponding to $a = \sigma = \text{id}$, the scheme (124)–(125) is no longer stiff when $\epsilon$ is small.

Example 3: from $\mathbb{R}^2$ to ellipse

In the last example, we compare the different numerical approaches studied in the previous sections. Let us define $\xi : \mathbb{R}^2 \to \mathbb{R}$ by

\[
\xi(x) = \frac{1}{2} \left( \frac{x_1^2}{c^2} + x_2^2 - 1 \right), \quad \forall x = (x_1, x_2)^T \in \mathbb{R}^2,
\]

where the constant $c = 3$. The level set $\Sigma = \{(x_1, x_2)^T \mid \frac{x_1^2}{c^2} + x_2^2 = 1\}$ is an ellipse in $\mathbb{R}^2$. We have $\nabla \xi = \left( \frac{2x_1}{c^2}, x_2 \right)^T$ and therefore $\det(\nabla \xi^T \nabla \xi) = |\nabla \xi|^2 = \frac{x_1^2}{c^2} + x_2^2$. For simplicity, we choose the potential $U = 0$ and the matrices $a = \sigma = \text{id} \in \mathbb{R}^{2 \times 2}$. The two probability measures in (32) on $\Sigma$ are

\[
d\mu_1 = \frac{1}{Z} \left( \frac{x_1^2}{c^2} + x_2^2 \right)^{-\frac{1}{2}} \, d\nu, \quad d\mu_2 = \frac{1}{Z} \, d\nu,
\]

where $Z$ denotes two different normalization constants and $\nu$ is the surface measure on $\Sigma$. Since $\Sigma$ is a one-dimensional manifold, it is helpful to consider the parametrization of $\Sigma$ by

\[
x_1 = c \cos \theta, \quad x_2 = \sin \theta,
\]

where the angle $\theta \in [0, 2\pi]$. Applying the chain rule $\frac{\partial}{\partial \theta} = -c \sin \theta \frac{\partial}{\partial x_1} + \cos \theta \frac{\partial}{\partial x_2}$, we can obtain the expressions of $\mu_1, \mu_2$ under this coordinate as

\[
d\mu_1 = \frac{1}{Z} \, d\theta, \quad d\mu_2 = \frac{1}{Z} \left( c^2 \sin^2 \theta + \cos^2 \theta \right)^{\frac{1}{2}} \, d\theta.
\]

With these preparations, we proceed to study the following four numerical approaches.

1. Numerical scheme (72) using $\Theta$. Since $U \equiv 0$ and $a = \text{id}, (72)$ becomes

\[
x^{(l+\frac{1}{2})}_i = x^{(l)}_i + \frac{1}{2} \beta^{-1} h \eta^{(l)}_i,
\]

\[
x^{(l+1)} = \Theta(x^{(l+\frac{1}{2})}),
\]

where $\Theta(x)$ is the limit of the flow map $\varphi$, given by

\[
\dot{y}_1(s) = -\frac{\xi(y(s))}{c^2} y_1(s), \quad \dot{y}_2(s) = -\xi(y(s)) y_2(s), \quad s \geq 0,
\]

starting from $y(0) = x$. 30
2. **Numerical scheme** \((101)\) using \(\Theta^A\). Let us choose the skew-symmetric matrix

\[
A = \begin{pmatrix} 0 & 1/2 \\ -1/2 & 0 \end{pmatrix}.
\]

Since \(U \equiv 0\) and \(a = \text{id}\), we have

\[
x^{(t+\frac{1}{2})} = x^{(t)} + \sqrt{2\beta^{-1}h} \eta(t),
\]

\[
x^{(t+1)} = \Theta^A(x^{(t+\frac{1}{2})}),
\]

where \(\Theta^A(x)\) is the limit of the flow map \(\varphi^A\), given by

\[
\dot{y}_1(s) = -\xi(y(s)) \left( \frac{y_1(s) - y_2(s)}{2c^2} \right), \quad \dot{y}_2(s) = -\xi(y(s)) \left( \frac{y_1(s) + y_2(s)}{2c^2} \right), \quad s \geq 0,
\]

starting from \(y(0) = x\).

3. **Numerical scheme** \((101)\) using \(\Pi\). Similarly, since \(U \equiv 0\) and \(a = \text{id}\), \((101)\) becomes

\[
x^{(t+\frac{1}{2})} = x^{(t)} + \sqrt{2\beta^{-1}h} \eta(t),
\]

\[
x^{(t+1)} = \Pi(x^{(t+\frac{1}{2})}),
\]

where \(\Pi\) is the projection map onto \(\Sigma\), defined in \((99)\).

4. **Euler-Maruyama discretization** of the SDE \((36)\). Notice that we have \(Pa = P\), and it is straightforward to compute

\[
P_{11} = \frac{c^4 x_2^4}{x_1^4 + c^4 x_2^4}, \quad P_{12} = P_{21} = -\frac{c^2 x_1 x_2}{x_1^4 + c^4 x_2^4}, \quad P_{22} = \frac{x_1^2}{x_1^4 + c^4 x_2^4}.
\]

Therefore, discretizing \((36)\), we obtain

\[
x_1^{(t+1)} = x_1^{(t)} + \frac{1}{\beta} \left( \frac{c^4 x_2^4}{x_1^4 + c^4 x_2^4} \right) h + \sqrt{2\beta^{-1}h} \left( \frac{c^4 x_2^4}{x_1^4 + c^4 x_2^4} \eta_1^{(t)} - \frac{c^2 x_1 x_2}{x_1^4 + c^4 x_2^4} \eta_2^{(t)} \right),
\]

\[
x_2^{(t+1)} = x_2^{(t)} + \frac{1}{\beta} \left( \frac{1 - 2c^3}{x_1^4 + c^4 x_2^4} \right) h + \sqrt{2\beta^{-1}h} \left( -\frac{c^2 x_1 x_2}{x_1^4 + c^4 x_2^4} \eta_1^{(t)} + \frac{x_1^2}{x_1^4 + c^4 x_2^4} \eta_2^{(t)} \right).
\]

Based on Theorem \((130)\) and Remark \((133)\) we study the performance of the schemes \((130)\), \((135)\), and \((137)\) in sampling the conditional measure \(\mu_1\), as well as the performance of the scheme \((135)\) in sampling the measure \(\mu_2\).

In the numerical experiment, we choose \(\beta = 1.0\) in each of the above schemes. For the first scheme using \(\Theta\), we simulate \((130)\) for \(n = 5 \times 10^6\) steps with the step-size \(h = 0.01\) (total time \(T = 50000\)). In each step, \(\Theta(x^{(t+\frac{1}{2})})\) is computed by solving the ODE \((131)\) starting from \(y(0) = x^{(t+\frac{1}{2})}\) until the time when \(|\xi(y(s))| < 10^{-7}\), using the 3rd order (Bogacki-Shampine) Runge-Kutta (RK) method. Since the right hand sides of \((131)\) decrease to zero exponentially (see Remark \((13)\), the step-size for solving the ODE is set to \(\Delta t = 0.1\) initially and is multiplied by 1.05 in each iteration of the RK method. On average, we find that 57 iterations of the RK method are needed in each step in order to meet the criterion \(|\xi(y(s))| < 10^{-7}\).
For the second scheme using $\Theta^A$, we simulate (133) for $n = 1.5 \times 10^7$ steps with the step-size $h = 0.002$ (total time $T = 30000$). Notice that, a smaller step-size $h$ is used, because in this case the non-gradient ODE flow (134) produces a drift force on the level set $\Sigma$. In each step, $\Theta^A(x^{(l+\frac{1}{2})})$ is computed by solving the ODE (134) in the same way (with the same parameters) as we did in the first scheme. On average, we find that 56 iterations of the RK method are needed in each step in order to meet the criterion $|ξ(y(s))| < 10^{-7}$.

For the third scheme using $\Pi$, (135) is simulated for $n = 5 \times 10^6$ steps with the step-size $h = 0.01$ (total time $T = 50000$). Using the parametrization (128), we have $\Pi(x) = (c \cos \theta^*, \sin \theta^*)^T$, where

$$\theta^* = \arg \min_{\theta \in [0, 2\pi]} \left( (x_1 - c \cos \theta)^2 + (x_2 - \sin \theta)^2 \right), \quad x = (x_1, x_2)^T. \quad (138)$$

Therefore, in each step, $\Pi(x^{(l+\frac{1}{2})})$ is computed by solving (138) using the simple gradient descent method. The step-size is fixed to $\Delta t = 0.1$ and the gradient descent iteration terminates when the derivative of the objective function in (138) has an absolute value that is less than $10^{-7}$. On average, it requires 28 gradient descent iterations in each step in order to meet the convergence criterion.

Let us make a comparison among the three schemes (130), (133) and (135). From Figure 1 and Figure 2, we can see that the three maps $\Theta$, $\Theta^A$ and $\Pi$ indeed have different effects. Roughly speaking, comparing to the projection map $\Pi$, both $\Theta$ and $\Theta^A$ tend to map states towards one of the two vertices $(\pm c, 0)$, where $|∇ξ|$ are smaller, while $\Pi^A$ introduces a further rotational force on $\Sigma$. Based on the states generated from these three schemes, in Figure 3, we show the empirical probability densities of the parameter $\theta$ in (128). From the agreement between the empirical densities and the densities computed from the analytical expressions in (129), we can make the conclusion that the trajectories generated from the two schemes using $\Theta$ and $\Theta^A$ indeed sample the probability measure $\mu_1$, while the trajectory generated from the scheme using $\Pi$ samples $\mu_2$.

Lastly, concerning the fourth scheme, we simulate (137) for $n = 10^7$ steps using the step-size $h = 0.0001$ (total time $T = 1000$). In this case, we find that it is necessary to choose a small step-size $h$ in order to keep the trajectory close to the level set $\Sigma$. As can be seen from Figure 4 even with this smaller step-size $h = 0.0001$, the generated trajectory departs from the level set $\Sigma$. This indicates the limited usefulness of the direct Euler-Maruyama discretization of the SDE (36) in long time simulations.

6 Conclusions

Ergodic diffusion processes on a submanifold of $\mathbb{R}^d$ and the related numerical sampling schemes have been considered in this work. A family of SDEs have been obtained whose invariant measures coincide with the given probability measure on the submanifold. In particular, for the conditional probability measure, we found that the corresponding SDEs have a relatively simple form. We proposed and analyzed a consistent numerical scheme which only requires 1st order derivatives of the reaction coordinate function. Different schemes (both constrained and unconstrained) sampling on the submanifolds are numerically evaluated.

Our work extends the results in the literature and may further contribute to both the mathematical analysis and the development of numerical methods on related problems, in particular...
Figure 1: Example 3. Given $x \in \mathbb{R}^2$, $\Pi(x)$ is the state on the ellipse $\Sigma$ which achieves the minimal distance to $x$, while $\Theta(x)$ and $\Theta^A(x)$ are the limits of the ODE flows (131) and (134) starting from $x$, respectively.

Figure 2: Example 3. Left: the streamline of the flow map $\varphi$ in (131). Middle: the streamline of the flow map $\varphi^A$ (134) with the matrix $A$ in (132). Right: illustration of the projection $\Pi$. Points on each straight line are mapped to the same point on $\Sigma$.

Figure 3: Example 3. The probability densities of the parameter $\theta$, computed from the scheme (130) using $\Theta$ (left plot), the scheme (133) using $\Theta^A$ (middle plot), and the scheme (135) using $\Pi$ (right plot). In each plot, dotted curves are the probability densities computed from the analytical expressions of $\mu_1, \mu_2$ in (129), respectively. Solid lines are the empirical probability densities of $\theta$ estimated using the states generated from the schemes (130), (133), and (135), respectively.
problems in molecular dynamics such as free energy calculation and model reduction of high-dimensional stochastic processes. Closely related to the current paper, in the future we would like to consider the following topics. Firstly, the “non-reversible” scheme \( \text{[97]} \) is supported by a simple numerical example but theoretical justification still needs to be done. This will be considered in future following the approach described in Remark \[5\]. Secondly, the constrained numerical schemes considered in the current work do not involve system’s momentum variables. In view of the work \[33\], it is interesting to study the Langevin dynamics under different constraints (such as certain variants of the map \( \Theta \) used in this work). The softly constrained Langevin dynamics is also a relevant topic in this direction. Thirdly, there is a research interest in the literature to study the effective dynamics of molecular systems along a given reaction coordinate \( \xi \). The coefficients of the effective dynamics are usually defined as averages on the level set of \( \xi \) \[28\]. As an application of the numerical scheme proposed in this work, we will study numerical algorithms to simulate the effective dynamics. This topic is related to the heterogeneous multiscale methods \[14\] and the equation-free approach \[27, 25\] in the literature.

**Acknowledgement**

This work is funded by the Einstein Center of Mathematics (ECMath) through project CH21. The author would like to thank Gabriel Stoltz for stimulating discussions on constrained Langevin processes at the Institut Henri Poincaré - Centre Émile Borel during the trimester “Stochastic Dynamics Out of Equilibrium”. The author appreciates the hospitality of this institution. The author also thanks the anonymous referees for their valuable comments and critics which helped improve the manuscript substantially.

**A Useful facts about the Riemannian manifold \( \mathcal{M} \)**

In this section, we present further details of Section \[2\] related to the Riemannian manifold \( \mathcal{M} = (\mathbb{R}^d, g) \), where \( g = a^{-1} \). In particular, we will prove Proposition \[1\] in Section \[2\] after deriving the expressions of several quantities on \( \mathcal{M} \).
Denote by $\nabla^M$ the Levi-Civita connection on $\mathcal{M}$. Given $x \in \mathcal{M}$ and a tangent vector $v \in T_x \mathcal{M}$, $\nabla^M_v$ is the covariant derivative operator on $\mathcal{M}$ along the vector $v$. For two vectors $u = (u_1, u_2, \cdots, u_d)^T$, $v = (v_1, v_2, \cdots, v_d)^T$, the Hessian of a smooth function $f : \mathcal{M} \to \mathbb{R}$ is defined as

$$
\text{Hess}^M f(u, v) = u(v f) - (\nabla^M_u v) = u_i v_j \text{Hess}^M f(e_i, e_j) = u_i v_j \left( \frac{\partial^2 f}{\partial x_i \partial x_j} - \Gamma^l_{ij} \frac{\partial f}{\partial x_l} \right),
$$

where

$$
\Gamma^l_{ij} = \frac{1}{2} g^{lr} \left( \frac{\partial g_{ir}}{\partial x_j} + \frac{\partial g_{jr}}{\partial x_i} - \frac{\partial g_{ij}}{\partial x_r} \right) = \frac{1}{2} \delta_{ij} \left( \frac{\partial (a^{-1})_{ir}}{\partial x_j} + \frac{\partial (a^{-1})_{jr}}{\partial x_i} - \frac{\partial (a^{-1})_{ij}}{\partial x_r} \right), \quad 1 \leq i, j, l \leq d
$$

are the Christoffel's symbols defined by $\nabla^M_e \epsilon_j = \Gamma^l_{ij} \epsilon_l$, for $1 \leq i, j \leq d$.

Recall that the vectors $\sigma_1, \sigma_2, \cdots, \sigma_d$ in $\Sigma$ form an orthonormal basis of the tangent space at each point of $\mathcal{M}$. Using (139) and $a = \sigma \sigma^T$, we can compute

$$
\Delta^M f = \text{tr}(\text{Hess}^M f) = \text{Hess}^M f(\sigma_i, \sigma_l) = a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} - a_{ij} \Gamma^l_{ij} \frac{\partial f}{\partial x_l}.
$$

Define $G = \text{det} g = (\text{det} a)^{-1}$, and recall that the Jacobi's formula [40] implies $\frac{\partial \ln G}{\partial x^l} = g^{ij} \frac{\partial a_{ij}}{\partial x^l} = a_{ij} \frac{\partial (a^{-1})_{ij}}{\partial x^l}$, where $1 \leq l \leq d$. Together with (140) and (141), we can verify the expression

$$
\Delta^M f = \frac{1}{\sqrt{G}} \frac{\partial (\sqrt{G} g^{ij} \frac{\partial f}{\partial x^i})}{\partial x^j}, \quad \forall f \in C^\infty(\mathcal{M}).
$$

For the submanifold $\Sigma$, it is direct to check that the Levi-Civita connection and the gradient operator on $\Sigma$ are given by $\nabla^\Sigma = P^\perp \nabla^M$ and $\text{grad}^\Sigma = P \text{grad}^M$, respectively. Concerning the divergence operator $\text{div}^\Sigma$, the Laplace-Beltrami operator $\Delta^\Sigma$, and the mean curvature vector $H$ on $\Sigma$, we have the following results.

**Lemma 2.** Let $f \in C^\infty(\Sigma)$ and $\tilde{f} \in C^\infty(\mathcal{M})$ be its extension to $\mathcal{M}$. $u \in \Gamma(T \mathcal{M})$ is a tangent vector field on $\mathcal{M}$ and we recall the vectors $p_i = P \sigma_i$, $1 \leq i \leq d$. We have

1. $\text{div}^\Sigma u = (\nabla^M_p u, p_i)_g$.
2. $(\text{div}^\Sigma p_i)_p_i + P \nabla^M_p p_i = 0$.
3. $\Delta^\Sigma f = \sum_{i=1}^d p_i^2 \tilde{f} + (\text{div}^\Sigma p_i)_p_i \tilde{f} = \sum_{i=1}^d p_i^2 \tilde{f} - (P \nabla^M_p p_i)_p_i \tilde{f}$.
4. $\Delta^\Sigma f = \text{Hess}^M \tilde{f}(p_i, p_i) + H \tilde{f}$, where $H$ is the mean curvature vector of the submanifold $\Sigma$.
5. In the special case when $g = a = \text{id}$, we have $(\text{div}^\Sigma p_i)_p_i = P \nabla^M_p p_i = 0$, and $\Delta^\Sigma = \sum_{i=1}^d p_i^2$.

**Proof.** Let $x \in \Sigma$ and assume that $v_i$, $1 \leq i \leq d - k$, is an orthonormal basis of $T_x \Sigma$. We have $v_i = (v_i, p_i)_g p_j$.

1. For the first assertion,

$$
\text{div}^\Sigma u = (\nabla^\Sigma_v u, v_j)_g = (P \nabla^M_v u, v_j)_g = (v_j, p_i)_g (\nabla^M_p u, p_i)_g = (\nabla^M_p u, p_i)_g.
$$
2. For the second assertion,
\[(\text{div}^\Sigma p_i) p_i + P \nabla^\Sigma p_i \]
\[= (\nabla^\Sigma p_i, p_j)_g p_j + (\nabla^\Sigma p_i, p_j)_g p_j \]
\[= (p_i, p_j)_g p_j - \nabla^\Sigma p_i - \nabla^\Sigma p_j = 0.\]

3. For the third assertion, by definition,
\[\Delta^\Sigma f = \text{div}^\Sigma (\text{grad}^\Sigma f) = \text{div}^\Sigma (P \text{grad}^\Sigma \tilde{f}) = \text{div}^\Sigma ((\text{grad}^\Sigma \tilde{f}, p_i)_g p_i) \]
\[= \text{div}^\Sigma ((p_i, \tilde{f}) p_i) = \sum_{i=1}^{d} p_i^2 \tilde{f} + (\text{div}^\Sigma p_i) p_i \tilde{f} = \sum_{i=1}^{d} p_i^2 \tilde{f} - (P \nabla^\Sigma p_i) \tilde{f},\]
where the second assertion has been used in the last equality.

4. For the fourth assertion, starting from the third assertion, using the definition of Hess\(^M\) in (139), and applying Proposition 5 below, we obtain
\[\Delta^\Sigma f = \sum_{i=1}^{d} p_i^2 \tilde{f} - P \nabla^\Sigma p_i \tilde{f} \]
\[= \text{Hess}^M \tilde{f}(p_i, p_i) + [(I - P) \nabla^\Sigma p_i] \tilde{f} = \text{Hess}^M \tilde{f}(p_i, p_i) + H \tilde{f}.\]

5. For the last assertion, when \(g = \text{id}\), we have \(\Gamma^l_{ij} \equiv 0\), for \(\forall 1 \leq i, j, l \leq d\). Also, it follows from (24) that \(P_{i,j} = P_{i,j} = P_{i,l} = P_{l,j}\). We obtain
\[\frac{(\text{div}^\Sigma p_i) p_i}{(\nabla^\Sigma p_i, p_j)_g p_j} = P_{j,i} P_{j,i} P_{j,j} \langle \nabla^\Sigma (P_{i,j} e_r), e_r \rangle_g e_r \]
\[= P_{j,i} \frac{\partial P_{i,j}}{\partial x_j} P_{i,j} e_r \]
\[= \left[ \frac{\partial P_{i,j}}{\partial x_j} P_{i,j} - \frac{\partial P_{i,j}}{\partial x_i} P_{i,j} \right] e_r \]
\[= 0,\]
and the other assertions follow accordingly.

\[\square\]

**Proposition 6.** Let \(H\) be the mean curvature vector defined in (20) on the submanifold \(\Sigma\). We have
\[H = (I - P) \nabla^\Sigma p_i \]
\[= - (\Psi^{-1})_{\alpha \gamma} \left[ \frac{1}{2} (P a)_{ij} (a \nabla \xi_{\alpha}) \frac{\partial (a^{-1})}_{ij} + P_{ij} \frac{\partial (a \nabla \xi_{\alpha})}{\partial x_i} \right] a \nabla \xi_{\gamma}. \quad (143)\]

In the special case when \(g = a = \text{id}\), we have
\[H = P_{ji} \frac{\partial P_{ij}}{\partial x_j} = - \left[ (\Psi^{-1})_{\alpha \gamma} P_{ij} \frac{\partial^2 \xi_{\alpha}}{\partial x_j \partial x_i} \right] a \nabla \xi_{\gamma}. \quad (144)\]
Proof. Given a tangent vector field \( v \) on \( \mathcal{M} \), from the definition of \( P \) we have \( v = P v + (\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha) \). Since \( P v \) is a tangent vector on \( \Sigma \), using (26) and the divergence theorem on \( \Sigma \), we know

\[
\int_{\Sigma} \langle H, v \rangle_g \; dv_g = - \int_{\Sigma} \text{div}^\Sigma [(I - P)v] \; dv_g = - \int_{\Sigma} \text{div}^\Sigma [(\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha)] \; dv_g. \tag{145}
\]

For the first expression, we notice that \( \langle (I - P)v, p_i \rangle_g \equiv 0, 1 \leq i \leq d \). Applying Lemma 2, we have

\[
- \int_{\Sigma} \text{div}^\Sigma [(I - P)v] \; dv_g = - \int_{\Sigma} \langle \nabla_p^M [(I - P)v], p_i \rangle_g \; dv_g = - \int_{\Sigma} p_i \langle (I - P)v, p_i \rangle_g \; dv_g + \int_{\Sigma} \langle (I - P)v, \nabla_p^M p_i \rangle_g \; dv_g = \int_{\Sigma} \langle v, (I - P)\nabla_p^M p_i \rangle_g \; dv_g.
\]

Comparing the last equality above with (145), we conclude that \( H = (I - P)\nabla_p^M p_i \).

For the second expression, we notice that \( \langle a \nabla_{\xi_l} a, p_i \rangle_g = 0 \), and also recall the expressions (140), (22) and (24). Applying Lemma 2 integrating by parts, and noticing the cancellation of some terms, we can derive

\[
\text{div}^\Sigma [(\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha)] = \langle \nabla_p^M [(\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha)], p_i \rangle_g = (\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha) \langle p_i, \nabla_p^M (a \nabla_{\xi_l} a), e_r \rangle_g.
\]

The second identity in (143) is obtained after comparing the above expression with (145).

In the case \( g = a = \text{id} \), we have \( \Gamma_{il}^j \equiv 0, 1 \leq i, l, r \leq d \). It follows that

\[
\text{div}^\Sigma [(\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha)] = (\Psi^{-1})_{\alpha\gamma}(v, a \nabla_{\xi_l} a \nabla_{\xi_l} \alpha) P_{jl} \partial^2_{ij} \alpha
\]

and we obtain that \( H = -[(\Psi^{-1})_{\alpha\gamma} P_{jl} \partial^2_{ij} \alpha \nabla_{\xi_l} \gamma]. \) Using (21) and (23), we have

\[
P_{jl} \partial^2_{ij} \alpha \nabla_{\xi_l} \gamma = -P_{jl} \partial^2_{ij} \alpha \nabla_{\xi_l} \gamma, \]

and therefore the first expression in (144) holds as well. \( \square \)

With the above preparations, we are ready to prove Proposition 1 in Section 2

Proof of Proposition 1. Let \( f \in C^\infty(\Sigma) \) and \( \tilde{f} \in C^\infty(\mathcal{M}) \) be its extension to \( \mathcal{M} \). Using Lemma 2 and Proposition 6 we have

\[
\Delta^\Sigma f = \text{Hess}^M \tilde{f}(p_r, p_r) + H \tilde{f}
\]
The other equality in (29) follows from Proposition 6.

Notice that we have already obtained the coefficients of the second order derivative terms. For the terms of the first order derivatives, let us denote

\[ I_1 = - (Pa)_{jl} \Gamma_{jl} \]

\[ I_2 = - \frac{1}{2} (\Psi^{-1})_{\alpha\gamma} (Pa)_{jl} (a \nabla \xi_{\gamma})_r (a \nabla \xi_{\alpha})_r \frac{\partial (a^{-1})_{jl}}{\partial x_r} \]

\[ I_3 = - (\Psi^{-1})_{\alpha\gamma} P_{ir} (a \nabla \xi_{\alpha})_r \frac{\partial (a \nabla \xi_{\gamma})_r}{\partial x_i} \]  \hspace{1cm} (146)

Using the expression of \( Pa \) in (24), the property \( Pa \nabla \xi_{\gamma} = 0 \), and integrating by parts, we easily obtain

\[ I_2 = \frac{1}{2} (Pa)_{ir} - a_{ir} (Pa)_{jl} \frac{\partial (a^{-1})_{jl}}{\partial x_r} \]

\[ I_3 = \frac{\partial P_{ir}}{\partial x_l} (a_{ir} - (Pa)_{ir}) \]  \hspace{1cm} (147)

For \( I_1 \), direct calculation using (140) gives

\[ I_1 = - \frac{1}{2} (Pa)_{jl} a_{ir} \left( \frac{\partial (a^{-1})_{ir}}{\partial x_j} + \frac{\partial (a^{-1})_{jr}}{\partial x_l} - \frac{\partial (a^{-1})_{jl}}{\partial x_r} \right) \]

\[ = - (Pa)_{jl} a_{ir} \frac{\partial (a^{-1})_{ir}}{\partial x_j} + \frac{1}{2} (Pa)_{jl} a_{ir} \frac{\partial (a^{-1})_{jl}}{\partial x_r} \]  \hspace{1cm} (148)

Therefore,

\[ I_1 + I_2 + I_3 = \frac{\partial (Pa)_{ij}}{\partial x_j} - \frac{\partial P_{ir}}{\partial x_l} (Pa)_{ir} + \frac{1}{2} (Pa)_{jl} a_{ir} \frac{\partial (a^{-1})_{jl}}{\partial x_r} + \frac{1}{2} ((Pa)_{ir} - a_{ir}) (Pa)_{jl} \frac{\partial (a^{-1})_{jl}}{\partial x_r} \]

\[ = \frac{\partial (Pa)_{ij}}{\partial x_j} - \frac{\partial P_{ir}}{\partial x_l} (Pa)_{ir} + \frac{1}{2} (Pa)_{jl} (Pa)_{jr} \frac{\partial (a^{-1})_{jl}}{\partial x_r} \]  \hspace{1cm} (149)

Applying Lemma \( \mathbb{B} \) below to handle the last term above, we conclude

\[ I_1 + I_2 + I_3 = \frac{\partial (Pa)_{ij}}{\partial x_j} - \frac{1}{2} (Pa)_{ir} \frac{\partial \ln \det a}{\partial x_r} + \frac{1}{2} (Pa)_{ir} \frac{\partial \ln \det \Psi}{\partial x_r} . \]

Finally, when \( g = a = \text{id} \), applying Lemma \( \mathbb{B} \) we can obtain

\[ \Delta^\Sigma f = \text{Hess}^M \tilde{f}(p_1, p_1) + H \tilde{f} \]

\[ = P_{ij} \frac{\partial^2 \tilde{f}}{\partial x_i \partial x_j} - \Gamma^i_{jl} \frac{\partial \tilde{f}}{\partial x_j} + H \tilde{f} \]

\[ = P_{ij} \frac{\partial^2 \tilde{f}}{\partial x_i \partial x_j} + H \frac{\partial \tilde{f}}{\partial x_i} . \]

The other equality in (29) follows from Proposition 6.  \( \square \)
The following identity has been used in the above proof, and will be useful in Appendix B and Appendix C as well.

**Lemma 3.**

\[
\frac{1}{2} (Pa)_{ir}(Pa)_{jl} \frac{\partial (a^{-1})_{jl}}{\partial x_r} = -\frac{1}{2} (Pa)_{ir} \frac{\partial \ln a}{\partial x_r} + (Pa)_{ir} \frac{\partial (P_{rj})}{\partial x_l} + \frac{1}{2} (Pa)_{ir} \frac{\partial \ln \det \Psi}{\partial x_r} .
\] (149)

**Proof.** Using the expression of \( Pa \) in (24), the relations

\[
P a \nabla \xi_\gamma = 0, \quad \frac{\partial \ln a}{\partial x_r} = (a^{-1})_{jl} \frac{\partial a_{jl}}{\partial x_r}, \quad \frac{\partial \ln \Psi}{\partial x_r} = (\Psi^{-1})_{\alpha \gamma} \frac{\partial \Psi_{\alpha \gamma}}{\partial x_r},
\]

and the integration by parts formula, we can compute

\[
\frac{1}{2} (Pa)_{ir}(Pa)_{jl} \frac{\partial (a^{-1})_{jl}}{\partial x_r} = \frac{1}{2} (Pa)_{ir} (a_{jl} - (\Psi^{-1})_{\alpha \gamma} (a \nabla \xi_\alpha)_j (a \nabla \xi_\gamma)_l) \frac{\partial (a^{-1})_{jl}}{\partial x_r}
\]

\[
= -\frac{1}{2} (Pa)_{ir} \frac{\partial \ln a}{\partial x_r} - \frac{1}{2} (Pa)_{ir} (\Psi^{-1})_{\alpha \gamma} (a \nabla \xi_\alpha)_j \frac{\partial a_{jl}}{\partial x_r} + \frac{1}{2} (Pa)_{ir} (\Psi^{-1})_{\alpha \gamma} \frac{\partial \nabla \xi_\alpha}{\partial x_r}
\]

\[
= -\frac{1}{2} (Pa)_{ir} \frac{\partial \ln a}{\partial x_r} - (Pa)_{ir} (\Psi^{-1})_{\alpha \gamma} (a \nabla \xi_\alpha)_j \frac{\partial a_{jl}}{\partial x_r} + \frac{1}{2} (Pa)_{ir} \frac{\partial \ln \det \Psi}{\partial x_r}.
\]

\[
\square
\]

### B Limiting flow map \( \Theta \)

In this section, we prove Proposition 4 in Section 4, which concerns the properties of the flow map \( \Theta \) defined in (68), (69), and (70). While the approach of the proof is similar to the one in [15], here we consider the specific function \( F \) in (69) and we will provide full details of the derivations.

**Proof of Proposition 4.** In this proof, we will always assume \( x \in \Sigma \). For a function which only depends on the state and is evaluated at \( x \), we will often omit its argument in order to keep the notations simple. Also notice that, repeated indices other than \( l \) and \( l' \) indicate that they are summed up, while for the indices \( l \), \( l' \) we assume that they are fixed by default unless the summation operator is used explicitly.

Since \( \nabla F = 0 \) on \( \Sigma \), from the equation (68) we know that \( \varphi(x, s) \equiv x, \forall s \geq 0 \). Let us denote by \( \nabla^2 F \) the Hessian matrix (on the standard Euclidean space) of the function \( F \) in (69), i.e., \( \nabla^2 F = (\partial^2 F)_{1 \leq i, j \leq d} \). Since \( \xi(x) = 0 \in \mathbb{R}^k \), direct calculation gives

\[
(a \nabla^2 F)_{ij} = a_{ir} \frac{\partial^2 F}{\partial x_r \partial x_j} = (a \nabla \xi \nabla \xi^T)_{ij}, \quad 1 \leq i, j \leq d.
\] (150)

Meanwhile, it is straightforward to verify that \( a \nabla^2 F \) satisfies

\[
\langle a \nabla^2 F u, v \rangle_g = \langle u, a \nabla^2 F v \rangle_g, \quad \forall \ u, v \in \mathbb{R}^d,
\]

\[
|a \nabla^2 F u|_g^2 = |\nabla \xi^T u|^2 \geq 0, \quad \forall \ u \in \mathbb{R}^d,
\]

\[
(a \nabla^2 F) u = a \nabla \xi \nabla \xi^T u = 0, \quad \forall \ u \in T_x \Sigma.
\] (151)
Therefore, we can assume that $a \nabla^2 F$ has real (non-negative) eigenvalues

$$\lambda_1 = \lambda_2 = \cdots = \lambda_{d-k} = 0 < \lambda_{d-k+1} \leq \cdots \leq \lambda_d,$$

and the corresponding eigenvectors, denoted by $v_i = (v_{i1}, v_{i2}, \cdots, v_{id})^T$, $1 \leq i \leq d$, are orthonormal with respect to the inner product $\langle \cdot, \cdot \rangle$ in (10), such that $v_1, v_2, \cdots, v_{d-k} \in T_x \Sigma$.

The projection matrix $P$ in (21) can be expressed using the vectors $v_i$ as

$$P_{ij} = \sum_{l=1}^{d-k} v_{li}(a^{-1})_{jr}v_{lr}, \quad 1 \leq i, j \leq d,$$

and we have

$$\sum_{l=1}^{d-k} v_{li}v_{lj} = (Pa)_{ij}, \quad a_{ij} - (Pa)_{ij} = \sum_{l=d-k+1}^{d} v_{li}v_{lj}.$$  \hfill (153)

It is also a simple fact that the eigenvalues of the $k \times k$ matrix $\Psi = \nabla \xi^T a \nabla \xi$ in (22) are $\lambda_{d-k+1}, \lambda_{d-k+2}, \cdots, \lambda_d$, with the corresponding eigenvectors given by $\nabla \xi^T v_{d-k+1}, \nabla \xi^T v_{d-k+2}, \cdots, \nabla \xi^T v_d$. In particular, this implies

$$\prod_{i=d-k+1}^{d} \lambda_i = \det(\nabla \xi^T a \nabla \xi) = \det \Psi.$$  \hfill (155)

In the following, we study the ODE (68) using the eigenvectors $v_i$. Differentiating the ODE (68) twice, using the facts that $\varphi(x, s) \equiv x, \forall s \geq 0$, and $\nabla F = 0$ on $\Sigma$, we obtain

$$\frac{d}{ds} \frac{\partial \varphi_i}{\partial x_j}(x, s) = - \left( a_{ir}, \frac{\partial^2 F}{\partial x_r \partial x_i} \right) \frac{\partial \varphi_r}{\partial x_j}(x, s)$$

$$\frac{d}{ds} \frac{\partial^2 \varphi_i}{\partial x_j \partial x_r}(x, s) = - \left( 2 a_{ir}, \frac{\partial^2 F}{\partial x_r \partial x_i}, a_{ir}, \frac{\partial^3 F}{\partial x_r \partial x_i \partial x_j} \right) \frac{\partial \varphi_r}{\partial x_j}(x, s) \frac{\partial \varphi_r}{\partial x_j}(x, s) \frac{\partial \varphi_r}{\partial x_j}(x, s)$$

$$\cdots$$

for $s \geq 0$ and $1 \leq i, j, r \leq d$.

1. The first equation of (155) implies

$$\frac{d}{ds} \left( v_{ij} \frac{\partial \varphi_i}{\partial x_j}(x, s) \right) = - \left( a_{ir}, \frac{\partial^2 F}{\partial x_r \partial x_i} \right) \left( v_{ij} \frac{\partial \varphi_r}{\partial x_j}(x, s) \right), \quad 1 \leq l \leq d.$$  \hfill (157)

Since $\varphi(\cdot, 0)$ is the identity map, we have

$$v_{ij} \frac{\partial \varphi_i}{\partial x_j}(x, 0) = v_{il}, \quad \text{at } s = 0.$$  \hfill (158)

Because $v_l$ is the eigenvector of $a \nabla^2 F$, we can directly solve the solution of (157)-(158) and obtain

$$v_{ij} \frac{\partial \varphi_i}{\partial x_j}(x, s) = e^{-\lambda_i s} v_{il}, \quad \frac{\partial \varphi_i}{\partial x_j}(x, s) = \sum_{l=1}^{d} e^{-\lambda_l s} v_{il}(a^{-1})_{jr}v_{lr}, \quad \forall s \geq 0,$$

for $1 \leq i, j \leq d$. Sending $s \to +\infty$, using (152) and (155), we obtain

$$\frac{\partial \Theta_i}{\partial x_j} = \lim_{s \to +\infty} \frac{\partial \varphi_i}{\partial x_j}(x, s) = \sum_{l=1}^{d-k} v_{il}(a^{-1})_{jr}v_{lr} = P_{ij}.$$  \hfill (160)
2. We proceed to compute \( a_{ijr} \frac{\partial^2 \varphi}{\partial x_j \partial x_r}, \ 1 \leq i \leq d \). For this purpose, let us define

\[
A_i(x, s) = (a^{-1})_{ijr} v_{jr} a_{ijr} \frac{\partial^2 \varphi}{\partial x_j \partial x_r}(x, s), \quad 1 \leq l \leq d, \nonumber
\]

\[
\iff \quad a_{ijr} \frac{\partial^2 \varphi}{\partial x_j \partial x_r}(x, s) = \sum_{l=1}^{d} v_l A_l(x, s).
\]

Using the second equation of (156), the solution (159), and the orthogonality of the eigenvectors, we can obtain

\[
\frac{dA_i}{ds}(x, s) = -\sum_{l=1}^{d} \sum_{l'=1}^{d} 2 \frac{\partial a_{ijr}}{\partial x_j} \frac{\partial^2 F}{\partial x_j \partial x_r} (a^{-1})_{ijr'} + \frac{\partial^3 F}{\partial x_j \partial x_r \partial x_j'} v_{l'i'} v_{l'r} e^{-2\lambda_i s} - \lambda_i A_i(x, s),
\]

for \( 1 \leq l \leq d \), from which we get

\[
P_{il} a_{jr} \frac{\partial^2 \varphi}{\partial x_j \partial x_r}(x, s) = \sum_{l=1}^{d} v_l A_l(x, s) \nonumber
\]

\[
= \sum_{l=1}^{d} \sum_{l'=1}^{d} \frac{\partial a_{ijr}}{\partial x_j} \frac{\partial^2 F}{\partial x_j \partial x_r} (a^{-1})_{ijr'} + \frac{\partial^3 F}{\partial x_j \partial x_r \partial x_j'} v_{l'i'} v_{l'r} e^{-\lambda_i s} \int_0^s e^{(\lambda_i - 2\lambda_i)u} \, du.
\]

To further simplify the last expression above, we differentiate the identity

\[
\frac{\partial^2 F}{\partial x_j \partial x_r} v_{l'i'} v_{l'r} \varphi = \lambda_i v_{l'i'},
\]

where \( l' \) is fixed, \( 1 \leq l' \leq d \), along the eigenvector \( v_l \), which gives

\[
\frac{\partial^3 F}{\partial x_j \partial x_r \partial x_j'} v_{l'i'} v_{l'r} \varphi.
\]

\[
= - 2 \frac{\partial^2 F}{\partial x_j \partial x_r} v_{l'i'} v_{l'r} + \frac{\partial \lambda_i}{\partial x_r} v_{l'r} \nonumber
\]

\[
= - 2 \lambda_i (a^{-1})_{l'i'} v_{l'i'} \frac{\partial^2 \varphi}{\partial x_j} v_{l'r} + \frac{\partial \lambda_i}{\partial x_r} v_{l'r}.
\]

Therefore, taking the limit \( s \to +\infty \), using the relations (157), (159), and Lemma 3 in Appendix A, we can compute

\[
P_{il} a_{jr} \frac{\partial^2 \varphi}{\partial x_j \partial x_r} = \lim_{s \to +\infty} P_{il} a_{jr} \frac{\partial^2 \varphi_{l'r}}{\partial x_j \partial x_r}(x, s) \nonumber
\]

\[
= \lim_{s \to +\infty} \sum_{l'=d-k+1}^{d} \sum_{l=1}^{d-k} \frac{\partial (a^{-1})_{l'i'}}{\partial x_j} v_{l'i'} v_{l'r} + 2 \lambda_i (a^{-1})_{l'i'} v_{l'i'} v_{l'r} \frac{\partial v_{l'r}}{\partial x_r} \nonumber
\]

\[
= \frac{\partial (a^{-1})_{l'i'}}{\partial x_j} (a_{l'i'} - (P a)_{l'i'})(P a)_{l'r} - \frac{1}{2} \frac{\partial (a^{-1})_{l'i'}}{\partial x_r} (a_{l'r} - (P a)_{l'r})(P a)_{l'r} - \frac{1}{2} (P a)_{l'r} \frac{\partial \ln \det \Psi}{\partial x_r}
\]
\[
\begin{align*}
\frac{\partial P}{\partial x^j} + \frac{\partial P}{\partial x^j} \frac{\partial (Pa)_{ij}}{\partial x_j} + \frac{\partial P}{\partial x^j} (Pa)_{ij} &= - P \frac{\partial a}{\partial x^j} + P \frac{\partial (Pa)_{ij}}{\partial x_j} \\
\frac{\partial P}{\partial x^j} + \frac{\partial P}{\partial x^j} \frac{\partial (Pa)_{ij}}{\partial x_j} + \frac{\partial P}{\partial x^j} (Pa)_{ij} &= - P \frac{\partial a}{\partial x^j} + P \frac{\partial (Pa)_{ij}}{\partial x_j}.
\end{align*}
\]

On the other hand, differentiating the relation \(\xi(\Theta(x)) \equiv 0\) twice and using (160), we get
\[
\begin{align*}
\frac{\partial^2 \Theta}{\partial x_i \partial x^j} &= - \frac{\partial^2 \xi}{\partial x_i \partial x^j} P_{ij} P_{jr} a_{jr} \\
&= \Psi \frac{\partial a}{\partial x^j} - \frac{\partial P}{\partial x^j} (Pa)_{ij} \frac{\partial P}{\partial x^j}.
\end{align*}
\]

for \(1 \leq \gamma \leq k\). Therefore, using \(PaP_T = PaP_a\) and \(Pa \nabla \xi = 0\), we can compute
\[
\begin{align*}
\frac{\partial^2 \Theta}{\partial x_i \partial x^j} &= \frac{\partial (Pa)_{ij}}{\partial x_j} - \frac{\partial P}{\partial x^j} \frac{\partial (Pa)_{ij}}{\partial x_j}.
\end{align*}
\]

Summing up (162) and (163), we conclude that
\[
\begin{align*}
a_{jr} \frac{\partial^2 \Theta_i}{\partial x_j \partial x^r} &= \frac{\partial (Pa)_{ij}}{\partial x_j} - \frac{\partial P}{\partial x^j} \frac{\partial a_{jr}}{\partial x^j}.
\end{align*}
\]

\[\square\]

C Projection map \(\Pi\)

In this section, we prove Proposition 5 in Section 4 which concerns the properties of the projection map \(\Pi\) defined in (99).

Proof of Proposition 5. For \(1 \leq l \leq d\), recall that \(p_l = (P\sigma)_{ij}e_v\) is the tangent vector field defined in Section 2 such that \(p_l \in T_x\Sigma\) at each \(x \in \Sigma\). Since \(\Pi_l(x) = x_i\) for \(x \in \Sigma, 1 \leq i \leq d\), taking derivatives along \(p_l\) twice, we obtain
\[
\begin{align*}
\frac{\partial \Pi_l}{\partial x_j} (P\sigma)_{ij} &= (P\sigma)_{il}, \\
\frac{\partial^2 \Pi_l}{\partial x_j \partial x^r} (P\sigma)_{ij} &= (P\sigma)_{il} \frac{\partial (P\sigma)_{il}}{\partial x_r} - \frac{\partial \Pi_l}{\partial x_j} (P\sigma)_{ij} \frac{\partial (P\sigma)_{ij}}{\partial x^r}.
\end{align*}
\]

Notice that, for a function which only depends on the state and is evaluated at \(x \in \Sigma\), we will often omit its argument in order to keep the notations simple.

On the other hand, the vector \(\sigma_l - p_l = ((I - P)\sigma)_{ij}e_v \in (T_x\Sigma)^z\) (the complement of the subspace \(T_x\Sigma\) in \(T_x\mathcal{M}\)). Let \(\phi(s)\) be the geodesic curve in \(\mathcal{M}\) such that \(\phi(0) = x\) and...
\( \phi'(0) = \sigma_t - p_t \). We have \( \Pi_i(\phi(s)) = x_i, \ \forall s \in [0, \epsilon) \) for some \( \epsilon > 0 \). Taking derivatives with respect to \( s \) twice, we obtain
\[
\frac{\partial \Pi_i}{\partial x_j}(\phi(s)) \frac{d\phi_j(s)}{ds} = 0,
\]
\[
\frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(\phi(s)) \frac{d\phi_j(s)}{ds} \frac{d\phi_r(s)}{ds} = - \frac{\partial \Pi_i}{\partial x_j}(\phi(s)) \frac{d^2 \phi_j(s)}{ds^2} = \frac{\partial \Pi_i}{\partial x_j}(\phi(s)) \Gamma^j_{rr} \frac{d\phi_r(s)}{ds} \frac{d\phi_r(s)}{ds},
\]
(165)
for \( 1 \leq i \leq d \), where \( \phi_j \) denotes the \( j \)-th component of \( \phi \), and the geodesic equation of the curve \( \phi \) has been used to obtain the last expression above. In particular, setting \( s = 0 \), we obtain
\[
\frac{\partial \Pi_i}{\partial x_j}(\sigma_{jl} - (P\sigma)_{jl}) = 0,
\]
\[
\frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(\sigma_{jl} - (P\sigma)_{jl})(\sigma_{rl} - (P\sigma)_{rl}) = \frac{\partial \Pi_i}{\partial x_j} \Gamma^j_{rr}(\sigma_{rl} - (P\sigma)_{rl})(\sigma_{rl} - (P\sigma)_{rl}).
\]
(166)
Combining the first equations in both (164) and (166), we can conclude that \( \frac{\partial \Pi_i}{\partial x_r} = P_{ij} \) at \( x \in \Sigma \). Since (166) holds at any \( x \in \Sigma \), taking the derivative in the first equation of (166) along the tangent vector \( p_t \in T_x \Sigma \), we obtain
\[
\frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(\sigma_{jl} - (P\sigma)_{jl})(\sigma_{rl} - (P\sigma)_{rl}) = - \frac{\partial \Pi_i}{\partial x_j}(P\sigma)_{rl} \frac{\partial(\sigma_{jl} - (P\sigma)_{jl})}{\partial x_r}.
\]
(167)
Combining (164), (166) and (167), using Lemma 3 in Appendix A, the expression in (140), the relations
\[
(P\sigma)_{jl}(P\sigma)_{rl} = (PaP^T)_{jr} = (Pa)_{jr},
\]
\[
(\sigma_{rl} - (P\sigma)_{rl})(\sigma_{rl} - (P\sigma)_{rl}) = a_{rr} - (Pa)_{rr},
\]
and the integration by parts formula, we can compute
\[
\frac{\partial^2 \Pi_i}{\partial x_j \partial x_r} \frac{\partial a_{jr}}{\partial x_r} = \frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(P\sigma + (\sigma - P\sigma))_{jl}(P\sigma + (\sigma - P\sigma))_{rl}
\]
\[
= \frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(P\sigma)_{jl}(P\sigma)_{rl} + 2 \frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(\sigma - P\sigma)_{jl}(P\sigma)_{rl} + \frac{\partial^2 \Pi_i}{\partial x_j \partial x_r}(\sigma - P\sigma)_{jl}(\sigma - P\sigma)_{rl}
\]
\[
= (P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} - P_{ij}(P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} - 2P_{ij}(P\sigma)_{rl} \frac{\partial(\sigma_{jl} - (P\sigma)_{jl})}{\partial x_r}
\]
\[
\quad + P_{ij} \Gamma^j_{rr}(\sigma_{rl} - (P\sigma)_{rl})(\sigma_{rl} - (P\sigma)_{rl})
\]
\[
= \left[ (P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} + P_{ij}(P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} - 2P_{ij}(P\sigma)_{rl} \frac{\partial(\sigma_{jl} - (P\sigma)_{jl})}{\partial x_r} \right] + P_{ij} \Gamma^j_{rr}(a_{rr} - (Pa)_{rr})
\]
\[
= \left[ 2(P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} - (P\sigma)_{jl}(P\sigma)_{rl} \frac{\partial P_{ij}}{\partial x_r} - 2(P\sigma)_{rl} \frac{\partial(P\sigma)_{jl}}{\partial x_r} + 2(P\sigma)_{rl} \sigma_{jl} \frac{\partial P_{ij}}{\partial x_r} \right]
\]
\[
\quad + (Pa)_{ij} \frac{\partial(a^{-1})_{jl}}{\partial x_r} (a_{rl} - (Pa)_{rl}) - \frac{1}{2} (Pa)_{ij} \frac{\partial(a^{-1})_{lr}}{\partial x_i} (a_{lr} - (Pa)_{lr})
\]
\[
= (Pa)_{ij} \frac{\partial P_{ij}}{\partial x_l} + \left[ -(Pa)_{ij} \frac{\partial P_{ij}}{\partial x_l} - (Pa)_{ij} \frac{\partial P_{ij}}{\partial x_j} + P_{ij} \frac{\partial (Pa)_{jl}}{\partial x_j} \right] + (Pa)_{ij} \frac{\partial P_{ij}}{\partial x_l} + \frac{1}{2} (Pa)_{ij} \frac{\partial \ln \det \Psi}{\partial x_j}
\]
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\[ -P_{ij} \frac{\partial a_{il}}{\partial x_l} + \frac{\partial (Pa)_{ij}}{\partial x_j} + \frac{1}{2}(Pa)_{ij} \frac{\partial \ln \det \Psi}{\partial x_j}. \]

References

[1] A. Abdulle, G. Vilmart, and K. Zygalakis. High order numerical approximation of the invariant measure of ergodic SDEs. *SIAM J. Numer. Anal.*, 52(4):1600–1622, 2014.

[2] L. Ambrosio and H. M. Soner. Level set approach to mean curvature flow in arbitrary codimension. *J. Differential Geom.*, 43(4):693–737, 1996.

[3] L. Ambrosio, N. Gigli, and G. Savaré. *Gradient Flows: In Metric Spaces And In The Space Of Probability Measures*. Lectures in Mathematics. Birkhäuser, 2005.

[4] D. Bakry and M. Émery. Hypercontractivité de semi-groupes de diffusion. *C. R. Math. Acad. Sci. Paris, Ser. I*, 299:775–778, 1984.

[5] A. Banyaga and D. Hurtubise. *Lectures on Morse Homology*. Texts in the Mathematical Sciences. Springer Netherlands, 2004.

[6] A. Bensoussan, J.-L. Lions, and G. Papanicolaou. *Asymptotic analysis for periodic structures*. Studies in mathematics and its applications. North-Holland, 1978.

[7] R. L. Bishop and R. J. Crittenden. *Geometry of Manifolds*. AMS/Chelsea Publication Series. American Mathematical Society, 1964.

[8] N. Bou-Rabee and H. Owhadi. Long-run accuracy of variational integrators in the stochastic context. *SIAM J. Numer. Anal.*, 48(1):278–297, 2010.

[9] M. Brubaker, M. Salzmann, and R. Urtasun. A family of MCMC methods on implicitly defined manifolds. In N. D. Lawrence and M. Girolami, editors, *Proceedings of the Fifteenth International Conference on Artificial Intelligence and Statistics*, volume 22 of *Proceedings of Machine Learning Research*, pages 161–172. PMLR, 2012.

[10] G. Ciccotti, R. Kapral, and E. Vanden-Eijnden. Blue moon sampling, vectorial reaction coordinates, and unbiased constrained dynamics. *ChemPhysChem*, 6(9):1809–1814, 2005.

[11] G. Ciccotti, T. Lelièvre, and E. Vanden-Eijden. Projection of diffusions on submanifolds: Application to mean force computation. *Commun. Pur. Appl. Math.*, 61(3):371–408, 2008.

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

[13] M. P. do Carmo. *Riemannian Geometry*. Mathematics (Boston, Mass.). Birkhäuser, 1992.

[14] W. E, B. Engquist, X. Li, W. Ren, and E. Vanden-Eijnden. Heterogeneous multiscale methods: A review. *Commun. Comput. Phys.*, 2(3):367–450, 2007.

[15] I. Fatkullin, G. Kovacic, and E. Vanden-Eijnden. Reduced dynamics of stochastically perturbed gradient flows. *Commun. Math. Sci.*, 8(2):439–461, 2010.
[16] G. Froyland, G. A. Gottwald, and A. Hammerlindl. A computational method to extract macroscopic variables and their dynamics in multiscale systems. *SIAM J. Appl. Dyn. Syst.*, 13(4):1816–1846, 2014.

[17] T. Funaki and H. Nagai. Degenerative convergence of diffusion process toward a submanifold by strong drift. *Stochastics and Stochastic Reports*, 44(1-2):1–25, 1993.

[18] M. Girolami and B. Calderhead. Riemann manifold Langevin and Hamiltonian Monte Carlo methods. *J. R. Stat. Soc. B.*, 73(2):123–214, 2011.

[19] D. Givon, R. Kupferman, and A. M. Stuart. Extracting macroscopic dynamics: model problems and algorithms. *Nonlinearity*, 17(6):R55–R127, 2004.

[20] I. Gyöngy. Mimicking the one-dimensional marginal distributions of processes having an Ito differential. *Probab. Th. Rel. Fields*, 71(4):501–516, 1986.

[21] C. Hartmann, C. Schütte, and W. Zhang. Jarzynski equality, fluctuation theorem, and variance reduction: Mathematical analysis and numerical algorithms. 2018. URL https://arXiv.org/abs/1803.09347

[22] E. P. Hsu. *Stochastic analysis on manifolds*. Graduate Studies in Mathematics. American Mathematical Society, 2002.

[23] J. Jost. *Riemannian Geometry and Geometric Analysis*. Universitext. Springer Berlin Heidelberg, 2008.

[24] G. S. Katzenberger. Solutions of a stochastic differential equation forced onto a manifold by a large drift. *Ann. Probab.*, 19(4):1587–1628, 1991.

[25] I. G. Kevrekidis and G. Samaey. Equation-free multiscale computation: Algorithms and applications. *Annu. Rev. Phys. Chem.*, 60(1):321–344, 2009.

[26] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G Kevrekidid, O. Runborg, and C. Theodoropoulos. Equation-free, coarse-grained multiscale computation: Enabling macroscopic simulators to perform system-level analysis. *Commun. Math. Sci.*, 1(4):715–762, 2003.

[27] I. G. Kevrekidis, C. W. Gear, and G. Hummer. Equation-free: The computer-aided analysis of complex multiscale systems. *AIChE J.*, 50(7):1346–1355, 2004.

[28] F. Legoll and T. Lelièvre. Effective dynamics using conditional expectations. *Nonlinearity*, 23(9):2131–2163, 2010.

[29] B. Leimkuhler and C. Matthews. Efficient molecular dynamics using geodesic integration and solvent–solute splitting. *Proc. Math. Phys. Eng. Sci.*, 472(2189), 2016.

[30] 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.

[31] T. Lelièvre and W. Zhang. Pathwise estimates for effective dynamics: the case of nonlinear vectorial reaction coordinates. 2018. URL https://arXiv.org/abs/1805.01928
[32] T. Lelièvre, M. Rousset, and G. Stoltz. *Free Energy Computations: A Mathematical Perspective*. Imperial College Press, 2010.

[33] T. Lelièvre, M. Rousset, and G. Stoltz. Langevin dynamics with constraints and computation of free energy differences. *Math Comput.*, 81(280):2071 – 2125, 2012.

[34] T. Lelièvre, M. Rousset, and G. Stoltz. Hybrid Monte Carlo methods for sampling probability measures on submanifolds. 2018. URL [https://arXiv.org/abs/1807.02356](https://arXiv.org/abs/1807.02356).

[35] J. S. Liu. *Monte Carlo Strategies in Scientific Computing*. Springer, first edition, 2008.

[36] A. J. Majda, C. Franzke, and B. Khouider. An applied mathematics perspective on stochastic modelling for climate. *Philos. Trans. R. Soc.*, A, 366(1875):2429–2455, 2008.

[37] L. Maragliano and E. Vanden-Eijnden. A temperature accelerated method for sampling free energy and determining reaction pathways in rare events simulations. *Chem. Phys. Lett.*, 426(13):168 – 175, 2006.

[38] 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.

[39] G. A. Pavliotis and A. M. Stuart. *Multiscale Methods: Averaging and Homogenization*. Texts in Applied Mathematics. Springer New York, 2008.

[40] K. B. Petersen and M. S. Pedersen. The Matrix Cookbook, 2012. URL [http://www2.imm.dtu.dk/pubdb/p.php?3274](http://www2.imm.dtu.dk/pubdb/p.php?3274). Version 20121115.

[41] P. Petersen. *Riemannian Geometry*. Graduate Texts in Mathematics. Springer New York, 2006.

[42] K. T. Sturm. Convex functionals of probability measures and nonlinear diffusions on manifolds. *J. Math. Pures Appl.*, 84(2):149 – 168, 2005.

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

[44] E. Vanden-Eijnden. Numerical techniques for multi-scale dynamical systems with stochastic effects. *Commun. Math. Sci.*, 1(2):385–391, 2003.

[45] E. Zappa, M. Holmes-Cerfon, and J. Goodman. Monte Carlo on Manifolds: Sampling Densities and Integrating Functions. *Commun. Pure Appl. Math.*, 71(12):2609–2647.

[46] W. Zhang, C. Hartmann, and C. Schütte. Effective dynamics along given reaction coordinates, and reaction rate theory. *Faraday Discuss.*, 195:365–394, 2016.