Riemannian Score-Based Generative Modelling

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Abstract

Score-based generative models (SGMs) are a powerful class of generative models that exhibit remarkable empirical performance. Score-based generative modelling (SGM) consists of a "noising" stage, whereby a diffusion is used to gradually add Gaussian noise to data, and a generative model, which entails a "denoising" process defined by approximating the time-reversal of the diffusion. Existing SGMs assume that data is supported on a Euclidean space, i.e. a manifold with flat geometry. In many domains such as robotics, geoscience or protein modelling, data is often naturally described by distributions living on Riemannian manifolds and current SGM techniques are not appropriate. We introduce here *Riemannian Score-based Generative Models* (RSGMs), a class of generative models extending SGMs to Riemannian manifolds. We demonstrate our approach on a variety of manifolds, and in particular with earth and climate science spherical data.

1 Introduction

Score-based Generative Models (SGMs) also called diffusion models (Song and Ermon, 2019; Song et al., 2021; Ho et al., 2020; Dhariwal and Nichol, 2021) formulate generative modelling as a denoising process. Noise is incrementally added to data using a diffusion process until it becomes approximately Gaussian. The generative model is then obtained by simulating an approximation of the corresponding time-reversal process, which progressively denoises a Gaussian sample to obtain a data sample. This process is also a diffusion whose drift depends on the logarithmic gradients of the noised data densities, i.e. the Stein scores, estimated using a neural network via score matching (Hyvärinen, 2005; Vincent, 2011).

SGMs have been primarily applied to data living on Euclidean spaces, i.e. manifolds with flat geometry. However, in a large number of scientific domains the distributions of interest are supported on Riemannian manifolds. These include, to name a few, protein modelling (Shapovalov and Dunbrack Jr, 2011), cell development (Klimovskaia et al., 2020), image recognition (Lui, 2012), geological sciences (Karpatne et al., 2018; Peel et al., 2001), graph-structured and hierarchical data (Roy et al., 2007; Steyvers and Tenenbaum, 2005), robotics (Feiten et al., 2013; Senanayake and Ramos, 2018) and high-energy physics (Brehmer and Cranmer, 2020).

We introduce in this work *Riemannian Score-based Generative Models* (RSGMs), an extension of SGMs to Riemannian manifolds which incorporate the geometry of the data by defining the forward diffusion process directly on the Riemannian manifold, inducing a manifold-valued reverse process. This requires constructing a noising process on the manifold that converges to an easy-to-sample reference distribution. We establish that, as in the Euclidean case, the corresponding time-reversal process is also a diffusion whose drift includes the Stein score which is intractable but can similarly be estimated via score matching. Methodological extensions are required as in most cases the transition kernel of the noising process cannot be sampled exactly. For example on compact manifolds it is

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typically only available as an infinite sum through the Sturm–Liouville decomposition (Chavel, 1984). To this end, we develop non-standard techniques for score estimation and rely on the use of Geodesic Random Walks for sampling (Jørgensen, 1975). We provide theoretical convergence bounds for RSGMs on compact manifolds and demonstrate our approach on a range of manifolds and tasks, including modelling a number of natural disaster occurrence datasets collected by Mathieu and Nickel (2020). We show that RGSMs achieve better performance than recent baselines (Mathieu and Nickel, 2020; Rozen et al., 2021) and scale better to high-dimensional manifolds.

2 Euclidean Score-based Generative Modelling

We recall here briefly the key concepts behind SGMs on the Euclidean space $\mathbb{R}^d$ and refer the readers to Song et al. (2021) for a more detailed introduction. We consider a forward *noising* process $(\mathbf{X}_t)_{t\geq 0}$ defined by the following Stochastic Differential Equation (SDE)

$$\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t \mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t, \quad \mathbf{X}_0 \sim p_0, \tag{1}$$

where $(\mathbf{B}_t)_{t\geq 0}$ is a d-dimensional Brownian motion and p_0 is the data distribution. The available data gives us an empirical approximation of p_0. The process $(\mathbf{X}_t)_{t\geq 0}$ is simply an Ornstein–Ulhenbeck (OU) process which converges with geometric rate to $\mathrm{N}(0, \mathrm{Id})$. Under mild conditions on p_0, the time-reversed process $(\mathbf{Y}_t)_{t\geq 0} = (\mathbf{X}_{T-t})_{t\in[0,T]}$ also satisfies an SDE (Cattiaux et al., 2021; Haussmann and Pardoux, 1986) given by

$$\mathrm{d}\mathbf{Y}_t = \{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t, \quad \mathbf{Y}_0 \sim p_T, \tag{2}$$

where p_t denotes the density of $\mathbf{X}_t$. By construction, the law of $\mathbf{Y}_{T-t}$ is equal to the law of $\mathbf{X}_t$ for $t \in [0, T]$ and in particular $\mathbf{Y}_T \sim p_0$. Hence, if one could sample from $(\mathbf{Y}_t)_{t\in[0,T]}$ then its final distribution would be the data distribution p_0. Unfortunately we cannot sample exactly from (2) as p_T and the scores $(\nabla \log p_t(x))_{t\in[0,T]}$ are intractable. Hence SGMs rely on a few approximations. First, p_T is replaced by the reference distribution $\mathrm{N}(0, \mathrm{Id})$ as we know that p_T converges geometrically towards it. Second, the following denoising score matching identity is exploited to estimate the scores

$$\nabla_{x_t} \log p_t(x_t) = \int_{\mathbb{R}^d} \nabla_{x_t} \log p_{t|0}(x_t|x_0)\, p_{0|t}(x_0|x_t)\mathrm{d}x_0,$$

where $p_{t|0}(x_t|x_0)$ is the transition density of the OU process (1) which is available in closed-form. It follows directly that $\nabla \log p_t$ is the minimizer of $\ell_t(\mathbf{s}) = \mathbb{E}[\|\mathbf{s}(\mathbf{X}_t) - \nabla_{x_t} \log p_{t|0}(\mathbf{X}_t|\mathbf{X}_0)\|^2]$ over functions $\mathbf{s}$ where the expectation is over the joint distribution of $\mathbf{X}_0, \mathbf{X}_t$. This result can be leveraged by considering a neural network $\mathbf{s}_\theta : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d$ trained by minimizing the loss function $\ell(\theta) = \int_0^T \lambda_t \ell_t(\mathbf{s}_\theta(t, \cdot))\mathrm{d}t$ for some weighting function $\lambda_t > 0$. Finally, an Euler–Maruyama discretization of (2) is performed using a discretization step γ such that $T = \gamma N$ for $N \in \mathbb{N}$

$$Y_{n+1} = Y_n + \gamma\{Y_n + 2\mathbf{s}_\theta(T - n\gamma, Y_n)\} + \sqrt{2\gamma} Z_{n+1}, \quad Y_0 \sim \mathrm{N}(0, \mathrm{Id}), \quad Z_n \overset{\text{i.i.d.}}{\sim} \mathrm{N}(0, \mathrm{Id}).$$

The above showcases the basics of SGMs but we highlight that many improvements have been proposed; see (e.g. Song and Ermon, 2020; Jolicoeur-Martineau et al., 2021; Dhariwal and Nichol, 2021). In particular, selecting an adaptive stepsize $(\gamma_n)_{n\in\mathbb{N}}$ (Bao et al., 2022; Watson et al., 2021) and using a predictor-corrector scheme (Song et al., 2021) instead of a simple Euler–Maruyama discretization drastically improves performance.

3 Riemannian Score-based Generative Modelling

We now move to the Riemannian manifold setting, and more specifically assume that $\mathcal{M}$ is a complete, orientable connected and boundaryless Riemannian manifold, endowed with a Riemannian metric g [4]. Four components are required to extend SGMs to this setting: i) a forward *noising* process on $\mathcal{M}$ which converges to an easy-to-sample reference distribution, ii) a time-reversal formula on $\mathcal{M}$ which defines a backward generative process, iii) a method for approximating samples of SDEs on manifolds, iv) a method to efficiently approximate the drift of the time-reversal process. Notation are gathered in **??**.

[4] Metrics g are sections of $\mathrm{T}^*\mathcal{M} \otimes \mathrm{T}^*\mathcal{M}$, the rank 2 tensor bundle of the dual tangent space, i.e. smooth varying bilinear maps on $\mathrm{T}\mathcal{M}$, verifying symmetry and positive semi-definiteness.

3.1 Noising processes on manifolds

The first necessary component is a suitable generic noising process on manifolds that will converge to a convenient stationary distribution. A simple choice is to use Langevin dynamics described by

$$\mathrm{d}\mathbf{X}_t = -\tfrac{1}{2}\,\nabla_{\mathbf{X}_t} U(\mathbf{X}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}, \tag{3}$$

which admits the invariant density (w.r.t. the volume form) given by $\mathrm{d}p_{\text{ref}}/\mathrm{dVol}_{\mathcal{M}}(x) \propto \mathrm{e}^{-U(x)}$ (Durmus, 2016, Section 2.4), where ∇ is the Riemannian gradient[5].

Two simple choices for $U(x)$ present themselves. Firstly, setting $U(x) = d_{\mathcal{M}}(x,\mu)^2/(2\gamma^2)$, where $d_{\mathcal{M}}$ is the geodesic distance and $\mu \in \mathcal{M}$ is an arbitrary mean location, induces the drift $\nabla_{\mathbf{X}_t} U(\mathbf{X}_t) = -\exp_{\mathbf{X}_t}^{-1}(\mu)/\gamma^2$ [6]. This is the potential of the 'Riemannian normal' (Pennec, 2006) distribution, from which it is in general neither trivial to sample nor to compute the normalisation constant (Hauberg, 2018; Mathieu et al., 2019). An alternative is to target the 'exponential wrapped' Gaussian. This is the pushforward of a Gaussian distribution in the tangent space at the mean location along the exponential map. The potential is given by $U(x) = d_{\mathcal{M}}(x,\mu)^2/(2\gamma^2) + \log|\partial \exp_{\mu}^{-1}(x)|$[7]. In contrast to the Riemannian normal, sampling and evaluating the density of this distribution is easy.

One recovers the standard Ornstein–Uhlenbeck noising process (Song et al., 2021) for both of these target distributions when $\mathcal{M} = \mathbb{R}^d$ and $\mu = 0$ since then the drift $b(t,\mathbf{X}_t) = \frac{1}{2}\,\exp_{\mathbf{X}_t}^{-1}(0) = -\frac{1}{2}\,\mathbf{X}_t$. On compact manifolds, the invariant measure $\mathrm{Vol}_{\mathcal{M}}$ has finite volume, thus a natural choice is to target the uniform distribution which is given by $\mathrm{Vol}_{\mathcal{M}}/|\mathcal{M}|$. In this case, $\nabla_{\mathbf{X}_t} U(\mathbf{X}_t) = 0$ and the noising process is simply a Brownian motion on $\mathcal{M}$.

3.2 Time-reversal on Riemannian manifolds

In order to use these noising processes we prove the time-reversal formula for manifolds, a generalisation of the results in the Euclidean case, e.g. see Cattiaux et al. (2021, Theorem 4.9). Consider an SDE of the form $\mathrm{d}\mathbf{X}_t = b(\mathbf{X}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$ where $\mathbf{B}_t^{\mathcal{M}}$ is a Brownian motion on $\mathcal{M}$. We refer to App. B.3 for an introduction to Brownian motions on manifolds. This result shows that if $(\mathbf{X}_t)_{t\in[0,T]}$ is a diffusion process then $(\mathbf{X}_{T-t})_{t\in[0,T]}$ is also a diffusion process w.r.t. the backward filtration whose coefficients can be computed, and are shown in Eq. (4). The proof relies on an extension of Cattiaux et al. (2021, Theorem 4.9) to the Riemannian manifold case and is postponed to App. G.

Theorem 1 (Time-reversed diffusion)**.** *Let $T \geq 0$ and $(\mathbf{B}_t^{\mathcal{M}})_{t\geq 0}$ be a Brownian motion on $\mathcal{M}$ such that $\mathbf{B}_0^{\mathcal{M}}$ has distribution the volume form p_{ref}*[8]*. Let $(\mathbf{X}_t)_{t\in[0,T]}$ be associated with the SDE $\mathrm{d}\mathbf{X}_t = b(\mathbf{X}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$. Let $(\mathbf{Y}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$ and assume that $\mathrm{KL}(\mathbb{P}|\mathbb{Q}) < +\infty$, where $\mathbb{Q}$ is the distribution of $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ and $\mathbb{P}$ the distribution of $(\mathbf{X}_t)_{t\in[0,T]}$. In addition, assume that $\mathbb{P}_t = \mathcal{L}(\mathbf{X}_t)$, the distribution of $\mathbf{X}_t$, admits a smooth positive density p_t w.r.t. p_{ref} for any $t \in [0,T]$. Then, $(\mathbf{Y}_t)_{t\in[0,T]}$ is associated with the SDE*

$$\mathrm{d}\mathbf{Y}_t = \{-b(\mathbf{Y}_t) + \nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}. \tag{4}$$

3.3 Approximate sampling of diffusions

Obtaining samples from SDEs on a manifold is non-trivial in general. If $\mathcal{M}$ is isometrically embedded into $\mathbb{R}^p$ (with $p \geq d$) one can define $(\mathbf{B}_t^{\mathcal{M}})_{t\geq 0}$ as a $\mathbb{R}^p$-valued process, see App. B.3. However, this approach is *extrinsic*, as it requires the knowledge of the projection operator to place points back on the manifold at each step which can accumulate errors. Here we consider an *intrisic* approach based on Geodesic Random Walks (GRWs), see Jørgensen (1975) for a review of their properties. GRWs can approximate *any* well-behaved diffusion on $\mathcal{M}$. Hence, we introduce GRWs in a general framework and consider a discrete-time process $(X_n^{\gamma})_{n\in\mathbb{N}}$ which approximates the diffusion $(\mathbf{X}_t)_{t\geq 0}$ defined by

$$\mathrm{d}\mathbf{X}_t = b(t,\mathbf{X}_t)\mathrm{d}t + \sigma(t,\mathbf{X}_t)\mathrm{d}\mathbf{B}_t^{\mathcal{M}}. \tag{5}$$

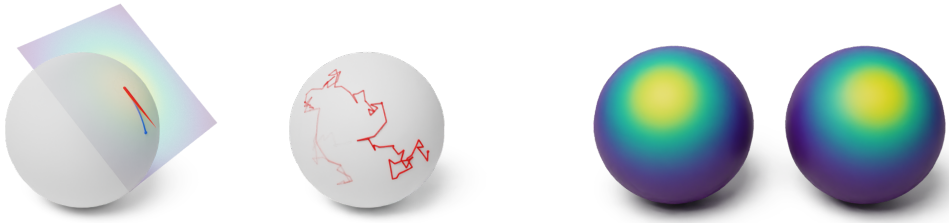
This generalisation is key to sampling the backward diffusion process defined in Theorem 1.

[5] The (Riemannian) gradient ∇ is defined s.t. for any $f : \mathcal{M} \to \mathbb{R}$, $x \in \mathcal{M}$, $v \in \mathrm{T}_x\mathcal{M}$, $\langle \nabla f, v\rangle_g = \mathrm{d}f(v)$.

[6] $\exp_x : \mathrm{T}_x\mathcal{M} \to \mathcal{M}$ denotes the exponential mapping on the manifold, see e.g. Lee (2013, Chapter 20).

[7] $|\cdot|$ denotes the absolute value of the determinant, and ∂f the Jacobian of f.

[8] Note that in the case of a non-compact manifold p_{ref} is only a measure and not a probability measure.



(a) A single step of a Geodesic Random Walk.

(b) Many steps yield an approximate Brownian motion trajectory.

(c) The density of a single step of Gaussian Random Walk [Left] and the Brownian motion density [Right] agree well for small time steps.

Figure 1: Geodesic Random Walks can be used to approximate Brownian motion and more generally SDEs on manifolds. (a) At each step, tangential noise is sampled (red), which is added the drift term (not pictured). This tangent vector is then pushed through the exponential map to produce a geodesics step on the manifold (blue). (b) Iterating this procedure yield approximate sample paths from the process.

Algorithm 1 GRW (Geodesic Random Walk)

Require: $T, N, X_0^\gamma, b, \sigma, \mathrm{P}$

$\gamma = T/N$ ▷ Step-size

for $k \in \{0, \dots, N-1\}$ **do**

  $Z_{k+1} \sim \mathrm{N}(0, \mathrm{Id})$ ▷ Sample a Gaussian in the tangent space of X_k^γ

  $W_{k+1} = \gamma b(k\gamma, X_k^\gamma) + \sqrt{\gamma}\sigma(k\gamma, X_k^\gamma) Z_{k+1}$ ▷ Compute the Euler–Maruyama step on tangent space

  $X_{k+1}^\gamma = \exp_{X_k^\gamma}[W_{k+1}]$ ▷ Move along the geodesic defined by W_{k+1} and X_k^γ on $\mathcal{M}$

end for

return $\{X_k^\gamma\}_{k=0}^N$

Definition 2 (Geodesic Random Walk)**.** *Let X_0^γ be a $\mathcal{M}$-valued random variable. For any $\gamma > 0$, we define $(X_n^\gamma)_{n\in\mathbb{N}}$ such that for any $n \in \mathbb{N}$, $X_{n+1}^\gamma = \exp_{X_n^\gamma}[\gamma\{b(X_n^\gamma) + \sqrt{\gamma}V_{n+1}\}]$, where $(V_n)_{n\in\mathbb{N}}$ is a sequence of $\mathrm{T}\mathcal{M}$-valued random variables such that for any $n \in \mathbb{N}$, $\mathbb{E}[V_{n+1}|\mathcal{F}_n] = 0$ and $\mathbb{E}[V_{n+1}V_{n+1}^\top|\mathcal{F}_n] = \sigma\sigma^\top(X_n^\gamma)$, where $\mathcal{F}_n$ is the filtration generated by $\{X_k^\gamma\}_{k=0}^n$. We say that the $\mathcal{M}$-valued process $(X_n^\gamma)_{n\in\mathbb{N}}$ is a Geodesic Random Walk.*

Algorithm 1 approximately simulates the diffusion $(\mathbf{X}_t)_{t\in[0,T]}$ defined in Eq. (5) using GRWs; see Kuwada (2012); Cheng et al. (2022) for quantitative error bounds in the time-homogeneous case and App. H.2 for a novel extentsion for the time-inhomogeneous case. Fig. 1 provides a graphical illustration of this procedure.

3.4 Score approximation on Riemannian manifolds

Score matching and loss functions. The reverse process from Eq. (4) involves the Stein score $\nabla \log p_t$ which is unfortunately intractable. To derive an approximation, we first remark that for any $s, t \in (0, T]$ with $t > s$ and $x_t \in \mathcal{M}$, $p_t(x_t) = \int_{\mathcal{M}} p_{t|s}(x_t|x_s)\mathrm{d}\mathbb{P}_s(x_s)$, where $\mathbb{P}_s = \mathcal{L}(\mathbf{X}_s)$, the distribution of $\mathbf{X}_s$. Thus, we have that for any $s, t \in [0, T]$ with $t > s$ and $x_t \in \mathcal{M}$

$$\nabla_{x_t} \log p_t(x_t) = \int_{\mathcal{M}} \nabla_{x_t} \log p_{t|s}(x_t|x_s)\mathbb{P}_{s|t}(x_t, \mathrm{d}x_s).$$

Hence, for any $s, t \in [0, T]$ with $t > s$ we have that $\nabla \log p_t = \arg\min\{\ell_{t|s}(\mathbf{s}_t) \,:\, \mathbf{s}_t \in \mathrm{L}^2(\mathbb{P}_t)\}$,

where $\ell_{t|s}(\mathbf{s}_t) = \int_{\mathcal{M}^2} \|\nabla_x \log p_{t|s}(x_t|x_s) - \mathbf{s}_t(x_t)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t)$, which is referred as the Denoising Score Matching (DSM) loss. It can also be written in an *implicit* fashion.

Proposition 3. *Let $t, s \in (0, T]$ with $t > s$. Then, for any $\mathbf{s}_t \in \mathrm{C}^\infty(\mathcal{M})$, $\ell_{t|s}(\mathbf{s}_t) = 2\ell_t^{\mathrm{im}}(\mathbf{s}_t) + \int_{\mathcal{M}^2} \|\nabla_{x_t} \log p_{t|s}(x_t|x_s)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t)$, where $\ell_t^{\mathrm{im}}(\mathbf{s}_t) = \int_{\mathcal{M}} \{\frac{1}{2}\|\mathbf{s}_t(x_t)\|^2 + \mathrm{div}(\mathbf{s}_t)(x_t)\}\mathrm{d}\mathbb{P}_t(x_t)$.*

The proof is postponed to App. I. For any $t \in (0, T]$ the minimizers of the loss ℓ_t^{im} on $\mathcal{X}(\mathcal{M})$ (where $\mathcal{X}(\mathcal{M})$ is the set of vector fields on $\mathcal{M}$) are the same as the ones for $\ell_{t|s}$. The loss ℓ_t^{im} is referred to as the *implicit* score matching (ISM) loss (Hyvärinen, 2005). These losses are direct analogous to the versions typically used in Euclidean space.

In the case where we have access to $\{\nabla \log p_{t|s} \,:\, T \leq t > s \geq 0\}$, the forward noising process transition kernels, or an approximation of this family, then we can use the DSM loss to learn

Algorithm 2 RSGM (Riemannian Score-Based Generative Model)

Require: $\varepsilon, T, N, \{X_0^m\}_{m=1}^M, \mathrm{loss}, \mathbf{s}, \theta_0, N_{\text{iter}}, p_{\text{ref}}, \mathrm{P}$

/// TRAINING ///
for $n \in \{0, \dots, N_{\text{iter}} - 1\}$ **do**
  $X_0 \sim (1/M) \sum_{m=1}^M \delta_{X_0^m}$ ▷ Random mini-batch from dataset
  $t \sim U([\varepsilon, T])$ ▷ Uniform sampling between ε and T
  $\mathbf{X}_t = \mathrm{GRW}(t, N, X_0, b, \mathrm{Id}, \mathrm{P})$ ▷ Approximate forward diffusion with Algorithm 1
  $\ell(\theta_n) = \ell_t(T, N, X_0, \mathbf{X}_t, \mathrm{loss}, \mathbf{s}_{\theta_n})$ ▷ Compute score matching loss from Table 2
  $\theta_{n+1} = \texttt{optimizer_update}(\theta_n, \ell(\theta_n))$ ▷ ADAM optimizer step
end for
$\theta^\star = \theta_{N_{\text{epoch}}}$
/// SAMPLING ///
$Y_0 \sim p_{\text{ref}}$ ▷ Sample from uniform distribution
$b_\theta^\star(t, x) = \mathbf{s}_{\theta^\star}(T - t, x)$ for any $t \in [0, T]$, $x \in \mathcal{M}$ ▷ Reverse process drift
$\{Y_k\}_{k=0}^N = \mathrm{GRW}(T, N, Y_0, b_{\theta^\star}, \mathrm{Id}, \mathrm{P})$ ▷ Approximate reverse diffusion with Algorithm 1
return $\theta^\star, \{Y_k\}_{k=0}^N$

Table 1: Differences between SGM on Euclidean spaces and RSGM on Riemannian manifolds.

Ingredient \ Space	Euclidean	'Generic' Manifold	Compact Manifold
Forward process $\mathrm{d}\mathbf{X}_t =$	$-\frac{1}{2}\mathbf{X}_t \mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$	$-\frac{1}{2}\nabla_{\mathbf{X}_t} U(\mathbf{X}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$	$\mathrm{d}\mathbf{B}_t^{\mathcal{M}}$
Easy-to-sample distribution	Gaussian	Wrapped Gaussian	Uniform
Time reversal	Cattiaux et al. (2021)	Theorem 1	
Sampling forward process	Direct	Geodesic Random Walk (Algorithm 1)	
Sampling backward process	Euler–Maruyama	Geodesic Random Walk (Algorithm 1)	

$\{\mathbf{s}_t \in \mathcal{X}(\mathcal{M}) \ : \ t \in [0, t]\}$. If this is not the case then we turn to ℓ_t^{im}. Note that ℓ_t^{im} requires the computation of a divergence term which requires d Jacobian-vector calls. In high dimension, a stochastic estimator is necessary (Hutchinson, 1989). Following Song and Ermon (2020); Nichol and Dhariwal (2021) the loss can be weighted with a term $\lambda_t > 0$.

Parametric family of vector fields. We approximate $(\nabla \log p_t)_{t \in [0,T]}$ by a family of functions $\{\mathbf{s}_\theta\}_{\theta \in \Theta}$ where Θ is a set of parameters and $\mathbf{s}_\theta : [0, T] \to \mathcal{X}(\mathcal{M})$. In a Euclidean space, vector fields are simply functions $\mathbf{s}_\theta : \mathbb{R}^d \to \mathbb{R}^d$. In manifolds, although for any $x \in \mathcal{M}$, $\mathrm{T}_x\mathcal{M} \cong \mathbb{R}^d$, there does not necessarily exist a set of d smooth vector fields $\{E_i\}_{i=1}^d$ such that span $\left(\{E_i(x)\}_{i=1}^d\right) = \mathrm{T}_x\mathcal{M}$ (Chapter 8, page 179, Lee, 2006) [9]. Fortunately, one can rely on a larger set of smooth vector fields $\{E_i(x)\}_{i=1}^n$ with $n > d$ that *does* span the tangent bundle. Then it suffices to construct a neural network $\mathbf{s}_\theta : [0, T] \times \mathcal{M} \to \mathbb{R}^n$ to parametrize the score network as $\mathbf{s}_\theta(t, x) = \sum_{i=1}^n \mathbf{s}_\theta^i(t, x) E_i(x)$. See App. D for a discussion on the different choices of generating sets $\{E_i(x)\}_{i=1}^n$.

Combining this parameterization with the score matching losses, the time-reversal formula of Theorem 1 and the sampling of forward and backward processes described in Sec. 3.3, we define our RGSM algorithm in Algorithm 2. This algorithm can also benefit from a predictor-corrector scheme as in (Song et al., 2021), see App. F.

4 RSGMs on compact manifolds

Assuming compactness of the manifold $\mathcal{M}$, we can leverage a number of special properties to implement a specific case of our algorithm. In particular we benefit from the fact that on compact manifolds we have a proper *uniform* distribution over the manifold, and have access to a variety of approximations of the heat kernel. As highlighted in Sec. 3.1, in the compact setting we use Brownian motion as the noising SDE, which targets the uniform distribution as the stationary distribution. Table 1 highlights the main differences between RSGMs on compact manifolds, generic manifolds and Euclidean score-based models.

[9] Manifolds for which there exists such a *global frame* $\{E_i(x)\}_{i=1}^d$ are referred as *parallelizable*. $\mathbb{S}^2$ is a well-known example of *non-parallelizable* manifold as per the *Hairy ball theorem*.

Heat kernel on compact Riemannian manifolds. For any $x_0 \in \mathcal{M}$ and $t \geq s \geq 0$, the heat kernel $p_{t|s}(\cdot|x_s)$ is defined as the density of $\mathbf{B}_t^{\mathcal{M}}$ w.r.t. the uniform measure on the manifold.

Contrary to the Gaussian transition density of the OU process (or the Brownian motion) in the Euclidean setting, it is typically only available as an infinite series. In order to circumvent this issue we consider two techniques: i) a truncation approach, ii) a Taylor expansion around $t = 0$ called a Varadhan asymptotics. First, we recall that in the case of compact manifolds the heat kernel is given by the Sturm–Liouville decomposition (Chavel, 1984) given for any $t > 0$ and $x_0, x_t \in \mathcal{M}$ by

$$p_{t|0}(x_t|x_0) = \sum_{j\in\mathbb{N}} \mathrm{e}^{-\lambda_j t}\phi_j(x_0)\phi_j(x_t), \tag{6}$$

where the convergence occurs in $\mathrm{L}^2(p_{\text{ref}} \otimes p_{\text{ref}})$, $(\lambda_j)_{j\in\mathbb{N}}$ and $(\phi_j)_{j\in\mathbb{N}}$ are the eigenvalues, respectively the eigenvectors, of $-\Delta_{\mathcal{M}}$, the Laplace-Beltrami operator in the manifold, in $\mathrm{L}^2(p_{\text{ref}})$ (see Saloff-Coste, 1994, Section 2). When the eigenvalues and eigenvectors are known, we rely on an approximation of the logarithmic gradient of $p_{t|0}$ by truncating the sum in Eq. (S8) with $J \in \mathbb{N}$ terms to obtain for any $t > 0$ and $x_0, x_t \in \mathcal{M}$

$$\nabla_{x_t} \log p_{t|0}(x_t|x_0) \approx S_{J,t}(x_0, x_t) \triangleq \nabla_{x_t} \log \sum_{j=0}^{J} \mathrm{e}^{-\lambda_j t}\phi_j(x_0)\phi_j(x_t). \tag{7}$$

Under regularity conditions on $\mathcal{M}$ it can be shown that for any $x, y \in \mathcal{M}$ and $t \geq 0$, $\lim_{J\to+\infty} S_{J,t}(x_0, x_t) = \nabla_{x_t} \log p_{t|0}(x_t|x_0)$ (see Jones et al., 2008, Lemma 1). In the case of the d-dimensional torus or sphere the eigenvalues and eigenvectors are computable (see Saloff-Coste, 1994, Section 2) and we can apply this method to approximate $p_{t|0}$ for any $t > 0$, see App. E

When the eigenvalues and eigenvectors are unknown or not tractable, we can still derive an approximation of the heat kernel for small times t. Using Varadhan's asymptotics—see Bismut (1984, Theorem 3.8) or Chen et al. (2021, Theorem 2.1)—for any $x, y \in \mathcal{M}$ with $y \notin \mathrm{Cut}(x)$ (where $\mathrm{Cut}(x)$ is the cut-locus of x in $\mathcal{M}$ (see Lee, 2018, Chapter 10)) we have that

$$\lim_{t\to 0} t\nabla_{x_t} \log p_{t|0}(x_t|x_0) = \exp_{x_t}^{-1}(x_0). \tag{8}$$

Using the previously defined score-matching losses and the approximations to the heat kernel above, we highlight three methods to compute $\nabla \log p_t$ in Table 2.

Table 2: Computational complexity of score matching losses w.r.t. score network forward and backward passes. ε is a random variable on $\mathrm{T}_{\mathbf{X}_t}\mathcal{M}$ such that $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{E}[\varepsilon\varepsilon^\top] = \mathrm{Id}$.

Loss	Approximation	Loss function	Requirements $p_{t\|0}$	Requirements $\exp_{\mathbf{X}_t}^{-1}$	Complexity
$\ell_{t\|0}$ (DSM)	None	$\frac{1}{2}\mathbb{E}\left[\|\mathbf{s}(\mathbf{X}_t) - \nabla \log p_{t\|0}(\mathbf{X}_t\|\mathbf{X}_0)\|^2\right]$	✓	✗	$\mathcal{O}(1)$
	Truncation (7)	$\frac{1}{2}\mathbb{E}\left[\|\mathbf{s}(\mathbf{X}_t) - S_{J,t}(\mathbf{X}_0, \mathbf{X}_t)\|^2\right]$	asymptotic expansion	✗	$\mathcal{O}(1)$
	Varhadan (8)	$\frac{1}{2}\mathbb{E}\left[\|\mathbf{s}(\mathbf{X}_t) - \exp_{\mathbf{X}_t}^{-1}(\mathbf{X}_0)/t\|^2\right]$	✗	✓	$\mathcal{O}(1)$
$\ell_{t\|s}$ (DSM)	Varhadan (8)	$\frac{1}{2}\mathbb{E}\left[\|\mathbf{s}(\mathbf{X}_t) - \exp_{\mathbf{X}_t}^{-1}(\mathbf{X}_s)/(t-s)\|^2\right]$	✗	✓	$\mathcal{O}(1)$
ℓ_t^{im} (ISM)	Deterministic	$\mathbb{E}\left[\frac{1}{2}\|\mathbf{s}(\mathbf{X}_t)\|^2 + \mathrm{div}(\mathbf{s})(\mathbf{X}_t)\right]$	✗	✗	$\mathcal{O}(d)$
	Stochastic	$\mathbb{E}\left[\frac{1}{2}\|\mathbf{s}(\mathbf{X}_t)\|^2 + \varepsilon^\top \partial\mathbf{s}(\mathbf{X}_t)\varepsilon\right]$	✗	✗	$\mathcal{O}(1)$

Convergence results in the compact setting We now provide a theoretical analysis of RSGM under the assumption that $\mathcal{M}$ is compact. The following result ensures that RSGM generates samples whose distribution is close to the data distribution p_0. Let us denote $\{Y_k\}_{n\in\{0,\dots,N\}}$ the sequence generated by Algorithm 2. This result relies on the following assumption, which is satisfied for a large class of manifolds $\mathcal{M}$ such as the d-dimensional sphere and torus, compact matrix groups and products of these manifolds.

A1. *There exist $C, \alpha > 0$ such that for any $t \in (0, 1]$ and $x \in \mathcal{M}$, $p_{t|0}(x|x) \leq Ct^{-\alpha/2}$, where $p_{t|0}(\cdot|x_0)$ is the density of the heat kernel, i.e. the density of $\mathbf{B}_t^{\mathcal{M}}$ with initial condition x_0* [10].

[10] The diagonal upper-bound is implied by Sobolev inequalities which control of the growth of some functions by the growth of their gradient. **A1** is satisfied in our experiments, see Saloff-Coste (1994); Gross (1992).

Theorem 4. *Assume* **A**1*, that* p_0 *is smooth and positive and that there exists* $\mathtt{M} \geq 0$ *such that for any* $t \in [0, T]$ *and* $x \in \mathcal{M}$*,* $\|\mathbf{s}_{\theta^\star}(t, x) - \nabla \log p_t(x)\| \leq \mathtt{M}$*, with* $\mathbf{s}_{\theta^\star} \in \mathrm{C}([0, T], \mathcal{X}(\mathcal{M}))$*. Then if* $T > 1/2$*, there exists* $C \geq 0$ *independent on* T *such that*

$$\mathbf{W}_1(\mathcal{L}(Y_N), p_0) = C(\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathtt{M} + \mathrm{e}^T \gamma^{1/2}),$$

where $\mathbf{W}_1$ *is the Wasserstein distance of order one on the probability measures on* $\mathcal{M}$*.*

The proof is postponed to App. H. In particular, for any $\varepsilon > 0$, choosing $T > 0$ large enough, $\mathtt{M}$ small enough (which can be achieved using the universal property of neural networks) and γ small enough, we get that $\mathbf{W}_1(\mathcal{L}(Y_N), p_0) \leq \varepsilon$. This result might seem weaker than the result obtained for Moser flows in (Rozen et al., 2021, Theorem 3), but we emphasize that our bound takes into account the time-discretization contrary to Rozen et al. (2021) which considers the continuous-time flow. If we consider the time-reversed continuous-time SDE then we recover a bound in total variation distance, see App. H. Note that the upper bound $\mathtt{M}$ encompasses both the bias introduced by the use of a neural network and the bias introduced by the use of an approximation of the score.

5 Related work

In this section we discuss previous work on parametrizing family of distributions for manifold-valued data. Here, the manifold structure is considered to be prescribed, in contrast with methods that jointly learn the manifold structure and density (e.g. Brehmer and Cranmer, 2020; Caterini et al., 2021).

Parametric family of distributions. The various parametric families of manifold-valued distributions that have been proposed can be categorized into three main approaches (Navarro et al., 2017): wrapping, projecting and conditioning. Wrapped distributions consider a parametric distribution on $\mathbb{R}^n$ that is pushed-forward along a surjective map $\psi : \mathbb{R}^n \to \mathcal{M}$. Projected distributions are defined by marginalizing out some distribution along the normal bundle of $\mathcal{M}$. Conditioning distributions encompass the von Mises-Fisher and Kent distributions (Fisher, 1953; Kent, 1982). Considering mixtures of these distributions is key to increase flexibility (Peel et al., 2001; Mardia et al., 2008).

Push-forward of Euclidean normalizing flows. More recently, approaches leveraging the flexibility of normalizing flows (Papamakarios et al., 2019) have been proposed. Following the wrapping method described above, these methods parametrize a normalizing flow in $\mathbb{R}^n$ before being pushed along an invertible map $\psi : \mathbb{R}^n \to \mathcal{M}$. However, to globally represent the manifold, the map ψ needs to be a homeomorphism, which can only happen if $\mathcal{M}$ is topologically equivalent to $\mathbb{R}^n$, hence limiting the scope of that approach. One natural choice for this map is the exponential map $\exp_x : \mathrm{T}_x\mathcal{M} \cong \mathbb{R}^d$. This approach has been taken, for instance, by Falorsi et al. (2019) and Bose et al. (2020), respectively parametrizing distributions on Lie groups and hyperbolic space.

Neural ODE on manifolds. To avoid artifacts or numerical instabilities due to the manifold embedding, another line of work uses tools from Riemannian geometry to define flows directly on the manifold of interest (Falorsi and Forré, 2020; Mathieu and Nickel, 2020; Falorsi, 2021). Since these methods do not require a specific embedding mapping, they are referred as *Riemannian*. They extend continuous normalizing flows (CNFs) (Grathwohl et al., 2019) to the manifold setting, by implicity parametrizing flows as solutions of Ordinary Differential Equations (ODEs). As such, the parametric flow is a *continuous* function of time. This approach has recently been extended by Rozen et al. (2021) introducing Moser flows, whose main appeal being that it circumvents the need to solve an ODE in the training process. We refer to App. J for an in-depth discussion on the links between our work and Moser flows.

Optimal transport on manifolds. Another line of work has developed flows on manifolds using tools from optimal transport. Sei (2013) introduced a flow that is given by $f_\theta : x \mapsto \exp_x(\nabla \psi_\theta^c)$ with ψ_θ^c a c-convex function and $c = d^2_{\mathcal{M}}$ the squared geodesic distance. This approach is motivated by the fact that the optimal transport map takes such an expression (Ambrosio, 2003). These methods operate directly on the manifold, similarly to CNFs, yet in contrast they are *discrete* in time. The benefits of this approach depend on the specific choice of parametric family of c-convex functions (Rezende and Racanière, 2021; Cohen et al., 2021), trading-off expressivity with scalability.

Table 3: Summary of computational complexity (w.r.t. neural network forward and backward passes) for different methods. d is the manifold dimension, k the number of Monte Carlo batches in Moser flow's regularizer, N is the number of steps in the (adaptive) ODE solver, whereas N^* is the number of steps in the SDE Euler-Maruyama solver–which can usually be lower than N. Moser flow and RSGM training complexity varies if the Hutchinson stochastic estimator is used. See Table 2 for score matching losses complexity.

Method	Training	Likelihood evaluation	Sampling
RCNF	Solving ODE $\mathcal{O}(dN)$	Solving augmented ODE $\mathcal{O}(dN)$	Solving ODE $\mathcal{O}(N)$
Moser flow	Computing div $\mathcal{O}(dk)$ or $\mathcal{O}(k)$	Solving augmented ODE $\mathcal{O}(dN)$	Solving ODE $\mathcal{O}(N)$
RSGM	Score matching $\mathcal{O}(d)$ or $\mathcal{O}(1)$	Solving augmented ODE $\mathcal{O}(dN)$	Solving SDE $\mathcal{O}(N^*)$

6 Experiments

In this section we benchmark the empirical performance of RSGMs along with other manifold-valued methods introduced in Sec. 5. We also compare to a 'Stereographic' score-based model, introduced in App. M. First, we assess their modelling capacity on earth and climate science spherical data. Then, we test the methods scalability with respect to manifold dimensions with a synthetic experiment on the torus $\mathbb{T}^d$. Eventually, we evaluate the models' regularity and time complexity with a synthetic $\mathrm{SO}_3(\mathbb{R})$ target. Experimental details are provided in App. N.

6.1 Earth and climate science datasets on the sphere

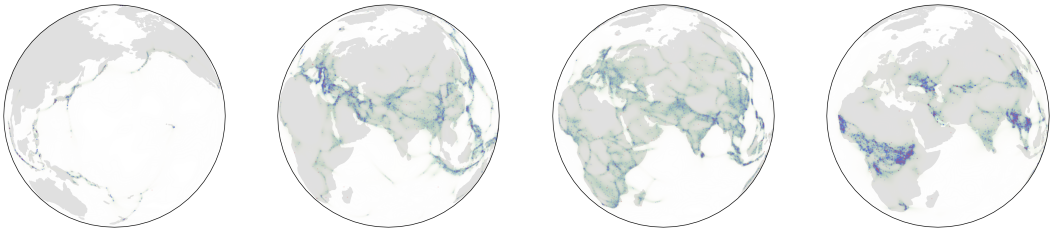
We start by evaluating RSGMs on a collection of simple datasets, each containing an empirical distribution of occurrences of earth and climate science events on the surface of the earth. These events are: volcanic eruptions (NGDC/WDS), earthquakes (NGDC/WDS), floods (Brakenridge, 2017) and wild fires (EOSDIS, 2020). We compare to previous baseline methods: Riemannian Continuous Normalizing Flows (Mathieu and Nickel, 2020), Moser Flows (Rozen et al., 2021) and a mixture of Kent distributions (Peel et al., 2001). Additionally, we consider a standard SGM on the 2D plane followed by the inverse stereographic projection which induces a density on the sphere (Gemici et al., 2016). We evaluate the log-likelihood of each model, extending to the manifold setting the likelihood computation techniques of SGMs, see App. C. We observe from Table 4, that all benchmarked methods have comparable performance when evaluated on these simple tasks with RSGM performing marginally better on most datasets. However, we empirically notice that Moser flows are slow to train and additionally that both Moser flows and stereographic SGMs are computationally expensive to evaluate.

6.2 Synthetic data on tori

We now move to another manifold, that is the torus $\mathbb{T}^d = \mathbb{S}^1 \times \cdots \times \mathbb{S}^1$, so as to assess the scalability of the different methods with respect to the dimension d. We consider a wrapped Gaussian target distribution on $\mathbb{T}^d$ with a random mean and unit variance. Moser flows' (Rozen et al., 2021) loss involves a regularization term which involves an integral over the manifold, approximated by a Monte Carlo (MC) estimator with uniform proposal. This term regularizes Moser flows towards probability measures, i.e. with unit volume. We thus expect Moser flows to fail in high-dimension as the number of samples K required for the MC estimator to be accurate will grows as $\mathcal{O}(\mathrm{e}^d)$, and the

Table 4: Negative log-likelihood scores for each method on the earth and climate science datasets. Bold indicates best results (up to statistical significance). Means and confidence intervals are computed over 5 different runs. Novel methods are shown with blue shading.

Method	Volcano	Earthquake	Flood	Fire
Mixture of Kent	$-0.80_{\pm 0.47}$	$0.33_{\pm 0.05}$	$0.73_{\pm 0.07}$	$-1.18_{\pm 0.06}$
Riemannian CNF	$\mathbf{-6.05_{\pm 0.61}}$	$0.14_{\pm 0.23}$	$1.11_{\pm 0.19}$	$\mathbf{-0.80_{\pm 0.54}}$
Moser Flow	$-4.21_{\pm 0.17}$	$\mathbf{-0.16_{\pm 0.06}}$	$\mathbf{0.57_{\pm 0.10}}$	$\mathbf{-1.28_{\pm 0.05}}$
Stereographic Score-Based	$-3.80_{\pm 0.27}$	$\mathbf{-0.19_{\pm 0.05}}$	$\mathbf{0.59_{\pm 0.07}}$	$\mathbf{-1.28_{\pm 0.12}}$
Riemannian Score-Based	$-4.92_{\pm 0.25}$	$\mathbf{-0.19_{\pm 0.07}}$	$\mathbf{0.45_{\pm 0.17}}$	$\mathbf{-1.33_{\pm 0.06}}$
Dataset size	827	6120	4875	12809



(a) Volcano (b) Earthquake (c) Flood (d) Fire

Figure 2: Trained score-based generative models on earth sciences data. The learned density is colored green-blue. Blue and red dots represent training and testing datapoints, respectively.

memory required to compute this estimator grows either in $\mathcal{O}(Kd)$ for exact divergences or $\mathcal{O}(K)$ for approximated divergences (see Table 3).

In Fig. 3, we observe that RSGMs are able to fit well the target distribution even in high dimension, with a linear or constant computational cost—depending on the divergence estimator. In contrast, Moser flows scale poorly with the dimension, to the extent that we are unable to train them for $d \geq 10$. This is due to the combination of the complexity which grows linearly with both the dimension d and the number of MC samples K, which itself ought to grow exponentially with d—as discussed in the previous paragraph. This is illustrated by the gap between the 'Moser' and 'ODE' likelihoods which increases with the manifold dimension (see left Fig. 3).

6.3 Synthetic data on the Special Orthogonal group

In order to demonstrate the broad range of applicability of our model we now turn to the task of density estimation on the special orthogonal group $\mathrm{SO}_d(\mathbb{R}) = \{\mathrm{Q} \in \mathrm{M}_d(\mathbb{R}) \,:\, \mathrm{Q}\mathrm{Q}^\top = \mathrm{Id},\ \det(\mathrm{Q}) = 1\}$. We consider the synthetic dataset consisting of samples in $\mathrm{SO}_3(\mathbb{R})$ from a mixture of wrapped normal distributions with M components.

We compare RSGMs against Moser flows and a wrapped-exponential baseline inspired by Falorsi et al. (2019)—where we parametrize a standard Euclidean SGM on $\mathfrak{so}(3)$ that is then pushed-forward on $\mathrm{SO}_3(\mathbb{R})$. RSGMs are trained using the $\ell_{t|0}$ (DSM) loss with the Varadhan approximation (see Table 2). From Table 5 we observe that, RSGMs perform consistently, whether the target distribution has few or many mixture components M, as opposed to Exp-wrapped SGMs and Moser flows which only perform well in some range of M. Similarly to Sec. 6.2, we find Moser flows to be much slower to train due to the large number of Monte Carlo samples needed in the reguralizer ($K = 10^4$). We also note from Table 5 that the number of score network evaluations (NFE) is significantly lower for RSGMs, and is particularly detrimental for Moser flows ($\gg 10^3$).

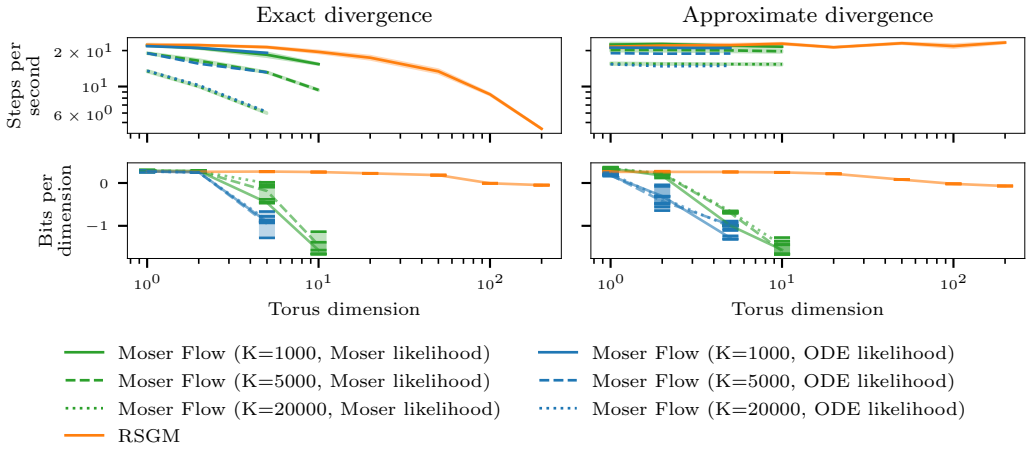
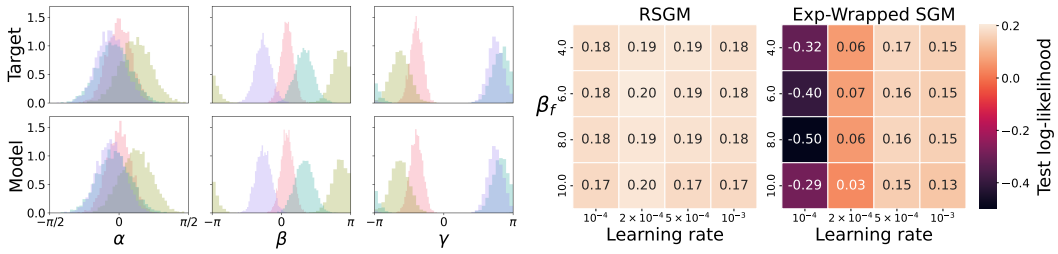


Figure 3: Comparison of Moser flows and RSGMs training speed and performance on the synthetic high-dimension torus task. Moser flows trained with $\lambda_{\min} = 1$. We report two likelihoods, the 'Moser' closed form density—not guaranteed to be normalized—and the 'ODE' likelihood given by solving an augmented ODE (as in CNFs) with the vector field induced by the Moser flow density—which is guaranteed to have unit volume.



(a) Histograms of $SO_3(\mathbb{R})$ samples from a target mixture distribution with $M = 4$ components, represented via their Euler angles.

(b) RSGMs are much more robust to hyperparameters than Exp-wrapped SGMs. The diffusion coefficient is given by $\sigma(t, \mathbf{X}_t) = \sqrt{\beta(t)}$, $\beta(t) = \beta_0 + (\beta_f - \beta_0)t$.

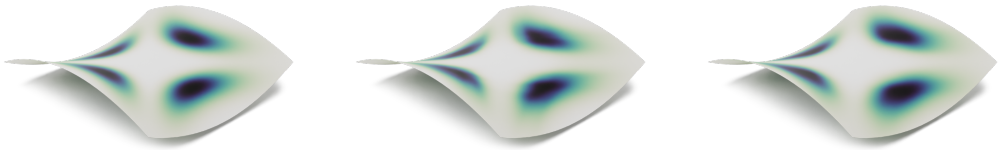
Figure 4: Trained score-based generative models on synthetic $SO_3(\mathbb{R})$ data.

Table 5: Test log-likelihood and associated number of function evaluations (NFE) in 10^3 on the synthetic mixture distribution with M components on $SO_3(\mathbb{R})$. Bold indicates best results (up to statistical significance). Means and standard deviations are computed over 5 different runs. Novel methods are shown with blue shading.

Method	$M = 16$		$M = 32$		$M = 64$	
	log-likelihood	NFE	log-likelihood	NFE	log-likelihood	NFE
Moser Flow	$0.85_{\pm 0.03}$	$2.3_{\pm 0.5}$	$0.17_{\pm 0.03}$	$2.3_{\pm 0.9}$	$\mathbf{-0.49_{\pm 0.02}}$	$7.3_{\pm 1.4}$
Exp-wrapped SGM	$\mathbf{0.87_{\pm 0.04}}$	$0.5_{\pm 0.1}$	$0.16_{\pm 0.03}$	$0.5_{\pm 0.0}$	$-0.58_{\pm 0.04}$	$0.5_{\pm 0.0}$
RSGM	$\mathbf{0.89_{\pm 0.03}}$	$\mathbf{0.1_{\pm 0.0}}$	$\mathbf{0.20_{\pm 0.03}}$	$\mathbf{0.1_{\pm 0.0}}$	$\mathbf{-0.49_{\pm 0.02}}$	$\mathbf{0.1_{\pm 0.0}}$

6.4 Synthetic data on hyperbolic space

Finally we demonstrate RSGM on a non-compact manifold: the two dimensional hyperbolic space $\mathbb{H}^2$, which is defined as the simply connected space of constant negative curvature. We use Langevin dynamics as the noising process (Eq. (3)) and target a wrapped Gaussian as the invariant distribution. We again consider a synthetic dataset of samples from a mixture of exp-wrapped normal distribution. From Fig. 5, we can qualitatively see that both score-based models are able to fit the target distribution.



(a) Target distribution. (b) Exp-wrapped SGM. (c) RSGM.

Figure 5: Samples from different probability distributions on $\mathbb{H}^2$ coloured w.r.t their density.

7 Discussion and limitations

In this paper we introduced Riemannian Score-Based Generative Models (RSGMs), a class of deep generative models that represent target densities supported on manifolds, as the time-reversal of Langevin dynamics. The main benefits of our method stems from its scalability to high dimensions, its applicability to a broad class of manifolds due to the diversity of available loss functions, its robustness and crucially its capacity to model complex datasets. We also provided theoretical guarantees on the convergence of RSGMs. In future work, we would like explore more generic classes of manifolds, such a ones with a boundary, along with alternative noising processes. Another promising extension concerns stochastic control on manifolds and more precisely, deriving efficient algorithms to solve Schrödinger bridges in the same spirit as De Bortoli et al. (2021) on Euclidean state spaces.

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References

Allgower, E. L. and Georg, K. (2012). *Numerical Continuation Methods: An Introduction*, volume 13. Springer Science & Business Media.

Ambrosio, L. (2003). Optimal transport maps in Monge-Kantorovich problem. *arXiv preprint arXiv:0304389v1*.

Atkinson, K. and Han, W. (2012). *Spherical Harmonics and Approximations on the Unit Sphere: An Introduction*, volume 2044. Springer Science & Business Media.

Bakry, D., Gentil, I., and Ledoux, M. (2014). *Analysis and Geometry of Markov Diffusion Operators*, volume 348. Springer.

Bao, F., Li, C., Zhu, J., and Zhang, B. (2022). Analytic-dpm: an analytic estimate of the optimal reverse variance in diffusion probabilistic models. *arXiv preprint arXiv:2201.06503*.

Barfoot, T., Forbes, J. R., and Furgale, P. T. (2011). Pose estimation using linearized rotations and quaternion algebra. *Acta Astronautica*, 68(1):101–112.

Batzolis, G., Stanczuk, J., Schönlieb, C.-B., and Etmann, C. (2021). Conditional image generation with score-based diffusion models. *arXiv preprint arXiv:2111.13606*.

Bismut, J.-M. (1984). Large deviations and the Malliavin calculus. *Birkhauser Prog. Math.*, 45.

Bose, J., Smofsky, A., Liao, R., Panangaden, P., and Hamilton, W. (2020). Latent variable modelling with hyperbolic normalizing flows. In *International Conference on Machine Learning*.

Bradbury, J., Frostig, R., Hawkins, P., Johnson, M. J., Leary, C., Maclaurin, D., Necula, G., Paszke, A., VanderPlas, J., Wanderman-Milne, S., and Zhang, Q. (2018). JAX: composable transformations of Python+NumPy programs.

Brakenridge, G. (2017). Global active archive of large flood events. http://floodobservatory.colorado.edu/Archives/index.html.

Brehmer, J. and Cranmer, K. (2020). Flows for simultaneous manifold learning and density estimation. *arXiv preprint arXiv:2003.13913*.

Caterini, A. L., Loaiza-Ganem, G., Pleiss, G., and Cunningham, J. P. (2021). Rectangular flows for manifold learning. *arXiv preprint arXiv:2106.01413*.

Cattiaux, P., Conforti, G., Gentil, I., and Léonard, C. (2021). Time reversal of diffusion processes under a finite entropy condition. *arXiv preprint arXiv:2104.07708*.

Chavel, I. (1984). *Eigenvalues in Riemannian Geometry*. Academic press.

Chen, X., Li, X. M., and Wu, B. (2021). Logarithmic heat kernels: estimates without curvature restrictions. *arXiv preprint arXiv:2106.02746*.

Chen, Y., Georgiou, T., and Pavon, M. (2016). Entropic and displacement interpolation: a computational approach using the Hilbert metric. *SIAM Journal on Applied Mathematics*, 76(6):2375–2396.

Cheng, X., Zhang, J., and Sra, S. (2022). Theory and algorithms for diffusion processes on Riemannian manifolds. *arXiv preprint arXiv:2204.13665*.

Choi, K., Meng, C., Song, Y., and Ermon, S. (2021). Density ratio estimation via infinitesimal classification. *arXiv preprint arXiv:2111.11010*.

Chung, H., Sim, B., and Ye, J. C. (2021). Come-closer-diffuse-faster: Accelerating conditional diffusion models for inverse problems through stochastic contraction. *arXiv preprint arXiv:2112.05146*.

Cohen, S., Amos, B., and Lipman, Y. (2021). Riemannian convex potential maps. *arXiv preprint arXiv:2106.10272*.

Croke, C. B. (1980). Some isoperimetric inequalities and eigenvalue estimates. In *Annales scientifiques de l'École normale supérieure*, volume 13, pages 419–435.

De Bortoli, V., Thornton, J., Heng, J., and Doucet, A. (2021). Diffusion Schrödinger bridge with applications to score-based generative modeling. In *Advances in Neural Information Processing Systems*.

Dhariwal, P. and Nichol, A. (2021). Diffusion models beat GAN on image synthesis. *arXiv preprint arXiv:2105.05233*.

Dormand, R. J. and Prince, J. P. (1980). A family of embedded Runge-Kutta formulae. *Journal of Computational and Applied Mathematics*, pages 19–26.

Durmus, A. (2016). *High Dimensional Markov Chain Monte Carlo Methods: Theory, Methods and Application*. Theses, Paris-Sud XI.

EOSDIS (2020). Land, atmosphere near real-time capability for eos (lance) system operated by nasa's earth science data and information system (esdis). https://earthdata.nasa.gov/earth-observation-data/near-real-time/firms/active-fire-data.

Falorsi, L. (2021). Continuous normalizing flows on manifolds. *arXiv:2104.14959*.

Falorsi, L., de Haan, P., Davidson, T. R., and Forré, P. (2019). Reparameterizing distributions on lie groups. In *International Conference on Artificial Intelligence and Statistics*, pages 3244–3253.

Falorsi, L. and Forré, P. (2020). Neural ordinary differential equations on manifolds. *arXiv preprint arXiv:2006.06663*.

Federer, H. (2014). *Geometric Measure Theory*. Springer.

Feiten, W., Lang, M., and Hirche, S. (2013). Rigid motion estimation using mixtures of projected Gaussians. In *International Conference on Information Fusion*, pages 1465–1472. IEEE.

Fisher, R. A. (1953). Dispersion on a sphere. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 217(1130):295–305.

Ganea, O.-E., Huang, X., Bunne, C., Bian, Y., Barzilay, R., Jaakkola, T. S., and Krause, A. (2022). Independent SE(3)-Equivariant models for end-to-end rigid protein docking. In *International Conference on Learning Representations*.

García-Zelada, D. and Huguet, B. (2021). Brenier–Schrödinger problem on compact manifolds with boundary. *Stochastic Analysis and Applications*, pages 1–29.

Gemici, M. C., Rezende, D., and Mohamed, S. (2016). Normalizing flows on Riemannian manifolds. *arXiv preprint arXiv:1611.02304*.

Grathwohl, W., Chen, R. T. Q., Bettencourt, J., and Duvenaud, D. (2019). Scalable reversible generative models with free-form continuous dynamics. In *International Conference on Learning Representations*.

Gretton, A., Borgwardt, K. M., Rasch, M. J., Schölkopf, B., and Smola, A. (2012). A kernel two-sample test. *Journal of Machine Learning Research*, 13(null):723–773.

Grigor'yan, A. (1999). Estimates of heat kernels on Riemannian manifolds. *London Math. Soc. Lecture Note Ser*, 273:140–225.

Gross, L. (1992). Logarithmic sobolev inequalities on lie groups. *Illinois journal of mathematics*, 36(3):447–490.

Gunther, M. (1991). Isometric embeddings of Riemannian manifolds, Kyoto, 1990. In *Proc. Intern. Congr. Math.*, pages 1137–1143. Math. Soc. Japan.

Hauberg, S. (2018). Directional Statistics with the Spherical Normal Distribution. In *2018 21st International Conference on Information Fusion (FUSION)*, pages 704–711, Cambridge, United Kingdom. IEEE.

Haussmann, U. G. and Pardoux, E. (1986). Time reversal of diffusions. *The Annals of Probability*, 14(4):1188–1205.

He, Y. (2013). A lower bound for the first eigenvalue in the Laplacian operator on compact Riemannian manifolds. *Journal of Geometry and Physics*, 71:73–84.

Ho, J., Jain, A., and Abbeel, P. (2020). Denoising diffusion probabilistic models. *Advances in Neural Information Processing Systems*.

Hou, B., Miolane, N., Khanal, B., Lee, M. C. H., Alansary, A., McDonagh, S., Hajnal, J. V., Rueckert, D., Glocker, B., and Kainz, B. (2018). Computing CNN Loss and Gradients for Pose Estimation with Riemannian Geometry. In Frangi, A. F., Schnabel, J. A., Davatzikos, C., Alberola-López, C., and Fichtinger, G., editors, *Medical Image Computing and Computer Assisted Intervention – MICCAI 2018*, pages 756–764, Cham. Springer International Publishing.

Hsu, E. (1999). Estimates of derivatives of the heat kernel on a compact Riemannian manifold. *Proceedings of the american mathematical society*, 127(12):3739–3744.

Hsu, E. P. (2002). *Stochastic Analysis on Manifolds*. Number 38. American Mathematical Society.

Hutchinson, M. F. (1989). A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines. *Communications in Statistics-Simulation and Computation*, 18(3):1059–1076.

Hyvärinen, A. (2005). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4).

Ikeda, N. and Watanabe, S. (1989). *Stochastic Differential Equations and Diffusion Processes*, volume 24 of *North-Holland Mathematical Library*. North-Holland Publishing Co., Amsterdam; Kodansha, Ltd., Tokyo, second edition.

Jolicoeur-Martineau, A., Piché-Taillefer, R., Tachet des Combes, R., and Mitliagkas, I. (2021). Adversarial score matching and improved sampling for image generation. *International Conference on Learning Representations*.

Jones, P. W., Maggioni, M., and Schul, R. (2008). Manifold parametrizations by eigenfunctions of the Laplacian and heat kernels. *Proceedings of the National Academy of Sciences of the United States of America*, 105(6):1803–1808.

Jørgensen, E. (1975). The central limit problem for geodesic random walks. *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, 32(1-2):1–64.

Karpatne, A., Ebert-Uphoff, I., Ravela, S., Babaie, H. A., and Kumar, V. (2018). Machine learning for the geosciences: Challenges and opportunities. *IEEE Transactions on Knowledge and Data Engineering*, 31(8):1544–1554.

Kawar, B., Vaksman, G., and Elad, M. (2021a). Snips: Solving noisy inverse problems stochastically. *arXiv preprint arXiv:2105.14951*.

Kawar, B., Vaksman, G., and Elad, M. (2021b). Stochastic image denoising by sampling from the posterior distribution. *arXiv preprint arXiv:2101.09552*.

Kent, J. T. (1982). The Fisher-Bingham distribution on the sphere. *Journal of the Royal Statistical Society: Series B (Methodological)*, 44(1):71–80.

Kingma, D. P. and Ba, J. (2015). Adam: A Method for Stochastic Optimization. *arXiv:1412.6980 [cs]*.

Klimovskaia, A., Lopez-Paz, D., Bottou, L., and Nickel, M. (2020). Poincaré maps for analyzing complex hierarchies in single-cell data. *Nature communications*, 11(1):1–9.

Kloeden, P. and Platen, E. (2011). *Numerical Solution of Stochastic Differential Equations*. Stochastic Modelling and Applied Probability. Springer Berlin Heidelberg.

Köhler, J., Klein, L., and Noé, F. (2020). Equivariant Flows: Exact likelihood generative learning for symmetric densities. *arXiv:2006.02425 [physics, stat]*.

Kullback, S. (1997). *Information Theory and Statistics*. Dover Publications, Inc., Mineola, NY. Reprint of the second (1968) edition.

Kurtz, T. G., Pardoux, É., and Protter, P. (1995). Stratonovich stochastic differential equations driven by general semimartingales. In *Annales de l'IHP Probabilités et statistiques*, volume 31, pages 351–377.

Kuwada, K. (2012). Convergence of time-inhomogeneous geodesic random walks and its application to coupling methods. *The Annals of Probability*, 40(5):1945–1979.

Lee, J. (2010). *Introduction to Topological Manifolds*, volume 202. Springer Science & Business Media.

Lee, J. M. (2006). *Riemannian Manifolds: An Introduction to Curvature*, volume 176. Springer Science & Business Media.

Lee, J. M. (2013). Smooth manifolds. In *Introduction to Smooth Manifolds*, pages 1–31. Springer.

Lee, J. M. (2018). *Introduction to Riemannian manifolds*. Springer.

Lee, S.-g., Kim, H., Shin, C., Tan, X., Liu, C., Meng, Q., Qin, T., Chen, W., Yoon, S., and Liu, T.-Y. (2021). Priorgrad: Improving conditional denoising diffusion models with data-driven adaptive prior. *arXiv preprint arXiv:2106.06406*.

Leobacher, G. and Steinicke, A. (2021). Existence, uniqueness and regularity of the projection onto differentiable manifolds. *Annals of Global Analysis and Geometry*, 60(3):559–587.

Léonard, C. (2012a). From the Schrödinger problem to the Monge–Kantorovich problem. *Journal of Functional Analysis*, 262(4):1879–1920.

Léonard, C. (2012b). Girsanov theory under a finite entropy condition. In *Séminaire de Probabilités XLIV*, pages 429–465. Springer.

Léonard, C., Rœlly, S., Zambrini, J.-C., et al. (2014). Reciprocal processes: a measure-theoretical point of view. *Probability Surveys*, 11:237–269.

Li, P. (1986). Large time behavior of the heat equation on complete manifolds with non-negative ricci curvature. *Annals of Mathematics*, 124(1):1–21.

Liptser, R. S. and Shiryaev, A. N. (2001). *Statistics of Random Processes. I*, volume 5 of *Applications of Mathematics (New York)*. Springer-Verlag, Berlin, expanded edition. General theory, Translated from the 1974 Russian original by A. B. Aries, Stochastic Modelling and Applied Probability.

Lui, Y. M. (2012). Advances in matrix manifolds for computer vision. *Image and Vision Computing*, 30(6-7):380–388.

Mardia, K. V., Hughes, G., Taylor, C. C., and Singh, H. (2008). A multivariate von Mises distribution with applications to bioinformatics. *Canadian Journal of Statistics*, 36(1):99–109.

Mathieu, E., Lan, C. L., Maddison, C. J., Tomioka, R., and Teh, Y. W. (2019). Continuous hierarchical representations with Poincaré variational auto-encoders. *arXiv preprint arXiv:1901.06033*.

Mathieu, E. and Nickel, M. (2020). Riemannian continuous normalizing flows. *arXiv preprint arXiv:2006.10605*.

Miolane, N., Guigui, N., Brigant, A. L., Mathe, J., Hou, B., Thanwerdas, Y., Heyder, S., Peltre, O., Koep, N., Zaatiti, H., Hajri, H., Cabanes, Y., Gerald, T., Chauchat, P., Shewmake, C., Brooks, D., Kainz, B., Donnat, C., Holmes, S., and Pennec, X. (2020a). Geomstats: A python package for riemannian geometry in machine learning. *Journal of Machine Learning Research*, 21(223):1–9.

Miolane, N., Guigui, N., Brigant, A. L., Mathe, J., Hou, B., Thanwerdas, Y., Heyder, S., Peltre, O., Koep, N., Zaatiti, H., Hajri, H., Cabanes, Y., Gerald, T., Chauchat, P., Shewmake, C., Brooks, D., Kainz, B., Donnat, C., Holmes, S., and Pennec, X. (2020b). Geomstats: A python package for riemannian geometry in machine learning. *Journal of Machine Learning Research*, 21(223):1–9.

Navarro, A. K., Frellsen, J., and Turner, R. E. (2017). The multivariate generalised von Mises distribution: inference and applications. In *AAAI Conference on Artificial Intelligence*.

(NGDC/WDS), N. G. D. C. . W. D. S. (2022a). Ncei/wds global significant earthquake database. https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.ngdc.mgg.hazards:G012153.

(NGDC/WDS), N. G. D. C. . W. D. S. (2022b). Ncei/wds global significant volcanic eruptions database. https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.ngdc.mgg.hazards:G10147.

Nichol, A. and Dhariwal, P. (2021). Improved denoising diffusion probabilistic models. *arXiv preprint arXiv:2102.09672*.

Papamakarios, G., Nalisnick, E., Rezende, D. J., Mohamed, S., and Lakshminarayanan, B. (2019). Normalizing flows for probabilistic modeling and inference. *arXiv preprint arXiv:1912.02762*.

Peel, D., Whiten, W. J., and McLachlan, G. J. (2001). Fitting mixtures of Kent distributions to aid in joint set identification. *Journal of the American Statistical Association*, 96(453):56–63.

Pennec, X. (2006). Intrinsic Statistics on Riemannian Manifolds: Basic Tools for Geometric Measurements. *Journal of Mathematical Imaging and Vision*, 25(1):127–154.

Prokudin, S., Gehler, P., and Nowozin, S. (2018). Deep directional statistics: Pose estimation with uncertainty quantification. In *European Conference on Computer Vision (ECCV)*.

Revuz, D. and Yor, M. (1999). *Continuous Martingales and Brownian Motion*, volume 293 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, third edition.

Rezende, D. J. and Racanière, S. (2021). Implicit Riemannian concave potential maps. *arXiv:2110.01288*.

Roy, D. M., Kemp, C., Mansinghka, V., and B Tenenbaum, J. (2007). Learning annotated hierarchies from relational data.

Rozen, N., Grover, A., Nickel, M., and Lipman, Y. (2021). Moser flow: Divergence-based generative modeling on manifolds. *Advances in Neural Information Processing Systems*.

Saloff-Coste, L. (1994). Precise estimates on the rate at which certain diffusions tend to equilibrium. *Mathematische Zeitschrift*, 217(1):641–677.

Santambrogio, F. (2017). {Euclidean, metric, and Wasserstein} gradient flows: an overview. *Bulletin of Mathematical Sciences*, 7(1):87–154.

Schrödinger, E. (1932). Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique. *Annales de l'Institut Henri Poincaré*, 2(4):269–310.

Sei, T. (2013). A Jacobian inequality for gradient maps on the sphere and its application to directional statistics. *Communications in Statistics-Theory and Methods*, 42(14):2525–2542.

Senanayake, R. and Ramos, F. (2018). Directional grid maps: modeling multimodal angular uncertainty in dynamic environments. In *2018 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, pages 3241–3248. IEEE.

Shapovalov, M. V. and Dunbrack Jr, R. L. (2011). A smoothed backbone-dependent rotamer library for proteins derived from adaptive kernel density estimates and regressions. *Structure*, 19(6):844–858.

Sinha, A., Song, J., Meng, C., and Ermon, S. (2021). D2c: Diffusion-denoising models for few-shot conditional generation. *arXiv preprint arXiv:2106.06819*.

Song, Y. and Ermon, S. (2019). Generative modeling by estimating gradients of the data distribution. In *Advances in Neural Information Processing Systems*.

Song, Y. and Ermon, S. (2020). Improved techniques for training score-based generative models. In *Advances in Neural Information Processing Systems*.

Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., and Poole, B. (2021). Score-based generative modeling through stochastic differential equations. In *International Conference on Learning Representations*.

Steyvers, M. and Tenenbaum, J. B. (2005). The large-scale structure of semantic networks: Statistical analyses and a model of semantic growth. *Cognitive science*, 29(1):41–78.

Sun, Y., Flammarion, N., and Fazel, M. (2019). Escaping from saddle points on Riemannian manifolds. *Advances in Neural Information Processing Systems*, 32.

Urakawa, H. (2006). Convergence rates to equilibrium of the heat kernels on compact Riemannian manifolds. *Indiana University Mathematics Journal*, pages 259–288.

Vargas, F., Thodoroff, P., Lawrence, N. D., and Lamacraft, A. (2021). Solving Schrödinger bridges via maximum likelihood. *arXiv preprint arXiv:2106.02081*.

Vincent, P. (2011). A connection between score matching and denoising autoencoders. *Neural Computation*, 23(7):1661–1674.

Watson, D., Ho, J., Norouzi, M., and Chan, W. (2021). Learning to efficiently sample from diffusion probabilistic models. *arXiv preprint arXiv:2106.03802*.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] Our main contribution is the extension of diffusion models on Riemannian manifolds.
   (b) Did you describe the limitations of your work? [Yes] See Sec. 7.
   (c) Did you discuss any potential negative societal impacts of your work? [No] The work presented in this paper focuses on the learning of score-based models on manifold. We do not foresee any immediate societal impact of such a study.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes] We have read the ethics review guidelines and our paper conforms to them.
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] Yes, see **A**1.
   (b) Did you include complete proofs of all theoretical results? [Yes] Yes, proofs are postponed to the supplementary material.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Experimental details are given in App. N.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Experimental details are given in App. N.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] Error bars are reported for each experiment.

(d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Experimental details are given in App. N.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes] See Sec. 6.1.
   (b) Did you mention the license of the assets? [Yes] See App. N.
   (c) Did you include any new assets either in the supplemental material or as a URL? [No] Not applicable.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [No] Not applicable.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [No] Not applicable.
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [No] Not applicable.
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [No] Not applicable.
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [No] Not applicable.

Supplementary to:
Riemannian Score-Based Generative Modelling

A Organization of the supplementary

In this supplementary we first introduce notation in **??**. We gather the proof of Theorem 1 as well as additional derivations on score-based generative models and Riemannian manifolds. In App. B, we recall basics on stochastic Riemannian geometry following Hsu (2002). In App. C, we introduce an extension to the Riemannian setting of the likelihood computation techniques in diffusion models. Details about parametric vector fields are given in App. D. In App. E, we recall some basic facts about eigenvalues and eigenfunctions of the Laplace–Beltrami operator on the d-dimensional sphere and torus. We present an extension of Algorithm 2 using predictor-corrector schemes in App. F. In App. G, we prove the extension of the time-reversal formula to manifold in Theorem 1. We prove the convergence of RSGM, i.e. Theorem 4, in App. H. The proof of Proposition 3 drawing links between the denoising score matching loss and the implicit score matching loss is presented App. I. We provide a thorough comparison between our approach and the one of Rozen et al. (2021) in App. J. We show how our method can be adapted to perform density estimation in App. K. Extensions to conditional SGM and Schrödinger Bridges are discussed in App. L. In Sec. 3.1, we briefly discuss the non compact setting. Details on the stereographic SGM are given in App. M. Experimental details are given in App. N.

B Preliminaries on stochastic Riemannian geometry

In this section, we recall some basic facts on Riemannian geometry and stochastic Riemannian geometry. We follow Hsu (2002); Lee (2018, 2006) and refer to Lee (2010, 2013) for a general introduction to topological and smooth manifolds. Throughout this section $\mathcal{M}$ is a d-dimensional smooth manifold, $\mathrm{T}\mathcal{M}$ its tangent bundle and $\mathrm{T}^\star\mathcal{M}$ it cotangent bundle. We denote $\mathrm{C}^\infty(\mathcal{M})$ the set of real-valued smooth functions on $\mathcal{M}$ and $\mathcal{X}(\mathcal{M})$ the set of vector fields on $\mathcal{M}$.

B.1 Tensor field, metric, connection and transport

Tensor field and Riemannian metric For a vector space V let $\mathrm{T}^{k,\ell}(V) = V^{\otimes k} \otimes (V^\star)^{\otimes \ell}$ with $k, \ell \in \mathbb{N}$. For any $k, \ell \in \mathbb{N}$ we define the space of (k,ℓ)-tensors as $\mathrm{T}^{k,\ell}\mathcal{M} = \sqcup_{p\in\mathcal{M}} \mathrm{T}^{k,\ell}(\mathrm{T}_p\mathcal{M})$. Note that $\Gamma(\mathcal{M}, \mathrm{T}^{0,0}\mathcal{M}) = \mathrm{C}^\infty(\mathcal{M})$, $\mathcal{X}(\mathcal{M}) = \Gamma(\mathcal{M}, \mathrm{T}^{1,0}\mathcal{M})$ and that the space of 1-form on $\mathcal{M}$ is given by $\Gamma(\mathcal{M}, \mathrm{T}^{0,1}\mathcal{M})$, where $\Gamma(\mathcal{M}, V(\mathcal{M}))$ is a section of a vector bundle $V(\mathcal{M})$ (see Lee, 2013, Chapter 10). For any $k \in \mathbb{N}$, we denote $\mathrm{T}^{|k|}\mathcal{M} = \sqcup_{j=0}^k \mathrm{T}^{j,k-j}\mathcal{M}$. $\mathcal{M}$ is said to be a Riemannian manifold if there exists $g \in \Gamma(\mathcal{M}, \mathrm{T}^{0,2}\mathcal{M})$ such that for any $x \in \mathcal{M}$, $g(x)$ is positive definite. g is called the Riemannian metric of $\mathcal{M}$. Every smooth manifold can be equipped with a Riemannian metric (see Lee, 2018, Proposition 2.4). In local coordinates we define $G = \{g_{i,j}\}_{1\le i,j\le d} = \{g(X_i, X_j)\}_{1\le i,j\le d}$, where $\{X_i\}_{i=1}^d$ is a basis of the tangent space. In what follows we consider that $\mathcal{M}$ is equipped with a metric g and for any $X, Y \in \mathcal{X}(\mathcal{M})$ we denote $\langle X, Y\rangle_{\mathcal{M}} = g(X, Y)$.

Connection A connection ∇ is a mapping which allows one to differentiate vector fields w.r.t other vector fields. ∇ is a linear map $\nabla : \mathcal{X}(\mathcal{M}) \times \mathcal{X}(\mathcal{M}) \to \mathcal{X}(\mathcal{M})$. In addition, we assume that i) for any $f \in \mathrm{C}^\infty(\mathcal{M})$, $X, Y \in \mathcal{X}(\mathcal{M})$, $\nabla_{fX}(Y) = f\nabla_X Y$, ii) for any $f \in \mathrm{C}^\infty(\mathcal{M})$, $X, Y \in \mathcal{X}(\mathcal{M})$, $\nabla_X(fY) = f\nabla_X Y + X(f)Y$. Given a system of local coordinates, the Christoffel symbols $\{\Gamma_{i,j}^k\}_{1\le i,j,k\le d}$ are given for any $i, j \in \{1, \dots, d\}$ by $\nabla_{X_i} X_j = \sum_{k=1}^d \Gamma_{i,j}^k X_k$. We also define the Levi–Civita connection ∇ by considering the additional two conditions: i) ∇ is torsion-free, i.e. for any $X, Y \in \mathcal{X}(\mathcal{M})$ we have $\nabla_X Y - \nabla_Y X = [X, Y]$, where $[X, Y]$ is the Lie bracket between X and Y, ii) ∇ is compatible with the metric g, i.e. for any $X, Y, Z \in \mathcal{X}(\mathcal{M})$, $X(\langle Y, Z\rangle_{\mathcal{M}}) = \langle \nabla_X Y, Z\rangle_{\mathcal{M}} + \langle Y, \nabla_X Z\rangle_{\mathcal{M}}$. We recall that the Levi–Civita connection is uniquely

defined since for any $X, Y, Z \in \mathcal{X}(\mathcal{M})$ we have

$$2\langle \nabla_X Y, Z\rangle_{\mathcal{M}} = X(\langle Y, Z\rangle_{\mathcal{M}}) + Y(\langle Z, X\rangle_{\mathcal{M}}) - Z(\langle X, Y\rangle_{\mathcal{M}}) + \langle [X, Y], Z\rangle_{\mathcal{M}} - \langle [Z, X], Y\rangle_{\mathcal{M}} - \langle [Y, Z], X\rangle_{\mathcal{M}}.$$

In this case, the Christoffel symbols are given for any $i, j, k \in \{1, \dots, d\}$ by

$$\Gamma_{i,j}^k = \tfrac{1}{2}\sum_{m=1}^d g^{km}(\partial_j g_{m,i} + \partial_i g_{m,j} - \partial_m g_{i,j}),$$

where $\{g^{i,j}\}_{1\leq i,j\leq d} = G^{-1}$. Note that if $\mathcal{M}$ is Euclidean then for any $i, j, k \in \{1, \dots, d\}$, $\Gamma_{i,j}^k = 0$. We also extend the connection so that for any $X \in \mathcal{X}(\mathcal{M})$ and $f \in \mathrm{C}^\infty(M)$ we have $\nabla_X f = X(f)$. In particular, we have that $\nabla_X f \in \mathrm{C}^\infty(\mathcal{M})$. In addition, we extend the connection such that for any $\alpha \in \Gamma(\mathcal{M}, \mathrm{T}^{0,1}\mathcal{M})$, $X, Y \in \mathcal{X}(\mathcal{M})$ we have $\nabla_X \alpha(Y) = \alpha(\nabla_X Y) - X(\alpha(Y))$. In particular, we have that $\nabla_X \alpha \in \Gamma(\mathcal{M}, \mathrm{T}^{1,0}\mathcal{M})$. Note that for any $X \in \mathcal{X}(\mathcal{M})$ and $\alpha, \beta \in \mathrm{T}^{|1|}\mathcal{M}$ we have $\nabla_X(\alpha \otimes \beta) = \nabla_X \alpha \otimes \beta + \alpha \otimes \nabla_X \beta$. Similarly, we can define recursively $\nabla_X \alpha$ for any $\alpha \in \Gamma(\mathcal{M}, \mathrm{T}^{k,\ell}\mathcal{M})$ with $k, \ell \in \mathbb{N}$. Such an extension is called a covariant derivative.

Parallel transport, geodesics and exponential mapping Given a connection, we can define the notion of parallel transport, which transports vector fields along a curve. Let $\gamma : [0, 1] \to \mathcal{M}$ be a smooth curve. We define the covariant derivative along the curve γ by $D_{\dot\gamma} : \mathcal{X}(\gamma) \to \mathcal{X}(\gamma)$ similarly to the connection, where $\mathcal{X}(\gamma) = \Gamma(\gamma([0, 1]), \mathrm{T}\mathcal{M})$. In particular if $\dot\gamma$ and $X \in \mathcal{X}(\gamma)$ can be extended to $\mathcal{X}(\mathcal{M})$ then we define $D_{\dot\gamma}(X) = \nabla_{\dot\gamma} X \in \mathcal{X}(\mathcal{M})$. In what follows, we denote $D = \nabla$ for simplicity. We say that $X \in \mathcal{X}(\gamma)$ is parallel to γ if for any $t \in [0, 1]$, $\nabla_{\dot\gamma} X(t) = 0$. In local coordinates, let $X \in \mathcal{X}(\gamma)$ be given for any $t \in [0, 1]$ by $X = \sum_{i=1}^d a_i(t)E_i(t)$ (assuming that $\gamma([0, 1])$ is entirely contained in a local chart), then we have that for any $t \in [0, 1]$ and $k \in \{1, \dots, d\}$

$$\dot a_k(t) + \sum_{i,j=1}^d \Gamma_{i,j}^k(x(t))\dot x_i(t)a_j(t) = 0. \tag{S1}$$

A curve γ on $\mathcal{M}$ is said to be a geodesics if $\dot\gamma$ is parallel to γ. Using Eq. (S1) we get that

$$\ddot x_k(t) + \sum_{i,j=1}^d \Gamma_{i,j}^k(x(t))\dot x_i(t)\dot x_j(t) = 0.$$

For more details on geodesics and parallel transport, we refer to Lee (2018, Chapter 4). In addition, we have that parallel transport provides a linear isomorphism between tangent spaces. Indeed, let $v \in \mathrm{T}_x\mathcal{M}$ and $\gamma : [0, 1] \to \mathcal{M}$ with $\gamma(0) = x$ a smooth curve. Then, there exists a unique vector field $X^v \in \mathcal{X}(\gamma)$ such that $X^v(x) = v$ and X^v is parallel to γ. For any $t \in [0, 1]$, we denote $\Gamma_0^t : \mathrm{T}_x\mathcal{M} \to \mathrm{T}_{\gamma(t)}\mathcal{M}$ the linear isomorphism such that $\Gamma_0^t(v) = X^v(\gamma(t))$.

For any $x \in \mathcal{M}$ and $v \in \mathrm{T}_x\mathcal{M}$ we denote $\gamma^{x,v} : [0, \varepsilon^{x,v}]$ the geodesics (defined on the maximal interval $[0, \varepsilon^{x,v}]$) on $\mathcal{M}$ such that $\gamma(0) = x$ and $\dot\gamma(0) = v$. We denote $\mathsf{U}^x = \{v \in \mathrm{T}_x\mathcal{M} : \varepsilon^{x,v} \geq 1\}$. Note that $0 \in \mathsf{U}^x$. For any $x \in \mathcal{M}$, we define the exponential mapping $\exp_x : \mathsf{U}^x \to \mathcal{M}$ such that for any $v \in \mathsf{U}^x$, $\exp_x(v) = \gamma^{x,v}(1)$. If for any $x \in \mathcal{M}$, $\mathsf{U}^x = \mathrm{T}_x\mathcal{M}$, the manifold is called *geodesically complete*. As any connected compact manifold is geodesically complete, there exists a geodesic between any two points $x, y \in \mathcal{M}$ (see Lee, 2018, Lemma 6.18). For any $x, y \in \mathcal{M}$, we denote $\mathrm{Geo}_{x,y}$ the sets of geodesics γ such that $\gamma(0) = x$ and $\gamma(y) = 1$. For any $x, y \in \mathcal{M}$ we denote $\Gamma_x^y(\gamma) : \mathrm{T}_x\mathcal{M} \to \mathrm{T}_y\mathcal{M}$ the linear isomorphism such that for any $v \in \mathrm{T}_x\mathcal{M}$, $\Gamma_x^y(v) = X^v(\gamma(1))$, where $\gamma \in \mathrm{Geo}_{x,y}$. Note that for any $x \in \mathcal{M}$ there exists $\mathsf{V}^x \subset \mathcal{M}$ such that $x \in \mathsf{V}^x$ and for any $y \in \mathsf{V}^x$ we have that $|\mathrm{Geo}_{x,y}| = 1$. In this case, we denote $\Gamma_x^y = \Gamma_x^y(\gamma)$ with $\gamma \in \mathrm{Geo}_{x,y}$.

Orthogonal projection We will make repeated use of orthonormal projections on manifolds. Recall that since $\mathcal{M}$ is a closed Riemannian manifold we can use the Nash embedding theorem (Gunther, 1991). In the rest of this paragraph, we assume that $\mathcal{M}$ is a Riemannian submanifold of $\mathbb{R}^p$ for some $p \in \mathbb{N}$ such that its metric is induced by the Euclidean metric. In order to define the projection we introduce

$$\mathrm{unpp}(\mathcal{M}) = \{x \in \mathbb{R}^d : \text{ there exists a unique } \xi_x \text{ such that } \|x - \xi_x\| = d(x, \mathcal{M})\}.$$

Let $\mathcal{E}(\mathcal{M}) = \mathrm{int}(\mathrm{unpp}(\mathcal{M}))$. By Leobacher and Steinicke (2021, Theorem 1), we have $\mathcal{M} \subset \mathcal{E}(\mathcal{M})$. We define $\tilde p : \mathcal{E}(\mathcal{M}) \to \mathcal{M}$ such that for any $x \in \mathcal{E}(\mathcal{M})$, $\tilde p(x) = \xi_x$. Using Leobacher and Steinicke (2021, Theorem 2), we have $\tilde p \in \mathrm{C}^\infty(\mathbb{R}^p, \mathcal{M})$ and for any $x \in \mathcal{M}$, $\tilde P(x) = \mathrm{d}\tilde p(x)$ is the orthogonal projection on $\mathrm{T}_x\mathcal{M}$. Since $\mathbb{R}^p$ is normal and $\mathcal{M}$ and $\mathcal{E}(\mathcal{M})^c$ are closed, there exists F open such that $\mathcal{M} \subset \mathsf{F} \subset \mathcal{E}(\mathcal{M})$. Let $p \in \mathrm{C}^\infty(\mathbb{R}^p, \mathbb{R}^p)$ such that for any $x \in \mathsf{F}$, $p(x) = \tilde p(x)$ (given by Whitney extension theorem for instance). Finally, we define $P : \mathbb{R}^p \to \mathbb{R}^p$ such that for any $x \in \mathbb{R}^p$, $P(x) = \mathrm{d}p(x)$. Note that for any $x \in \mathcal{M}$, $P(x)$ is the orthogonal projection $\mathrm{T}_x\mathcal{M}$ and that $P \in \mathrm{C}^\infty(\mathbb{R}^p, \mathbb{R}^p)$.

B.2 Stochastic Differential Equations on manifolds

Stratanovitch integral For reasons that will become clear in the next paragraph, it is easier to define Stochastic Differential Equations (SDEs) on manifolds w.r.t the Stratanovitch integral (Kloeden and Platen, 2011, Part II, Chapter 3). We consider a filtered probability space $(\Omega, (\mathcal{F}_t)_{t\geq 0}, \mathbb{P})$. Let $(\mathbf{X}_t)_{t\geq 0}$ and $(\mathbf{Y}_t)_{t\geq 0}$ be two real continuous semimartingales. We define the quadratic covariation $([\mathbf{X}, \mathbf{Y}]_t)_{t\geq 0}$ such that for any $t \geq 0$

$$[\mathbf{X}, \mathbf{Y}]_t = \mathbf{X}_t\mathbf{Y}_t - \mathbf{X}_0\mathbf{Y}_0 - \int_0^t \mathbf{X}_s \mathrm{d}\mathbf{Y}_s - \int_0^t \mathbf{Y}_s \mathrm{d}\mathbf{X}_s.$$

We refer to Revuz and Yor (1999, Chapter IV) for more details on semimartingales and quadratic variations. We denote $[\mathbf{X}] = [\mathbf{X}, \mathbf{X}]$. In particular, we have that $([\mathbf{X}, \mathbf{Y}]_t)_{t\geq 0}$ is an adapted continuous process with finite-variation and therefore $[[\mathbf{X}, \mathbf{Y}]] = 0$. Let $(\mathbf{X}_t)_{t\geq 0}$ and $(\mathbf{Y}_t)_{t\geq 0}$ be two real continuous semimartingales, then we define the Stratanovitch integral as follows for any $t \geq 0$

$$\int_0^t \mathbf{X}_s \circ \mathrm{d}\mathbf{Y}_s = \int_0^t \mathbf{X}_s \mathrm{d}\mathbf{Y}_s + \tfrac{1}{2}[\mathbf{X}, \mathbf{Y}]_t.$$

In particular, denoting $(\mathbf{Z}_t^1)_{t\geq 0}$ and $(\mathbf{Z}_t^2)_{t\geq 0}$ the processes such that for any $t \geq 0$, $\mathbf{Z}_t^1 = \int_0^t \mathbf{X}_s \circ \mathrm{d}\mathbf{Y}_s$ and $\mathbf{Z}_t^2 = \int_0^t \mathbf{X}_s \mathrm{d}\mathbf{Y}_s$, we have that $[\mathbf{Z}^1] = [\mathbf{Z}^2]$. We refer to Kurtz et al. (1995) for more details on Stratanovitch integrals. Note that if for any $t \geq 0$, $\mathbf{X}_t = \int_0^t f(\mathbf{X}_s) \circ \mathrm{d}\mathbf{Y}_s$ with $\mathrm{C}^1(\mathbb{R}, \mathbb{R})$, then $[\mathbf{X}, \mathbf{Y}]_t = \int_0^t f(\mathbf{X}_s) f'(\mathbf{X}_s) \mathrm{d}\mathbf{Y}_s$. Assuming that $f \in \mathrm{C}^3(\mathbb{R}, \mathbb{R})$ we have that (Revuz and Yor, 1999, Chapter IV, Exercise 3.15)

$$f(\mathbf{X}_t) = f(\mathbf{X}_0) + \int_0^t f'(\mathbf{X}_s) \circ \mathrm{d}\mathbf{X}_s.$$

The proof relies on the fact that for any $t \geq 0$, $\mathrm{d}[\mathbf{X}, f'(\mathbf{X})]_t = f''(\mathbf{X}_t)\mathrm{d}[\mathbf{X}]_t$. This result should be compared with Itô's lemma. In particular, Stratanovitch calculus satisfies the ordinary chain rule making it a useful tool in differential geometry which makes a heavy use of diffeomorphism. Finally, we have the following correspondence between Stratanovitch and Itô SDEs. Assume that $(\mathbf{X}_t)_{t\in[0,T]}$ is a strong solution to $\mathrm{d}\mathbf{X}_t = b(t, \mathbf{X}_t)\mathrm{d}t + \sigma(t, \mathbf{X}_t) \circ \mathrm{d}\mathbf{B}_t$, with $b \in \mathrm{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ and $\sigma \in \mathrm{C}^\infty(\mathbb{R}^d, \mathbb{R}^{d\times d})$. Then, we have that

$$\mathrm{d}\mathbf{X}_t = \{b(t, \mathbf{X}_t) + \bar{b}(\mathbf{X}_t)\}\mathrm{d}t + \sigma(t, \mathbf{X}_t)\mathrm{d}\mathbf{B}_t, \qquad \bar{b} = (-1/2)[\mathrm{div}(\sigma\sigma^\top) - \sigma\mathrm{div}(\sigma^\top)]. \tag{S2}$$

where for any $\mathrm{A} \in \mathrm{C}^\infty(\mathbb{R}^d, \mathbb{R}^{d\times d})$ we have that $\mathrm{div}(\mathrm{A}) \in \mathrm{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ and for any $i \in \{1, \ldots, d\}$ and $x \in \mathbb{R}^d$, $\mathrm{div}(\mathrm{A})_i(x) = \sum_{j=1}^d \partial_j \mathrm{A}_{i,j}(x)$. In particular, note that if for $x_0 \in \mathbb{R}^d$, $\sigma(x_0)$ is an orthogonal projection, then $\sigma(x_0)\bar{b}(x_0) = 0$.

SDEs on manifolds We define semimartingales and SDEs on manifold through the lens of their actions on functions. A continuous $\mathcal{M}$-valued stochastic process $(\mathbf{X}_t)_{t\geq 0}$ is called a $\mathcal{M}$-valued semimartingale if for any $f \in \mathrm{C}^\infty(\mathcal{M})$ we have that $(f(\mathbf{X}_t))_{t\geq 0}$ is a real valued semimartingale. Let $\ell \in \mathbb{N}$, $V^{1:\ell} = \{V_i\}_{i=1}^\ell \in \mathcal{X}(\mathcal{M})^\ell$ and $Z^{1:\ell} = \{Z^i\}_{i=1}^\ell$ a collection of ℓ real-valued semimartingales. A $\mathcal{M}$-valued semimartingale $(\mathbf{X}_t)_{t\geq 0}$ is said to be the solution of $\mathrm{SDE}(V^{1:\ell}, Z^{1:\ell}, \mathbf{X}_0)$ up to a stopping τ with $\mathbf{X}_0$ a $\mathcal{M}$-valued random variable if for all $f \in \mathrm{C}^\infty(\mathcal{M})$ and $t \in [0, \tau]$ we have

$$f(\mathbf{X}_t) = f(\mathbf{X}_0) + \sum_{i=1}^\ell \int_0^t V_i(f)(\mathbf{X}_s) \circ \mathrm{d}\mathbf{Z}_s^i.$$

Since the previous SDE is defined w.r.t the Stratanovitch integral we have that if $(\mathbf{X}_t)_{t\geq 0}$ is a solution of $\mathrm{SDE}(V^{1:\ell}, Z^{1:\ell}, \mathbf{X}_0)$ and $\mathbf{\Phi} : \mathcal{M} \to \mathcal{N}$ is a diffeomorphism then $(\mathbf{\Phi}(\mathbf{X}_t))_{t\geq 0}$ is a solution of $\mathrm{SDE}(\mathbf{\Phi}_\star V^{1:\ell}, Z^{1:\ell}, \mathbf{\Phi}(\mathbf{X}_0))$, where $\mathbf{\Phi}_\star$ is the pushforward operation (see Hsu, 2002, Proposition 1.2.4). Because the vector fields $\{V_i\}_{i=1}^\ell$ are smooth we have that for any $\ell \in \mathbb{N}$, $V^{1:\ell} = \{V_i\}_{i=1}^\ell \in \mathcal{X}(\mathcal{M})^\ell$ and $Z^{1:\ell} = \{Z^i\}_{i=1}^\ell$ a collection of ℓ real-valued semimartingales, there exists a unique solution to $\mathrm{SDE}(V^{1:\ell}, Z^{1:\ell}, \mathbf{X}_0)$ (see Hsu, 2002, Theorem 1.2.9).

B.3 Brownian motion on manifolds

In this section, we introduce the notion of Brownian motion on manifolds. We derive some of its basic convergence properties and provide alternative definitions (stochastic development, isometric embedding, random walk limit). These alternative definitions are the basis for our alternative

methodologies to sample from the time-reversal. To simplify our discussion, we assume that $\mathcal{M}$ is a connected compact orientable Riemannian manifold equipped with the Levi–Civita connection ∇. We denote p_{ref}^m the Haussdorff measure of the manifold (which coincides with the measure associated with the Riemannian volume form (see Federer, 2014, Theorem 2.10.10) and $p_{\text{ref}} = p_{\text{ref}}^m / p_{\text{ref}}(\mathcal{M})$ the associated probability measure.

Gradient, divergence and Laplace operators Let $f \in \mathrm{C}^\infty(\mathcal{M})$. We define $\nabla f \in \mathcal{X}(\mathcal{M})$ such that for any $X \in \mathcal{X}(\mathcal{M})$ we have $\langle X, \nabla f \rangle_{\mathcal{M}} = X(f)$. Let $\{X_i\}_{i=1}^d \in \mathcal{X}(\mathcal{M})^d$ such that for any $x \in \mathcal{M}$, $\{X_i(x)\}_{i=1}^d$ is an orthonormal basis of $\mathrm{T}_x\mathcal{M}$. Then, we define $\mathrm{div} : \mathcal{X}(\mathcal{M}) \to \mathrm{C}^\infty(\mathcal{M})$ (linear) such that for any $X \in \mathcal{X}(\mathcal{M})$, $\mathrm{div}(X) = \sum_{i=1}^d \langle \nabla_{X_i} X, X_i \rangle_{\mathcal{M}}$. The following Stokes formula (also called divergence theorem, see Lee (2018, p.51)) holds for any $f \in \mathrm{C}^\infty(\mathcal{M})$ and $X \in \mathcal{X}(\mathcal{M})$, $\int_M \mathrm{div}(X)(x) f(x) \mathrm{d}p_{\text{ref}}(x) = -\int_M X(f)(x) \mathrm{d}p_{\text{ref}}(x)$. Let $X = \sum_{i=1}^d a_i X_i$ in local coordinates. Using the Stokes formula and the definition of the gradient we get that in local coordinates

$$\nabla f = \sum_{i,j=1}^d g^{i,j} \partial_i f X_j, \qquad \mathrm{div}(X) = \det(G)^{-1/2} \sum_{i=1}^d \partial_i (\det(G)^{1/2} a_i).$$

The Laplace–Beltrami operator is given by $\Delta_{\mathcal{M}} : \mathrm{C}^\infty(M) \to \mathrm{C}^\infty(M)$ and for any $f \in \mathrm{C}^\infty(M)$ by $\Delta_{\mathcal{M}}(f) = \mathrm{div}(\mathrm{grad}(f))$. In local coordinates we obtain $\Delta_{\mathcal{M}}(f) = \det(G)^{-1/2} \sum_{i=1}^d \partial_i (\det(G)^{1/2} \sum_{j=1}^d g^{i,j} \partial_j f)$. Using the Nash isometric embedding theorem (Gunther, 1991) we will see that $\Delta_{\mathcal{M}}$ can always be written as a sum of squared operators. However, this result requires an *extrinsic* point of view as it relies on the existence of projection operators. In contrast, if we consider the orthonormal bundle $\mathrm{O}\mathcal{M}$, see (Hsu, 2002, Chapter 2), we can define the Laplace–Bochner operator $\Delta_{\mathrm{O}\mathcal{M}} : \mathrm{C}^\infty(\mathrm{O}\mathcal{M}) \to \mathrm{C}^\infty(\mathrm{O}\mathcal{M})$ as $\Delta_{\mathrm{O}\mathcal{M}} = \sum_{i=1}^d H_i^2$, where we recall that for any $i \in \{1, \dots, d\}$, H_i is the horizontal lift of e_i. In this case, $\Delta_{\mathrm{O}\mathcal{M}}$ is a sum of squared operators and we have that for any $f \in \mathrm{C}^\infty(\mathcal{M})$, $\Delta_{\mathrm{O}\mathcal{M}}(f \circ \pi) = \Delta_{\mathcal{M}}(f)$ (see Hsu, 2002, Proposition 3.1.2). Being able to express the various Laplace operators as a sum of squared operators is key to express the associated diffusion process as the solution of an SDE.

Alternatives definitions of Brownian motion We are now ready to define a Brownian motion on the manifold $\mathcal{M}$. Using the Laplace–Beltrami operator, we can introduce the Brownian motion through the lens of diffusion processes.

Definition S5 (Brownian motion)**.** *Let $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ be a $\mathcal{M}$-valued semimartingale. $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ is a Brownian motion on $\mathcal{M}$ if for any $f \in \mathrm{C}^\infty(\mathcal{M})$, $(\mathbf{M}_t^f)_{t \geq 0}$ is a local martingale where for any $t \geq 0$*

$$\mathbf{M}_t^f = f(\mathbf{B}_t^{\mathcal{M}}) - f(\mathbf{B}_0^{\mathcal{M}}) - \tfrac{1}{2} \int_0^t \Delta_{\mathcal{M}} f(\mathbf{B}_s^{\mathcal{M}}) \mathrm{d}s.$$

Note that this definition is in accordance with the definition of the Brownian motion as a diffusion process in the Euclidean space $\mathbb{R}^d$, since in this case $\Delta_{\mathcal{M}} = \Delta$. A key property of frame bundles and orthonormal bundles is that any semimartingale on $\mathcal{M}$ can be associated to a process on $\mathrm{F}\mathcal{M}$ (or $\mathrm{O}\mathcal{M}$) and a process on $\mathbb{R}^d$. The proof of the following result can be found in Hsu (2002, Propositions 3.2.1 and 3.2.2).

Proposition S6 (Intrinsic view of Brownian motion)**.** *Let $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ be a $\mathcal{M}$-valued semimartingales. Then $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ is a Brownian motion on $\mathcal{M}$ if and only on the following conditions hold:*

a) The horizontal lift $(\mathbf{U}_t)_{t \geq 0}$ is a $\Delta_{\mathrm{O}\mathcal{M}}/2$ diffusion process, i.e. for any $f \in \mathrm{C}^\infty(\mathrm{O}\mathcal{M})$, we have that $(\mathbf{M}_t^f)_{t \geq 0}$ is a local martingale where for any $t \geq 0$

$$\mathbf{M}_t^f = f(\mathbf{U}_t) - f(\mathbf{U}_0) - \tfrac{1}{2} \int_0^t \Delta_{\mathrm{O}\mathcal{M}} f(\mathbf{U}_s) \mathrm{d}s.$$

b) The stochastic antidevelopment of $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ is a $\mathbb{R}^d$-valued Brownian motion $(\mathbf{B}_t)_{t \geq 0}$.

In particular the previous proposition provides us with an *intrisic* way to sample the Brownian motion on $\mathcal{M}$ with initial condition $\mathbf{B}_0^{\mathcal{M}}$. First sample $(\mathbf{U}_t)_{t \geq 0}$ solution of $\mathrm{SDE}(H^{1:d}, \mathbf{B}^{1:d}, \mathbf{U}_0)$ with $H^{1:d} = \{H_i\}_{i=1}^d$ and $\pi(\mathbf{U}_0) = \mathbf{B}_0^{\mathcal{M}}$ and $\mathbf{B}^{1:d}$ the Euclidean d-dimensional Brownian motion. Then, we recover the $\mathcal{M}$-valued Brownian motion $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0}$ upon letting $(\mathbf{B}_t^{\mathcal{M}})_{t \geq 0} = (\pi(\mathbf{U}_t))_{t \geq 0}$.

We now consider an *extrinsic* approach to the sampling of Brownian motions on $\mathcal{M}$. Using the Nash embedding theorem (Gunther, 1991), there exists $p \in \mathbb{N}$ such that without loss of generality

we can assume that $\mathcal{M} \subset \mathbb{R}^p$. For any $x \in \mathcal{M}$, we denote $\mathrm{P}(x) : \mathbb{R}^p \to \mathrm{T}_x\mathcal{M}$ the projection operator. In addition for any $x \in \mathcal{M}$, we denote $\{\mathrm{P}_i(x)\}_{i=1}^p = \{\mathrm{P}(x)e_i\}_{i=1}^p$, where $\{e_i\}_{i=1}^p$ is the canonical basis of $\mathbb{R}^p$. For any $i \in \{1, \dots, p\}$, we smoothly extend P_i to $\mathbb{R}^p$. In this case, we have the following proposition (Hsu, 2002, Theorem 3.1.4):

Proposition S7 (Extrinsic view of Brownian motion)**.** *For any $f \in \mathrm{C}^\infty(\mathcal{M})$ we have that $\Delta_{\mathcal{M}}(f) = \sum_{i=1}^p \mathrm{P}_i(\mathrm{P}_i(f))$. Hence, we have that $(\mathbf{B}_t^{\mathcal{M}})_{t\geq 0}$ solution of $\mathrm{SDE}(\{\mathrm{P}_i\}_{i=1}^p, \mathbf{B}^{1:p}, \mathbf{B}_0^{\mathcal{M}})$ with $\mathbf{B}_0^{\mathcal{M}}$ a $\mathcal{M}$-valued random variable and $\mathbf{B}^{1:p}$ a $\mathbb{R}^p$-valued Brownian motion.*

The second part of this proposition, stems from the fact that any solution of $\mathrm{SDE}(\{V_i\}_{i=1}^\ell, \mathbf{B}^{1:\ell}, \mathbf{X}_0)$, where $\mathbf{X}_0$ is a $\mathcal{M}$-valued random variable and $\mathbf{B}^{1:\ell}$ a $\mathbb{R}^\ell$-valued Brownian motion is a diffusion process with generator $\mathcal{A}$ such that for any $f \in \mathrm{C}^\infty(\mathcal{M})$, $\mathcal{A}(f) = \sum_{i=1}^\ell V_i(V_i(f))$. The *extrinsic* approach is particularly convenient since the SDE appearing in Proposition S7 can be seen as an SDE on the Euclidean space $\mathbb{R}^p$.

We finish this paragraph, by investigating the behaviour of the Brownian motion in local coordinates. For simplicity, we assume here that we have access to a system of global coordinates. In the case where the coordinates are strictly local then we refer to Ikeda and Watanabe (1989, Chapter 5, Theorem 1) for a construction of a global solution by patching local solutions. We denote $\{X_k, X_{i,j}\}_{1\leq i,j,k\leq d}$ such that for any $u \in \mathrm{F}\mathcal{M}$, $\{X_k(u), X_{i,j}(u)\}_{1\leq i,j,k\leq d}$ is a basis of $\mathrm{T}_u\mathrm{F}\mathcal{M}$, Using properties of the horizontal lift, see (Hsu, 2002, Chapter 2), we get that $(\mathbf{U}_t)_{t\geq 0} = (\{\mathbf{X}_t^k, \mathbf{E}_t^{i,j}\}_{1\leq i,j,k\leq d})$ obtained in Proposition S6 is given in the global coordinates for any $i, j, k \in \{1, \dots, d\}$ by

$$\mathrm{d}\mathbf{X}_t^k = \sum_{j=1}^d \mathbf{E}_t^{k,j} \circ \mathrm{d}\mathbf{B}_t^k, \qquad \mathrm{d}\mathbf{E}_t^{i,j} = -\sum_{n=1}^d \{\sum_{\ell,m=1}^d \mathbf{E}_t^{\ell,n}\mathbf{E}_t^{m,j}\Gamma_{\ell,m}^i(\mathbf{X}_t)\} \circ \mathrm{d}\mathbf{B}_t^n.$$

By definition of the Stratanovitch integral we have that for any $k \in \{1, \dots, d\}$

$$\mathrm{d}\mathbf{X}_t^k = \sum_{j=1}^d \{\mathbf{E}_t^{k,j}\mathrm{d}\mathbf{B}_t^k + \tfrac{1}{2}\mathrm{d}[\mathbf{E}_t^{k,j}, \mathbf{B}_t^j]_t\}.$$

Let $(\mathbf{M}_t)_{t\geq 0} = (\{\mathbf{M}_t^k\}_{k=1}^d)_{t\geq 0}$ such that for any $t \geq 0$ and $k \in \{1, \dots, d\}$ $\mathbf{M}_t^k = \sum_{j=1}^d \int_0^t \mathbf{E}_t^{k,j}\mathrm{d}\mathbf{B}_t^k$. We obtain that $\mathrm{d}\mathbf{M}_t = G(\mathbf{X}_t)^{-1/2}\mathrm{d}\mathbf{B}_t$ for some d-dimensional Brownian motion $(\mathbf{B}_t)_{t\geq 0}$, using Lévy's characterization of Brownian motion. In addition, we have that for any $k, j \in \{1, \dots, d\}$

$$[\mathbf{E}^{k,j}, \mathbf{B}^j]_t = -\sum_{\ell,m=1}^d \int_0^t \mathbf{E}_t^{\ell,j}\mathbf{E}_t^{m,j}\Gamma_{\ell,m}^k(\mathbf{X}_t)\mathrm{d}t$$

Hence, using this result and the fact that $\sum_{j=1}^d \mathbf{E}_t^{\ell,j}\mathbf{E}_t^{m,j} = g^{\ell,m}(\mathbf{X}_t)$, we get that for any $k \in \{1, \dots, d\}$

$$\mathrm{d}\mathbf{X}_t^k = -\tfrac{1}{2}\sum_{\ell,m=1}^d g^{\ell,m}(\mathbf{X}_t)\Gamma_{\ell,m}^k(\mathbf{X}_t)\mathrm{d}t + (G(\mathbf{X}_t)^{-1/2}\mathrm{d}\mathbf{B}_t)^k.$$

Note that this result could also have been obtained using the expression of the Laplace–Beltrami in local coordinates.

Brownian motion and random walks In the previous paragraph we consider three SDEs to obtain a Brownian motion on $\mathcal{M}$ (stochastic development, isometric embedding and local coordinates). In this section, we summarize results from Jørgensen (1975) establishing the limiting behaviour of Geodesic Random Walks (GRWs) when the stepsize of the random walk goes to 0. This will be of particular interest when considering the time-reversal process. We start by defining the geodesic random walk on $\mathcal{M}$, following Jørgensen (1975, Section 2).

Let $\{\nu_x\}_{x\in\mathcal{M}}$ such that for any $x \in \mathcal{M}$, $\nu_x : \mathcal{B}(\mathrm{T}_x\mathcal{M}) \to [0, 1]$ with $\nu_x(\mathrm{T}_x\mathcal{M}) = 1$, i.e. for any $x \in \mathcal{M}$, ν_x is a probability measure on $\mathrm{T}_x\mathcal{M}$. Assume that for any $x \in \mathcal{M}$, $\int_{\mathcal{M}} \|v\|^3\mathrm{d}\nu_x(v) < +\infty$. In addition assume that there exists $\mu^{(1)} \in \mathcal{X}(\mathcal{M})$ and $\mu^{(2)} \in \mathcal{X}^2(\mathcal{M})$, where $\mathcal{X}^2(\mathcal{M})$ is the section $\Gamma(\mathcal{M}, \sqcup_{x\in\mathcal{M}}\mathcal{L}(\mathrm{T}_x\mathcal{M}))$, such that for any $x \in \mathcal{M}$, $\int_{\mathcal{M}} v\mathrm{d}\nu_x(v) = \mu^{(1)}(x)$ and $\int_{\mathcal{M}} v \otimes v\mathrm{d}\nu_x(v) = \mu^{(2)}(x)$. In addition, we assume that for any $x \in \mathcal{M}$, $\Sigma(x) = \mu^{(2)}(x) - \mu^{(1)}(x) \otimes \mu^{(1)}(x)$ is strictly positive definite and that there exists $\mathrm{L} \geq$ such that for any $x, y \in \mathcal{M}$, $\|\nu_x - \nu_y\|_{\mathrm{TV}} \leq \mathrm{L}d_{\mathcal{M}}(x, y)$. Where we have that for any $\nu_1 \in \mathcal{P}(\mathrm{T}_x\mathcal{M})$ and $\nu_2 \in \mathcal{P}(\mathrm{T}_y\mathcal{M})$,

$$\|\nu_x - \nu_y\|_{\mathrm{TV}} = \sup\{\nu_1[f] - \Gamma_x^y(\gamma)_\#\nu_2[f] \,:\, \gamma \in \mathrm{Geo}_{x,y},\ f \in \mathrm{C}(\mathrm{T}_x\mathcal{M})\}.$$

Note that if $d_{\mathcal{M}}(x, y) \leq \varepsilon$ then for some $\varepsilon > 0$ we have that $|\mathrm{Geo}_{x,y}| = 1$.

Definition S8 (Geodesic random walk)**.** *Let X_0 be a $\mathcal{M}$-valued random variable. For any $\gamma > 0$, we define $(\mathbf{X}_t^\gamma)_{t\geq 0}$ such that $\mathbf{X}_0^\gamma = X_0$ and for any $n \in \mathbb{N}$ and $t \in [0, \gamma]$, $\mathbf{X}_{n\gamma+t} = \exp_{\mathbf{X}_{n\gamma}}[t\gamma\{\mu_n + (1/\sqrt{\gamma})(V_n - \mu_n)\}]$, where $(V_n)_{n\in\mathbb{N}}$ is a sequence of random variables in such that for any $n \in \mathbb{N}$, V_n has distribution $\nu_{\mathbf{X}_{n\gamma}}$ conditionally to $\mathbf{X}_{n\gamma}$.*

For any $\gamma > 0$, the process $(X_n^\gamma)_{n\in\mathbb{N}} = (\mathbf{X}_{n\gamma}^\gamma)_{n\in\mathbb{N}}$ is called a geodesic random walk. In particular, for any $\gamma > 0$ we denote $(\mathrm{R}_n^\gamma)_{n\in\mathbb{N}}$ the sequence of Markov kernels such that for any $n \in \mathbb{N}$, $x \in \mathcal{M}$ and $\mathsf{A} \in \mathcal{B}(\mathcal{M})$ we have that $\delta_x \mathrm{R}(\mathsf{A}) = \mathbb{P}(X_n^\gamma \in \mathsf{A})$, with $X_0^\gamma = x$. The following theorem establishes that the limiting dynamics of a geodesic random walk is associated with a diffusion process on $\mathcal{M}$ whose coefficients only depends on the properties of ν (see Jørgensen, 1975, Theorem 2.1).

Theorem S9 (Convergence of geodesic random walks)**.** *For any $t \geq 0$, $f \in \mathrm{C}(\mathcal{M})$ and $x \in \mathcal{M}$ we have that $\lim_{\gamma\to 0} \|\mathrm{R}_\gamma^{\lceil t/\gamma \rceil}[f] - \mathrm{P}_t[f]\|_\infty = 0$, where $(\mathrm{P}_t)_{t\geq 0}$ is the semi-group associated with the infinitesimal generator $\mathcal{A} : \mathrm{C}^\infty(\mathcal{M}) \to \mathrm{C}^\infty(\mathcal{M})$ given for any $f \in \mathrm{C}^\infty(\mathcal{M})$ by $\mathcal{A}(f) = \langle \mu^{(1)}, \nabla f\rangle_{\mathcal{M}} + \frac{1}{2}\langle \Sigma, \nabla^2 f\rangle_{\mathcal{M}}$.*

In particular if $\mu^{(1)} = 0$ and $\mu^{(2)} = \mathrm{Id}$ then the random walk converges towards a Brownian motion on $\mathcal{M}$ in the sense of the convergence of semi-groups. For any $x \in \mathcal{M}$ in local coordinates we have that $\Phi_\# \nu_x$ has zero mean and covariance matrix $G(x)$, where Φ is a local chart around x and $G(x) = (g_{i,j}(x))_{1\leq i,j\leq d}$ the coordinates of the metric in that chart.

Convergence of Brownian motion We finish this section with a few considerations regarding the convergence of the Brownian motion on $\mathcal{M}$. Since we have assumed that $\mathcal{M}$ is compact we have that there exist $(\Phi_k)_{k\in\mathbb{N}}$ an orthonormal basis of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(p_{\text{ref}})$, $(\lambda_k)_{k\in\mathbb{N}}$ such that for any $i, j \in \mathbb{N}$, $i \leq j$, $\lambda_i \leq \lambda_j$ and $\lambda_0 = 0$, $\Phi_0 = 1$ and for any $k \in \mathbb{N}$, $\Delta_{\mathcal{M}}\Phi_k = -\lambda_k \Phi_k$. For any $t \geq 0$ and $x, y \in \mathcal{M}$, $p_{t|0}(y|x) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-\lambda_k t}\Phi_k(x)\Phi_k(y)$ where for any $f \in \mathrm{C}^\infty$ we have

$$\mathbb{E}[f(\mathbf{B}_t^{\mathcal{M},x})] = \int_{\mathcal{M}} p_{t|0}(x, y) f(y) \mathrm{d}p_{\text{ref}}(y),$$

where $(\mathbf{B}_t^{\mathcal{M},x})_{t\geq 0}$ is the Brownian motion on $\mathcal{M}$ with $\mathbf{B}_0^{\mathcal{M},x} = x$ and p_{ref} is the probability measure associated with the Haussdorff measure on $\mathcal{M}$. We also have the following result (see Urakawa, 2006, Proposition 2.6).

Proposition S10 (Convergence of Brownian motion)**.** *For any $t > 0$, P_t admits a density $p_{t|0}$ w.r.t p_{ref} and $p_{\text{ref}}\mathrm{P}_t = p_{\text{ref}}$, i.e. p_{ref} is an invariant measure for $(\mathrm{P}_t)_{t\geq 0}$. In addition, if there exists $C, \alpha \geq 0$ such that for any $t \in (0, 1]$, $p_{t|0}(x|x) \leq Ct^{-\alpha/2}$ then for any $p_0 \in \mathcal{P}(\mathcal{M})$ and for any $t \geq 1/2$ we have*

$$\|p_0\mathrm{P}_t - p_{\text{ref}}\|_{\mathrm{TV}} \leq C^{1/2}\mathrm{e}^{\lambda_1/2}\mathrm{e}^{-\lambda_1 t},$$

where λ_1 is the first non-negative eigenvalue of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(p_{\text{ref}})$ and we recall that $(\mathrm{P}_t)_{t\geq 0}$ is the semi-group of the Brownian motion.

A review on lower bounds on the first positive eigenvalue of the Laplace–Beltrami operator can be found in (He, 2013). These lower bounds usually depend on the Ricci curvature of the manifold or its diameter. We conclude this section by noting that in the non-compact case (Li, 1986) establishes similar estimates in the case of a manifold with non-negative Ricci curvature and maximal volume growth.

C Likelihood computation

C.1 ODE likelihood computation

Similarly to Song et al. (2021), once the score is learned we can use it in conjunction with an Ordinary Differential Equation (ODE) solver to compute the likelihood of the model. Let $(\Phi_t)_{t\in[0,T]}$ be a family of vector fields. We define $(\mathbf{X}_t)_{t\in[0,T]}$ such that $\mathbf{X}_0$ has distribution p_0 (the data distribution) and satisfying $\mathrm{d}\mathbf{X}_t = \Phi_t(\mathbf{X}_t)\mathrm{d}t$. Assuming that p_0 admits a density w.r.t. p_{ref} then for any $t \in [0, T]$, the distribution of $\mathbf{X}_t$ admits a density w.r.t. p_{ref} and we denote p_t this density. We recall that $\mathrm{d}\log p_t(\mathbf{X}_t) = -\mathrm{div}(\Phi_t)(\mathbf{X}_t)\mathrm{d}t$, see Mathieu and Nickel (2020, Proposition 2) for instance.

Recall that we consider a Brownian motion on the manifold as a forward process $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ with $\{p_t\}_{t\in[0,T]}$ the associated family of densities. Thus we have that for any $t \in [0,T]$ and $x \in \mathcal{M}$

$$\partial_t p_t(x) = \tfrac{1}{2}\Delta_{\mathcal{M}} p_t(x) = \operatorname{div}\left(\tfrac{1}{2} p_t \nabla \log p_t\right)(x).$$

Hence, we can define $(\mathbf{X}_t)_{t\in[0,T]}$ satisfying $\mathrm{d}\mathbf{X}_t = -\frac{1}{2}\nabla \log p_t(\mathbf{X}_t)\mathrm{d}t$ such that $\mathbf{X}_0$ has distribution p_0. Defining $(\hat{\mathbf{X}}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$, it follows that $\hat{\mathbf{X}}_0$ has distribution $\mathcal{L}(\mathbf{X}_T)$ and satisfies

$$\mathrm{d}\hat{\mathbf{X}}_t = \tfrac{1}{2}\nabla \log p_{T-t}(\hat{\mathbf{X}}_t)\mathrm{d}t. \tag{S3}$$

Finally, we introduce $(\mathbf{Y}_t)_{t\in[0,T]}$ satisfying (S3) but such that $\mathbf{Y}_0 \sim p_{\text{ref}}$. Note that if $T \geq 0$ is large then the two processes $(\mathbf{Y}_t)_{t\in[0,T]}$ and $(\hat{\mathbf{X}}_t)_{t\in[0,T]}$ are close since $\mathcal{L}(\mathbf{X}_T)$ is close to p_{ref}.

Therefore, using the score network and a manifold ODE solver (as in Mathieu and Nickel, 2020), we are able to approximately solve the following ODE

$$\mathrm{d}\log q_t(\hat{\mathbf{X}}_t^\theta) = -\tfrac{1}{2}\operatorname{div}(\mathbf{s}_\theta(T-t,\cdot))(\hat{\mathbf{X}}_t^\theta)\mathrm{d}t,$$

with q_t the density of $\mathbf{Y}_t^\theta$ w.r.t. p_{ref} and $\log q_0(\mathbf{Y}_0) = 0$ with $\mathrm{d}\mathbf{Y}_t^\theta = \frac{1}{2}\operatorname{div}(\mathbf{s}_\theta(T-t,\mathbf{Y}_t^\theta))\mathrm{d}t$ and $\mathbf{Y}_0^\theta \sim p_{\text{ref}}$. The likelihood approximation of the model is then given by $\mathbb{E}[\log q_T(\hat{\mathbf{X}}_T^\theta)] = \int_{\mathcal{M}} \log q_T(x)\mathrm{d}p_{\text{data}}(x)$, where $(\hat{\mathbf{X}}_t^\theta)_{t\in[0,T]} = (\mathbf{X}_{T-t}^\theta)_{t\in[0,T]}$ with $\mathrm{d}\mathbf{X}_t^\theta = -\frac{1}{2}\operatorname{div}(\mathbf{s}_\theta(t,\mathbf{X}_t^\theta))\mathrm{d}t$ and $\mathbf{X}_0 \sim p_{\text{data}}$. In App. C.2, we highlight that this is *not* the likelihood of the SDE model.

C.2 Difference between ODE and SDE likelihood computations

In this section, we show that the likelihood computation from Song et al. (2021) does not coincide with the likelihood computation obtained with the SDE model. We present our findings in the Riemannian setting but our results can be adapted to the Euclidean setting with arbitrary forward dynamics. Recall that we consider a Brownian motion on the manifold as a forward process $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ with $(p_t)_{t\in[0,T]}$ the associated family of densities. We have that for any $t \in [0,T]$ and $x \in \mathcal{M}$

$$\partial_t p_t(x) = \tfrac{1}{2}\Delta_{\mathcal{M}} p_{t|0}(x) = \operatorname{div}(\tfrac{1}{2} p_t \nabla \log p_t)(x). \tag{S4}$$

ODE model. In the case of the ODE model, we define $(\mathbf{X}_t)_{t\in[0,T]}$ such that $\mathbf{X}_0 \sim p_0$ and satisfies $\mathrm{d}\mathbf{X}_t = -\frac{1}{2}\nabla \log p_t(\mathbf{X}_t)\mathrm{d}t$. The family of densities $(q_t)_{t\in[0,T]}$ associated with $(\mathbf{X}_t)_{t\in[0,T]}$ also satisfies (S4). Now consider $(\hat{\mathbf{X}}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$, this satisfies $\hat{\mathbf{X}}_0 \sim p_T$ with

$$\mathrm{d}\hat{\mathbf{X}}_t = \tfrac{1}{2}\nabla \log p_{T-t}(\hat{\mathbf{X}}_t)\mathrm{d}t. \tag{S5}$$

Finally, we consider $(\mathbf{Y}_t^{\text{ODE}})_{t\in[0,T]}$ which also satisfies Eq. (S5) and such that $\mathbf{Y}_0^{\text{ODE}} \sim p_{\text{ref}}$. Denoting $(q_t^{\text{ODE}})_{t\in[0,T]}$ the densities of $(\mathbf{Y}_t^{\text{ODE}})_{t\in[0,T]}$ w.r.t. p_{ref} we have for any $t \in [0,T]$ and $x \in \mathcal{M}$

$$\partial_t q_t^{\text{ODE}}(x) = -\operatorname{div}(\tfrac{1}{2} q_t^{\text{ODE}} \nabla \log p_{T-t})(x). \tag{S6}$$

SDE model. When sampling we consider a process $(\mathbf{Y}_t^{\text{SDE}})_{t\in[0,T]}$ such that $\mathbf{Y}_0^{\text{SDE}}$ has distribution p_{ref} and whose family of densities $(q_t^{\text{SDE}})_{t\in[0,T]}$ satisfies for any $t \in [0,T]$ and $x \in \mathcal{M}$

$$\partial_t q_t^{\text{SDE}}(x) = -\operatorname{div}(\nabla \log p_{T-t} q_t^{\text{SDE}}(x)) + \tfrac{1}{2}\Delta_{\mathcal{M}} q_t^{\text{SDE}}(x) = -\operatorname{div}(q_t^{\text{SDE}}\{\nabla \log p_{T-t} - \tfrac{1}{2}\nabla \log q_t^{\text{SDE}}\})(x). \tag{S7}$$

Hence, Eq. (S6) and Eq. (S7) do not agree, except if $q_t^{\text{SDE}} = q_t^{\text{ODE}} = p_{T-t}$ which is the case if and only if $\mathbf{Y}_0^{\text{SDE}}$ and $\mathbf{Y}_0^{\text{ODE}}$ have the same distribution as $\mathbf{X}_T$. Note that it is possible to evaluate the likelihood of the SDE model using that

$$\partial_t \log q_t^{\text{SDE}}(\mathbf{Y}_t^{\text{SDE}}) = \left\{\nabla \log p_{T-t}(\mathbf{Y}_t^{\text{SDE}}) - \tfrac{1}{2}\nabla \log q_t^{\text{SDE}}(\mathbf{Y}_t^{\text{SDE}})\right\}\mathrm{d}t.$$

We can use the score approximation $\boldsymbol{s}_\theta(t,x)$ to approximate $\nabla \log p_t(x)$ for any $t \in [0,T]$ and $x \in \mathcal{M}$. In order to approximate $\nabla \log q_t^{\text{SDE}}$, one can consider another neural network $\boldsymbol{t}_\theta(t,x)$ approximating $\nabla \log q_t^{\text{SDE}}(x)$ for any $t \in [0,T]$ and $x \in \mathcal{M}$. This approximation can be obtained using the implicit score loss presented in Sec. 3.4.

D Parametric family of vector fields

We approximate $(\nabla \log p_t)_{t\in[0,T]}$ by a family of functions $\{\mathbf{s}_\theta\}_{\theta\in\Theta}$ where Θ is a set of parameters and for any $\theta \in \Theta$, $\mathbf{s}_\theta : [0,T] \to \mathcal{X}(\mathcal{M})$. In this work, we consider several parameterisations of vector fields:

• **Projected vector field**. We define $\mathbf{s}_\theta(t,x) = \mathrm{proj}_{T_x\mathcal{M}}(\tilde{\mathbf{s}}_\theta(t,x)) = P(x)\tilde{\mathbf{s}}_\theta(t,x)$ for any $t \in [0,T]$ and $x \in \mathcal{M}$, with $\tilde{\mathbf{s}}_\theta : \mathbb{R}^p \times [0,T] \to \mathbb{R}^p$ an ambient vector field and $P(x)$ the orthogonal projection over $\mathrm{T}_x\mathcal{M}$ at $x \in M$. According to Rozen et al. (2021, Lemma 2), then $\mathrm{div}(\mathbf{s}_\theta)(x,t) = \mathrm{div}_E(\mathbf{s}_\theta)(x,t)$ for any $x \in \mathcal{M}$, where div_E denotes the standard Euclidean divergence.

• **Divergence-free vector fields**: For any Lie group G, any basis of the Lie algebra $\mathfrak{g} = \mathrm{T}_eG$ yields a global frame. Indeed, let $v \in \mathfrak{g}$ and define the flow $\Phi : \mathbb{R} \times \mathcal{M} \to \mathcal{M}$ given for any $t \in \mathbb{R}$ and $x \in M$ by $\Phi_t^v(x) = x \exp_e(tv)$. Then defining $\{E_i\}_{i=1}^d = \{\partial_t \Phi_0^{v_i}\}_{i=1}^d$, where $\{v_i\}_{i=1}^d$ is a basis of $\mathfrak{g}$, we get that $\{E_i\}_{i=1}^d$ is a left-invariant global frame. As a result, we have that for any $i \in \{1,\dots,d\}$, $\mathrm{div}(E_i) = 0$ (for the classical left invariant metric). This result simplifies the computation of $\mathrm{div}(\mathbf{s}_\theta)$ where $\mathbf{s}_\theta(t,x) = \sum_{i=1}^d s_\theta^i(t,x)E_i(x)$ for any $t \in [0,T]$ and $x \in \mathcal{M}$ since we have that $\mathrm{div}(\mathbf{s}_\theta)(t,x) = \sum_{i=1}^d E_i(s_\theta^i)(t,x) + \sum_{i=1}^d s_\theta^i(t,x)\mathrm{div}(E_i)(x) = \sum_{i=1}^d ds_\theta^i(E_i)(t,x)$ (see Falorsi and Forré, 2020). Note that this approach can be extended to any homogeneous space (G,H).

• **Coordinates vector fields**. We define $\mathbf{s}_\theta(t,x) = \sum_{i=1}^d \mathbf{s}_\theta^i(t,x)E_i(x)$ for any $t \in [0,T]$ and $x \in \mathcal{M}$, with $\{E_i\}_{i=1}^d = \{\partial_i \varphi(\varphi^{-1}(x))\}_{i=1}^d$ the vector fields induced by a choice of local coordinates, where φ is a local parameterization $\varphi : \mathsf{U} \to \mathcal{M}$ and $z \in \mathsf{U} \subset \mathbb{R}^d$. Then the divergence can be computed in these local coordinates $\mathrm{div}(\mathbf{s}_\theta)(t,\varphi(z)) = |\det G|^{-1/2} \sum_{i=1}^d \partial_i\{|\det G|^{1/2}\mathbf{s}_\theta^i(t,\varphi(\cdot))\}(z)$. In the case of the sphere, one recovers the standard divergence in spherical coordinates using this formula. Note that $\{E_i\}_{i=1}^d$ does not span the tangent bundle except if the manifold is parallelizable. The sphere is a well-known example of non-parallelizable manifold, as per the *hairy ball theorem*.

E Eigensystems of the Laplace–Beltrami operator and heat kernels

In this section, we recall the eigenfunctions and eigenvalues of the Laplace–Beltrami operator in two specific cases: the d-dimensional torus and the d-dimensional sphere. We also highlight that the heat kernel on compact manifold can be written as an infinite series using the Sturm–Liouville decomposition.

The case of the torus Let $\{b_i\}_{i=1}^d$ be a basis of $\mathbb{R}^d$. We consider the associated lattice on $\mathbb{R}^d$, i.e. $\Gamma = \{\sum_{i=1}^d \alpha_i b_i : \{\alpha_i\}_{i=1}^d \in \mathbb{Z}^d\}$. Finally, the associated d-dimensional torus is defined as $\mathbb{T}_\Gamma = \mathbb{R}^d/\Gamma$. Denote $\mathrm{B} = (b_1,\dots,b_d) \in \mathbb{R}^{d\times d}$. Let $\{\bar{b}_i\}_{i=1}^d \in (\mathbb{R}^d)^d$ such that $(\mathrm{B}^{-1})^\top = (\bar{b}_1,\dots,\bar{b}_d)$. We define $\Gamma^\star = \{\sum_{i=1}^d \alpha_i \bar{b}_i : \{\alpha_i\}_{i=1}^d \in \mathbb{Z}^d\}$, the dual lattice. Note that for any $x \in \Gamma$ and $y \in \Gamma^\star$ we have that $\langle x,y\rangle \in \mathbb{Z}$ and that if $\{b_i\}_{i=1}^d$ is an orthonormal basis then $\Gamma = \Gamma^\star$. The torus $\mathbb{R}^d/\Gamma$ is a (flat) compact Riemannian manifold. The set of eigenvalues of the Laplace–Beltrami operator is given by $\{-4\pi^2\|y\|^2 : y \in \Gamma^\star\}$. The eigenfunctions of the Laplace–Beltrami operator are given by $\{x \mapsto \sin(2\pi\langle x,y\rangle) : y \in \Gamma^\star\}$ and $\{x \mapsto \cos(2\pi\langle x,y\rangle) : y \in \Gamma^\star\}$.

The case of the sphere Next, we investigate the case of the d-dimensional sphere (see Saloff-Coste, 1994). The set of eigenvalues of the Laplace–Beltrami operator is given by $\{-k(k+d-1) : k \in \mathbb{N}\}$. Note that $\lambda_k = k(k+d-1)$ has multiplicity $d_k = (k+d-2)!/\{(d-1)!k\}(2k+d-1)$. The eigenfunctions of the Laplace–Beltrami operator are known as the spherical harmonics and can be defined in terms of Legendre polynomials. When investigating the heat kernel on the d-dimensional sphere, we are interested in the product $(x,y) \mapsto \sum_{\phi\in\Phi_n} \phi(x)\phi(y)$, where Φ_n is the set of eigenfunctions associated with the eigenvalue λ_n for $n \in \mathbb{N}$. This function can be described using the Gegenbauer polynomials (see Atkinson and Han, 2012, Theorem 2.9). More precisely, we have that for any $n \in \mathbb{N}$ and $x,y \in \mathbb{S}^d$

$$\begin{aligned} G_n(x,y) &= \textstyle\sum_{\phi\in\Phi_n} \phi(x)\phi(y) \\ &= n!\Gamma((d-1)/2)\textstyle\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k(1-\langle x,y\rangle^2)\langle x,y\rangle^{n-2k}/(4^k k!(n-2k)!\Gamma(k+(d-1)/2)), \end{aligned}$$

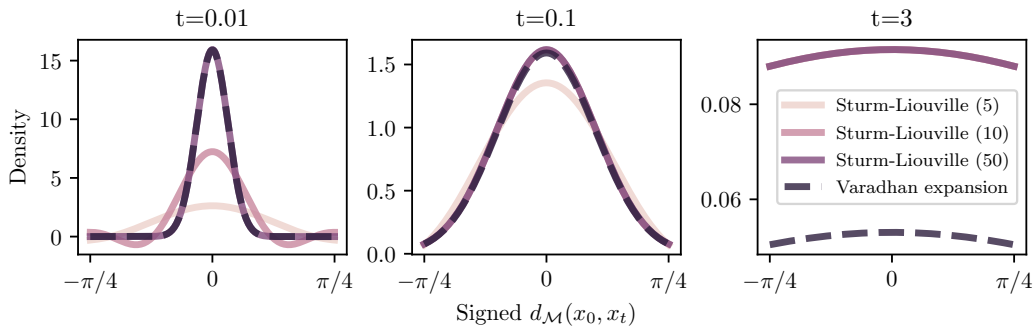


Figure S1: Slice of heat kernel $p_{t|0}(x_t|x_0)$ on $\mathbb{S}^2$ for different approximations.

where here $\Gamma : \mathbb{R}_+ \to \mathbb{R}$ is given for any $v > 0$ by $\Gamma(v) = \int_0^{+\infty} t^{v-1}\mathrm{e}^{-t}\mathrm{d}t$. In the special case where $d = 1$, then the heat kernel coincide with the wrapped Gaussian density and can be easily evaluated.

Heat kernel on compact Riemannian manifolds. We recall that in the case of compact manifolds the heat kernel is given by the Sturm–Liouville decomposition Chavel (1984) given for any $t > 0$ and $x, y \in \mathcal{M}$ by

$$p_{t|0}(y|x) = \sum_{j\in\mathbb{N}} \mathrm{e}^{-\lambda_j t}\phi_j(x)\phi_j(y), \tag{S8}$$

where the convergence occurs in $\mathrm{L}^2(p_{\text{ref}} \otimes p_{\text{ref}})$, $(\lambda_j)_{j\in\mathbb{N}}$ and $(\phi_j)_{j\in\mathbb{N}}$ are the eigenvalues, respectively the eigenvectors, of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(p_{\text{ref}})$ (see Saloff-Coste, 1994, Section 2). When the eigenvalues and eigenvectors are known, we approximate the logarithmic gradient of $p_{t|0}$ by truncating the sum in (S8) with $J \in \mathbb{N}$ terms. Another possibility to approximate $\nabla \log p_{t|0}$ is to rely on the so-called Varadhan approximation, see Sec. 3.4, which is valid for small $t > 0$. Fig. S1 illustrates these different approximations of the heat kernel and Table 1 compares the different loss functions.

Table 1: Riemannian score matching losses.

Loss	Approximation	Loss function	Unbiased	Consistent	Variance
$\ell_{t\|0}$ (DSM)	Truncation (7)	$\frac{1}{2}\mathbb{E}\left[\|s(\mathbf{X}_t) - S_{J,t}(\mathbf{X}_0, \mathbf{X}_t)\|^2\right]$	✗	✓$(J \to \infty)$	0
	Varhadan (8)	$\frac{1}{2}\mathbb{E}\left[\|s(\mathbf{X}_t) - \log_{\mathbf{X}_t}(\mathbf{X}_0)/t\|^2\right]$	✗	✓$(t \to 0)$	0
$\ell_{t\|s}$ (DSM)	Varhadan (8)	$\frac{1}{2}\mathbb{E}\left[\|s(\mathbf{X}_t) - \log_{\mathbf{X}_t}(\mathbf{X}_s)/(t-s)\|^2\right]$	✗	✓$(t \to s)$	0
ℓ_t^{im} (ISM)	Deterministic	$\mathbb{E}\left[\frac{1}{2}\|s(\mathbf{X}_t)\|^2 + \mathrm{div}(s)(\mathbf{X}_t)\right]$	✓	✓	0
	Stochastic	$\mathbb{E}\left[\frac{1}{2}\|s(\mathbf{X}_t)\|^2 + \varepsilon^\top \partial s(\mathbf{X}_t)\varepsilon\right]$	✓	✓	$2\|\partial s\|_F$

F Predictor-corrector schemes

In this section, we present a predictor-corrector scheme, adapting the techniques of Allgower and Georg (2012); Song et al. (2021) to the manifold setting. Changes between Algorithm 1, Algorithm 2 and Algorithm 3, Algorithm 4 are highlighted in red. Let $t \in [0, T]$, $\gamma > 0$ and $k = \lfloor t/\gamma \rfloor$. We remark that Algorithm 3 (Line 11) corresponds to the recursion associated with $(X_j^{t,\gamma})_{j\in\mathbb{N}}$ such that for any $j \in \mathbb{N}$

$$X_{j+1}^{t,\gamma} = \exp_{X_j^{t,\gamma}}[\tfrac{\gamma}{2}\nabla \log p_{T-k\gamma}(X_j^{t,\gamma}) + \sqrt{\gamma}Z_{j+1}],$$

where $\{\bar{Z}_j\}_{j\in\mathbb{N}}$ is a family of i.i.d Gaussian random variables with zero mean and identity covariances matrix in $\mathbb{R}^p$ and for any $j \in \mathbb{N}$, $Z_j = \mathrm{P}(X_j^{t,\gamma})\bar{Z}_j$. Note that here $k \in \{0, N-1\}$ is fixed. Letting $\gamma \to 0$, we obtain that under mild assumptions, see (Kuwada, 2012, Theorem 3.1), $(X_j^{t,\gamma})_{j\in\mathbb{N}}$ converges to $(\mathbf{X}_s^t)_{s\geq 0}$ such that

$$\mathrm{d}\mathbf{X}_s^t = \tfrac{1}{2}\nabla \log p_{T-t}(\mathbf{X}_s^t)\mathrm{d}s + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}.$$

We have that p_{T-t} is the invariant measure of $(\mathbf{X}_s^t)_{s\geq 0}$. Hence, the role of the corrector step is to project the distribution back onto p_{T-t} for all times $t \in [0, T]$, see Fig. S2.

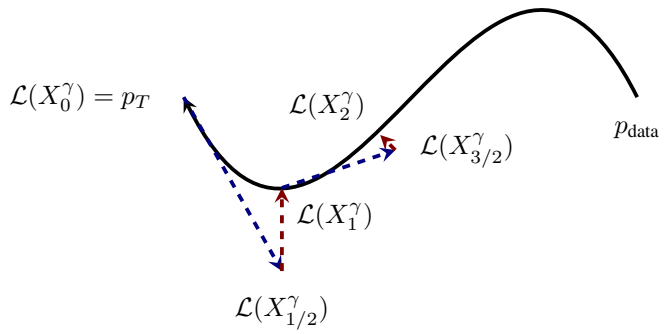


Figure S2: Illustration of the effect of the corrector step on RSGM. The black line corresponds to the dynamics of the noising process $(p_t)_{t\in[0,T]}$. The green dashed lines correspond to the predictor step (going backward in time) and the red dashed lines correspond to the corrector step (projecting back onto the initial dynamics). Note that $\mathcal{L}(X_1^\gamma) \approx p_{T-\gamma}$ and $\mathcal{L}(X_2^\gamma) \approx p_{T-2\gamma}$.

Algorithm 3 GRW-c (Geodesic Random Walk with corrector)

Require: $T, N, X_0^\gamma, b, \sigma, \mathrm{P}$

$\gamma = T/N$ ▷ Step-size
for $k \in \{0, \dots, N-1\}$ **do**
  /// PREDICTOR STEP
  $\bar{Z}_{k+1/2} \sim \mathrm{N}(0, \mathrm{I}_p)$ ▷ Standard Gaussian in ambient space $\mathbb{R}^p$
  $Z_{k+1/2} = \mathrm{P}(X_k^\gamma)\bar{Z}_{k+1/2}$ ▷ Projection in the tangent space $\mathrm{T}_x\mathcal{M}$
  $W_{k+1/2} = \gamma b(k\gamma, X_k^\gamma) + \sqrt{\gamma}\sigma(k\gamma, X_k^\gamma)Z_{k+1/2}$ ▷ Euler–Maruyama step on tangent space
  $X_{k+1/2}^\gamma = \exp_{X_k^\gamma}[W_{k+1/2}]$ ▷ Geodesic projection onto $\mathcal{M}$
  /// CORRECTOR STEP
  $\bar{Z}_{k+1} \sim \mathrm{N}(0, \mathrm{I}_p)$ ▷ Standard Gaussian in ambient space $\mathbb{R}^p$
  $Z_{k+1} = \mathrm{P}(X_{k+1/2}^\gamma)\bar{Z}_{k+1}$ ▷ Projection in the tangent space $\mathrm{T}_x\mathcal{M}$
  $W_{k+1} = \frac{\gamma}{2} b(k\gamma, X_{k+1/2}^\gamma) + \sqrt{\gamma}\sigma(k\gamma, X_{k+1/2}^\gamma)Z_{k+1}$ ▷ Euler–Maruyama step on tangent space
  $X_{k+1}^\gamma = \exp_{X_{k+1/2}^\gamma}[W_{k+1}]$ ▷ Geodesic projection onto $\mathcal{M}$
end for
return $\{X_k^\gamma\}_{k=0}^N$

G Time-reversal formula: extension to compact Riemannian manifolds

In this section, we provide the proof of Theorem 1. The proof follows the arguments of Cattiaux et al. (2021, Theorem 4.9). We could have also applied the abstract results of Cattiaux et al. (2021, Theorem 5.7) to obtain our results. Note that the time-reversal on manifold could also be obtained by readily extending arguments from Haussmann and Pardoux (1986), however the entropic conditions found by Cattiaux et al. (2021) are more natural when it comes to the study of the Schrödinger Bridge problem. For the interested reader we provide an informal derivation of the time-reversal formula obtained by Haussmann and Pardoux (1986) in App. G.1. The proof of Theorem 1 is given in App. G.2. Finally, we emphasize that García-Zelada and Huguet (2021) have developed a Girsanov theory for stochastic processes defined on compact manifolds with boundary in order to study the Brenier-Schrödinger problem.

Algorithm 4 RSGM-c (Riemannian Score-Based Generative Model with corrector)

Require: $\varepsilon, T, N, \{X_0^m\}_{m=1}^M, \mathrm{loss}, \mathbf{s}, \theta_0, N_{\text{iter}}, p_{\text{ref}}, \mathrm{P}$

/// TRAINING ///
for $n \in \{0, \dots, N_{\text{iter}} - 1\}$ **do**
  $X_0 \sim (1/M) \sum_{m=1}^M \delta_{X_0^m}$ ▷ Random mini-batch from dataset
  $t \sim U([\varepsilon, T])$ ▷ Uniform sampling between ε and T
  $\mathbf{X}_t = \mathrm{GRW}(t, N, X_0, 0, \mathrm{Id}, \mathrm{P})$ ▷ Approximate forward diffusion with Algorithm 1
  $\ell(\theta_n) = \ell_t(T, N, X_0, \mathbf{X}_t, \mathrm{loss}, \mathbf{s}_{\theta_n})$ ▷ Compute score matching loss from Table 2
  $\theta_{n+1} = \texttt{optimizer_update}(\theta_n, \ell(\theta_n))$ ▷ ADAM optimizer step
end for
$\theta^\star = \theta_{N_{\text{epoch}}}$
/// SAMPLING ///
$Y_0 \sim p_{\text{ref}}$ ▷ Sample from uniform distribution
$b_\theta^\star(t, x) = \mathbf{s}_{\theta^\star}(T - t, x)$ for any $t \in [0, T]$, $x \in \mathcal{M}$ ▷ Reverse process drift
$\{Y_k\}_{k=0}^N = \text{GRW-c}(T, N, Y_0, b_{\theta^\star}, \mathrm{Id}, \mathrm{P})$ ▷ Approximate reverse diffusion with Algorithm 3
return $\theta^\star, \{Y_k\}_{k=0}^N$

G.1 Informal derivation

In this section, we provide a non-rigorous derivation of Theorem 1 following the approach of Haussmann and Pardoux (1986). Let $(\mathbf{X}_t)_{t\in[0,T]}$ be a continuous process such that for any $f \in \mathrm{C}^2(\mathcal{M})$ we have that $(\mathbf{M}_t^{\mathbf{X},f})_{t\in[0,T]}$ is a $\mathbf{X}$-martingale where for any $t \in [0, T]$

$$\mathbf{M}_t^{\mathbf{X},f} = f(\mathbf{X}_t) - \int_0^t \{\langle b(\mathbf{X}_s), \nabla f(\mathbf{X}_s)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(\mathbf{X}_s)\}\mathrm{d}s. \tag{S9}$$

Let $(\mathbf{Y}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$. Our goal is to show that for any $f \in \mathrm{C}^2(\mathcal{M})$, $(\mathbf{M}_t^{\mathbf{Y},f})_{t\in[0,T]}$ is a $\mathbf{Y}$-martingale where for any $t \in [0, T]$

$$\mathbf{M}_t^{\mathbf{Y},f} = f(\mathbf{Y}_t) - \int_0^t \{\langle -b(\mathbf{Y}_s) + \nabla \log p_{T-s}(\mathbf{Y}_s), \nabla f(\mathbf{Y}_s)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(\mathbf{Y}_s)\}\mathrm{d}s.$$

Note that here we implicitly assume that for any $t \in [0, T]$, $\mathbf{X}_t$ admits a smooth positive density w.r.t. p_{ref} denoted p_t. In other words, we want to show that for any $g \in \mathrm{C}^2(\mathcal{M})$ and $s, t \in [0, T]$ with $t \geq s$ we have

$$\begin{aligned}&\mathbb{E}[g(\mathbf{Y}_s)(f(\mathbf{Y}_t) - f(\mathbf{Y}_s))] \\ &\quad = \mathbb{E}[g(\mathbf{Y}_s) \int_s^t \{\langle -b(\mathbf{Y}_u) + \nabla \log p_{T-u}(\mathbf{Y}_u), \nabla f(\mathbf{Y}_u)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(\mathbf{Y}_u)\}\mathrm{d}u].\end{aligned} \tag{S10}$$

We introduce the infinitesimal generator $\mathcal{A} : \mathrm{C}^2(\mathcal{M}) \to \mathrm{C}(\mathcal{M})$ given for any $f \in \mathrm{C}^2(\mathcal{M})$ and $x \in \mathcal{M}$ by

$$\mathcal{A}(f)(x) = \langle b(x), \nabla f(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(x).$$

Similarly, we introduce the infinitesimal generator $\tilde{\mathcal{A}} : [0, T] \times \mathrm{C}^2(\mathcal{M}) \to \mathrm{C}(\mathcal{M})$ given for any $f \in \mathrm{C}^2(\mathcal{M})$, $t \in [0, T]$ and $x \in \mathcal{M}$ by

$$\tilde{\mathcal{A}}(t, f)(x) = \langle -b(x) + \nabla \log p_{T-t}(x), \nabla f(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(x).$$

With these notations, (S11) can be written as follows: we want to show that for any $g \in \mathrm{C}^2(\mathcal{M})$ and $s, t \in [0, T]$ with $t \geq s$ we have

$$\mathbb{E}[g(\mathbf{Y}_s)(f(\mathbf{Y}_t) - f(\mathbf{Y}_s))] = \mathbb{E}[g(\mathbf{Y}_s) \int_s^t \tilde{\mathcal{A}}(u, \mathbf{Y}_u)\mathrm{d}u]. \tag{S11}$$

The rest of this section follows the first part of the proof of Haussmann and Pardoux (1986, Theorem 2.1). Let $t, s \in [0, T]$ with $t \geq s$. We have

$$\begin{aligned}\mathbb{E}[g(\mathbf{Y}_s)(f(\mathbf{Y}_t) - f(\mathbf{Y}_s))] &= \mathbb{E}[g(\mathbf{X}_{T-s})(f(\mathbf{X}_{T-t}) - f(\mathbf{X}_{T-t}))] \\ &= \mathbb{E}[\mathbb{E}[g(\mathbf{X}_{T-s})|\mathbf{X}_{T-t}]f(\mathbf{X}_{T-t})] - \mathbb{E}[g(\mathbf{X}_{T-s})f(\mathbf{X}_{T-s})] \\ &= \mathbb{E}[v(T-t, \mathbf{X}_{T-t})f(\mathbf{X}_{T-t})] - \mathbb{E}[v(T-s, \mathbf{X}_{T-s})f(\mathbf{X}_{T-s})],\end{aligned} \tag{S12}$$

with $v : [0, T-s] \times \mathcal{M} \to \mathbb{R}$ given for any $u \in [0, T-s]$ and $x \in \mathcal{M}$ by $v(u, x) = \mathbb{E}[g(\mathbf{X}_{T-s})|\mathbf{X}_u = x]$. We have that v satisfies the backward Kolmogorov equation, i.e. we have for any $u \in [0, T-s]$ and $x \in \mathcal{M}$

$$\partial_u v(u, x) = -\mathcal{A}v(u, x). \tag{S13}$$

Note that it is not trivial to show that v is regular enough to satisfy the backward Kolmogorov equation. In this informal derivation, we assume that v is regular enough and will provide a different rigorous proof of the time-reversal formula in App. G.2. However, note that it is possible to show that v indeed satisfies the backward Kolmogorov equation by adapting arguments from Haussmann and Pardoux (1986) to the manifold framework.

Let $h: [0, T-s] \times \mathcal{M} \to \mathbb{R}$ given for any $u \in [0, T-s]$ and $x \in \mathcal{M}$ by $h(u,x) = v(u,x)f(x)$. Using (S13), we have for any $u \in [0, T-s]$ and $x \in \mathcal{M}$

$$\begin{aligned}\partial_u h(u,x) + \mathcal{A}h(u,x) &= f(x)\partial_u v(u,x) + f(x)\mathcal{A}v(u,x) + v(u,x)\mathcal{A}f(x) + \langle \nabla f(x), \nabla v(u,x)\rangle \\ &= v(u,x)\mathcal{A}f(x) + \langle \nabla f(x), \nabla v(u,x)\rangle. \end{aligned} \tag{S14}$$

In addition, using the divergence theorem (see Lee, 2018, p.51), we have for any $u \in [0, T-s]$

$$\begin{aligned}\mathbb{E}[\langle \nabla f(\mathbf{X}_u), \nabla v(u, \mathbf{X}_u)\rangle] &= \int_{\mathcal{M}} \langle \nabla f(x_u), \nabla v(u, x_u) p_u(x_u)\rangle \mathrm{d}p_{\text{ref}}(x_u) \\ &= -\int_{\mathcal{M}} v(u,x_u)\mathrm{div}(p_u \nabla f)(x_u)\mathrm{d}p_{\text{ref}}(x_u) \\ &= -\int_{\mathcal{M}} v(u,x_u)\Delta_{\mathcal{M}} f(x_u) p_u(x_u)\mathrm{d}p_{\text{ref}}(x_u) \\ &\quad - \int_{\mathcal{M}} v(u,x_u)\langle \nabla f(x_u), \nabla \log p_u(x_u)\rangle p_u(x_u)\mathrm{d}p_{\text{ref}}(x_u) \\ &= -\mathbb{E}[v(u,\mathbf{X}_u)\Delta_{\mathcal{M}} f(\mathbf{X}_u)] - \mathbb{E}[v(u,\mathbf{X}_u)\langle \nabla f(\mathbf{X}_u), \nabla \log p_u(\mathbf{X}_u)\rangle].\end{aligned}$$

Therefore, using this result and (S14) we get that for any $u \in [0, T-s]$

$$\begin{aligned}\mathbb{E}[\partial_u h(u,\mathbf{X}_u) + \mathcal{A}h(u,\mathbf{X}_u)] &= \mathbb{E}[v(u,\mathbf{X}_u)\{\langle b(\mathbf{X}_u) - \nabla \log p_u(\mathbf{X}_u), \nabla f(\mathbf{X}_u)\rangle - \tfrac{1}{2}\Delta_{\mathcal{M}} f(\mathbf{X}_u)\}] \\ &= -\mathbb{E}[v(u,\mathbf{X}_u)\tilde{\mathcal{A}}(T-u, f)(\mathbf{X}_u)].\end{aligned}$$

Combining this result and (S9) and that for any $u \in [0, T-s]$ and $x \in \mathcal{M}$, $v(u,x) = \mathbb{E}[g(\mathbf{X}_{T-s})|\mathbf{X}_u = x]$ we get

$$\begin{aligned}&\mathbb{E}[v(T-t, \mathbf{X}_{T-t})f(\mathbf{X}_{T-t})] - \mathbb{E}[v(T-s, \mathbf{X}_{T-s})f(\mathbf{X}_{T-s})] \\ &\quad = \mathbb{E}[h(T-t, \mathbf{X}_{T-t}) - h(T-s, \mathbf{X}_{T-s})] \\ &\quad = \int_{T-t}^{T-s} \mathbb{E}[v(u,\mathbf{X}_u)\tilde{\mathcal{A}}(T-u, \mathbf{X}_u)]\mathrm{d}u \\ &\quad = \mathbb{E}[g(\mathbf{X}_{T-s}) \int_{T-t}^{T-s} \tilde{\mathcal{A}}(T-u, \mathbf{X}_u)\mathrm{d}u].\end{aligned}$$

Using this result, (S12) and the change of variable $u \mapsto T-u$ we obtain

$$\mathbb{E}[g(\mathbf{Y}_s)(f(\mathbf{Y}_t) - f(\mathbf{Y}_s))] = \mathbb{E}[g(\mathbf{X}_{T-s}) \int_{T-t}^{T-s} \tilde{\mathcal{A}}(T-u, \mathbf{X}_u)\mathrm{d}u] = \mathbb{E}[g(\mathbf{Y}_s) \int_s^t \tilde{\mathcal{A}}(u, \mathbf{Y}_u)\mathrm{d}u].$$

Hence, (S11) holds and we have proved Theorem 1. Again, we emphasize that in order to make the proof completely rigourous one needs to derive regularity properties of v.

G.2 Proof of Theorem 1

In this section, we follow another approach to prove the time-reversal formula. We are going to use the integration by part formula of Cattiaux et al. (2021, Theorem 3.17) in a similar spirit as Cattiaux et al. (2021, Theorem 4.9) in the Euclidean setting. In order to adapt arguments from Cattiaux et al. (2021) to our Riemannian setting, we use the Nash embedding theorem in order to embed our processes in a Euclidean space and leverage tools from Girsanov theory. The rest of the section is organized as follows. First in App. G.2.1, we recall basic properties of infinitesimal generators and recall the integration by part formula of Cattiaux et al. (2021, Theorem 3.17). Then in App. G.2.2, we extend some Girsanov theory to compact Riemannian manifolds using the Nash embedding theorem. We conclude the proof in App. G.2.3.

G.2.1 Diffusion processes and integration by part formula

In this section, we state a simplified version of Cattiaux et al. (2021, Theorem 3.17) for Markov continuous path (probability) measure on Polish spaces. Let $(\mathsf{X}, \mathcal{X})$ be a Polish space. We say that $\mathbb{P}$ is a path measure if $\mathbb{P} \in \mathcal{P}(\mathrm{C}([0,T], \mathsf{X}))$. Let $(\mathbf{X}_t)_{t\in[0,T]}$ with distribution $\mathbb{P}$. We denote $(\mathcal{F}_t)_{t\in[0,T]}$ the filtration such that for any $t \in [0,T]$, $\mathcal{F}_t = \sigma(\mathbf{X}_s,\ s \in [0,t])$. Let $(\mathbf{M}_t)_{t\in[0,T]}$ be a Polish-valued stochastic process. We say that $(\mathbf{M}_t)_{t\in[0,T]}$ is a $\mathbb{P}$-local martingale if it is a local martingale w.r.t. the filtration $(\mathcal{F}_t)_{t\in[0,T]}$. A function $u: [0,T] \times \mathsf{X} \to \mathbb{R}$ is said to be in the domain of the extended generator of $\mathbb{P}$ if there exists a process $(\bar{\mathcal{A}}_{\mathbb{P}} u(t, \mathbf{X}_{[0,t]}))_{t\in[0,T]}$ such that:

(a) $(\bar{\mathcal{A}}_{\mathbb{P}} u(t, \mathbf{X}_{[0,t]}))_{t\in[0,T]}$ is adapted w.r.t. $(\mathcal{F}_t)_{t\in[0,T]}$.

(b) $\int_0^T |\bar{\mathcal{A}}_{\mathbb{P}} u(t, \mathbf{X}_{[0,t]})| \mathrm{d}t < +\infty$, $\mathbb{P}$-a.s.

(c) The process $(\mathbf{M}_t)_{t\in[0,T]}$ is a $\mathbb{P}$-local martingale, where for any $t \in [0,T]$

$$\mathbf{M}_t = u(t, \mathbf{X}_t) - u(0, \mathbf{X}_0) - \int_0^t \bar{\mathcal{A}}_{\mathbb{P}} u(s, \mathbf{X}_{[0,s]}) \mathrm{d}s.$$

The domain of the extended generator is denoted $\mathrm{dom}(\bar{\mathcal{A}}_{\mathbb{P}})$. We say that (u, v) with $u, v : [0,T] \times \mathsf{X} \to \mathbb{R}$ is in the domain of the carré du champ if $u, v, uv \in \mathrm{dom}(\bar{\mathcal{A}}_{\mathbb{P}})$. In this case, we define the carré du champ $\bar{\Upsilon}_{\mathbb{P}}$ as

$$\bar{\Upsilon}_{\mathbb{P}}(u, v) = \bar{\mathcal{A}}_{\mathbb{P}}(uv) - \bar{\mathcal{A}}_{\mathbb{P}}(u)v - \bar{\mathcal{A}}_{\mathbb{P}}(v)u.$$

Note that if $\mathsf{X} = \mathcal{M}$ is a Riemannian manifold, $\mathrm{C}^2(\mathcal{M}) \subset \mathrm{dom}(\bar{\mathcal{A}}_{\mathbb{P}})$ and for any $u \in \mathrm{C}^2(\mathcal{M})$ $\bar{\mathcal{A}}_{\mathbb{P}}(u) = \langle \nabla u, X \rangle + \frac{1}{2}\Delta_{\mathcal{M}} u$ with $X \in \Gamma(\mathrm{T}\mathcal{M})$ then we have that $\mathrm{C}^2(\mathcal{M}) \times \mathrm{C}^2(\mathcal{M}) \subset \mathrm{dom}(\bar{\Upsilon}_{\mathbb{P}})$ and for any $u, v \in \mathrm{C}^2(\mathcal{M})$, $\bar{\Upsilon}_{\mathbb{P}}(u, v) = \langle \nabla u, \nabla v \rangle$. Assume that there exists $\mathcal{U}_{\mathbb{P}} \subset \mathrm{dom}(\bar{\mathcal{A}}_{\mathbb{P}}) \cap \mathrm{C}_b(\mathsf{X})$ such that $\mathcal{U}_{\mathbb{P}}$ is an algebra. We denote $\mathcal{U}_{\mathbb{P},2}$ such that

$$\mathcal{U}_{\mathbb{P},2} = \{u \in \mathcal{U}_{\mathbb{P}} \,:\, \bar{\mathcal{A}}_{\mathbb{P}} u \in \mathrm{L}^2(\mathbb{P}),\ \bar{\Upsilon}_{\mathbb{P}}(u, u) \in \mathrm{L}^1(\mathbb{P})\}.$$

Finally we denote $R(\mathbb{P})$ the time-reverse path measure, i.e. for any $\mathsf{A} \in \mathcal{B}(\mathrm{C}([0,T], \mathsf{X}))$ we have $R(\mathbb{P})(\mathsf{A}) = \mathbb{P}(R(\mathsf{A}))$, where $R(\mathsf{A}) = \{t \mapsto \omega_{T-t} \,:\, \omega \in \mathsf{A}\}$. In what follows, we assume $\mathbb{P}$ is Markov. It is well-known, see (Léonard et al., 2014, Theorem 1.2) for instance, that in this case $R(\mathbb{P})$ is also Markov. In addition, since $\mathbb{P}$ is Markov, for any $u \in \mathrm{dom}(\bar{\mathcal{A}}_{\mathbb{P}})$ and $t \in [0,T]$ there exists $\mathcal{A}_{\mathbb{P}}$ such that $\bar{\mathcal{A}}_{\mathbb{P}} u(t, \mathbf{X}_{[0,t]}) = \mathcal{A}_{\mathbb{P}} u(t, \mathbf{X}_t)$ with $\mathcal{A}_{\mathbb{P}} u : [0,T] \times \mathsf{X} \to \mathbb{R}$. Similarly, we define $\Upsilon_{\mathbb{P}}(u, v) : [0,T] \times \mathsf{X} \to \mathbb{R}$ from $\bar{\Upsilon}_{\mathbb{P}}(u, v)$.

We are now ready to state the integration by part formula, (Cattiaux et al., 2021, Theorem 3.17).

Theorem S11. *Let $u, v \in \mathcal{U}_{\mathbb{P},2}$. The following hold:*

(a) If $u \in \mathrm{dom}(\mathcal{A}_{R(\mathbb{P})})$ and $\mathcal{A}_{R(\mathbb{P})} u \in \mathrm{L}^1(\mathbb{P})$ then for almost any $t \in [0,T]$

$$\mathbb{E}[\{\mathcal{A}_{\mathbb{P}} u(t, \mathbf{X}_t) + \mathcal{A}_{R(\mathbb{P})} u(T-t, \mathbf{X}_t)\} v(\mathbf{X}_t) + \Upsilon_{\mathbb{P}}(u, u)(t, \mathbf{X}_t)] = 0.$$

(b) If the following hold:

i) $\Upsilon_{\mathbb{P}}(u, v) \in \mathrm{C}([0,T] \times \mathsf{X}, \mathbb{R})$.

ii) $\mathcal{U}_{2,\mathbb{P}}$ determines the weak convergence of Borel measures.

iii) μ defines a finite measure on $[0,T] \times \mathsf{X}$ where for any $\omega \in \bar{\mathcal{U}}_{2,\mathbb{P}}$ we have

$$\mu[\omega] = \mathbb{E}[\int_0^T \Upsilon_{\mathbb{P}}(u, \omega_t)(t, \mathbf{X}_t) \mathrm{d}t],$$

where $\bar{\mathcal{U}}_{2,\mathbb{P}} = \{\omega \in \mathrm{C}([0,T] \times \mathsf{X}, \mathbb{R}) \,:\, \omega(t, \cdot) \in \mathcal{U}_{2,\mathbb{P}}$ for any $t \in [0,T]\}$.

Then $u \in \mathrm{dom}(\mathcal{A}_{R(\mathbb{P})})$ and $\mathcal{A}_{R(\mathbb{P})} u \in \mathrm{L}^1(\mathbb{P})$.

Note that this theorem is a simplified version of Cattiaux et al. (2021, Theorem 3.17) where we restrict ourselves to the case of Markov path measures. In what follows, we wish to apply Theorem S11 to diffusion processes on manifolds. To do so, we will verify that under a finite entropy assumption, the conditions $u \in \mathrm{dom}(\mathcal{A}_{R(\mathbb{P})})$ and $\mathcal{A}_{R(\mathbb{P})} u \in \mathrm{L}^1(\mathbb{P})$ are fullfilled for a class of regular functions u. These integrability results are obtained using Girsanov theory.

G.2.2 Girsanov theory on compact Riemannian manifolds

In this section, we will consider two types of martingale problems: one on Euclidean spaces and one on the compact Riemannian manifold $\mathcal{M}$. Let $\mathbb{P} \in \mathcal{P}(\mathrm{C}([0,T], \mathbb{R}^p))$. We say that $\mathbb{P}$ satisfies the (Euclidean) martingale problem with infinitesimal generator $\mathcal{A} : [0,T] \times \mathrm{C}^2(\mathbb{R}^p) \times \mathbb{R}^p \to \mathbb{R}$ if for any $u \in \mathrm{C}^2_c(\mathbb{R}^p)$, $(\mathbf{M}_t)_{t\in[0,T]}$ is a $\mathbb{P}$-martingale where for any $t \in [0,T]$ we have

$$\mathbf{M}_t = \mathbf{M}_0 + \int_0^t \mathcal{A}(t, u)(\mathbf{X}_s) \mathrm{d}s,$$

where $(\mathbf{X}_t)_{t\in[0,T]}$ has distribution $\mathbb{P}$ and $\int_0^T |\mathcal{A}(t,u)(\mathbf{X}_s)\mathrm{d}t| < +\infty$, $\mathbb{P}$-a.s. Let $\mathbb{P} \in \mathcal{P}(\mathrm{C}([0,T],\mathcal{M}))$. We say that $\mathbb{P}$ satisfies the (Riemannian) martingale problem with infinitesimal generator $\tilde{\mathcal{A}}:\ [0,T]\times \mathrm{C}^2(\mathcal{M})\times\mathcal{M}\to\mathbb{R}$ if for any $u\in\mathrm{C}^2(\mathcal{M})$, $(\mathbf{M}_t)_{t\in[0,T]}$ is a $\mathbb{P}$-martingale where for any $t\in[0,T]$ we have

$$\mathbf{M}_t = \mathbf{M}_0 + \int_0^t \tilde{\mathcal{A}}(t,u)(\mathbf{X}_s)\mathrm{d}s,$$

where $(\mathbf{X}_t)_{t\in[0,T]}$ has distribution $\mathbb{P}$ and $\int_0^T |\tilde{\mathcal{A}}(t,u)(\mathbf{X}_s)\mathrm{d}t| < +\infty$, $\mathbb{P}$-a.s. We now prove the following theorem.

Proposition S12. *Let $\mathbb{Q}$ be the path measure of a Brownian motion on $\mathcal{M}$. Let $\mathbb{P}$ be a Markov path measure on $\mathrm{C}([0,T],\mathcal{M})$ such that $\mathrm{KL}\left(\mathbb{P}|\mathbb{Q}\right) < +\infty$. Then there exists β such that for any $t\in[0,T]$ and $x\in\mathcal{M}$, $\beta(t,x)\in\mathrm{T}_x\mathcal{M}$ and we have that $\mathbb{P}$ satisfies the martingale problem with infinitesimal generator $\mathcal{A}$ where for any $t\in[0,T]$, $u\in\mathrm{C}^2(\mathcal{M})$ and $x\in\mathcal{M}$ we have*

$$\mathcal{A}(t,u)(x) = \langle \beta(t,x), \nabla u(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} u(x).$$

In addition, we have that

$$\mathrm{KL}\left(\mathbb{P}|\mathbb{Q}\right) = \mathrm{KL}\left(\mathbb{P}_0|\mathbb{Q}_0\right) + \tfrac{1}{2}\int_0^T \mathbb{E}[\|\beta(t,\mathbf{X}_t)\|^2]\mathrm{d}t,$$

where $(\mathbf{X}_t)_{t\in[0,T]}$ has distribution $\mathbb{P}$.

Proof. First, we extend $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ to $\mathbb{R}^p$ using the Nash embedding theorem (see Gunther, 1991). $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ can be seen as a process on $\mathbb{R}^p$ (for some $p\in\mathbb{N}$) which satisfies in a weak sense

$$\mathrm{d}\mathbf{B}_t^{\mathcal{M}} = \textstyle\sum_{i=1}^p \mathrm{P}_i(\mathbf{B}_t^{\mathcal{M}})\circ \mathrm{d}\mathbf{B}_t^i = P(\mathbf{B}_t^{\mathcal{M}})\circ\mathrm{d}\mathbf{B}_t,$$

where $(\mathbf{B}_t)_{t\in[0,T]}$ is a p-dimensional Brownian motion and $\mathrm{P}\in\mathrm{C}^\infty(\mathbb{R}^p,\mathbb{R}^{p\times p})$ is such that for any $x\in\mathcal{M}$, $\mathrm{P}(x)$ is the projection onto $\mathrm{T}_x\mathcal{M}$ and for any $i\in\{1,\dots,p\}$, $\mathrm{P}_i\in\mathrm{C}^\infty(\mathbb{R}^p,\mathbb{R}^p)$ with $\mathrm{P}_i = \mathrm{P}e_i$ where $\{e_j\}_{j=1}^p$ is the canonical basis of $\mathbb{R}^p$. We refer to App. B.1 for more details on the projection operator and its extension to $\mathbb{R}^p$. Using the link between Stratanovitch and Itô integral, there exists $\bar{b}\in\mathrm{C}^\infty(\mathbb{R}^p,\mathbb{R}^p)$ such that $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ can be seen as a process on $\mathbb{R}^p$ which satisfies in a weak sense

$$\mathrm{d}\mathbf{B}_t^{\mathcal{M}} = \bar{b}(\mathbf{B}_t^{\mathcal{M}})\mathrm{d}t + \mathrm{P}(\mathbf{B}_t^{\mathcal{M}})\mathrm{d}\mathbf{B}_t,$$

where $\bar{b}$ is given in (S2) and satisfies $\mathrm{P}\bar{b}(x) = 0$ for any $x\in\mathcal{M}$, see the remark following (S2). For any $u,v\in\mathrm{C}_c^2(\mathcal{M})$, we consider $\bar{u},\bar{v}$ extensions to $\mathrm{C}_c^2(\mathbb{R}^p)$ and we have for any $s,t\in[0,T]$

$$\begin{aligned}&\mathbb{E}[\bar{v}(\mathbf{B}_s^{\mathcal{M}})\textstyle\int_s^t \tfrac{1}{2}\Delta_{\mathcal{M}} u(\mathbf{B}_u^{\mathcal{M}})\mathrm{d}u]\\ &\quad= \mathbb{E}[\bar{v}(\mathbf{B}_s^{\mathcal{M}})\textstyle\int_s^t\{\langle\nabla\bar{u}(\mathbf{B}_w^{\mathcal{M}}),\bar{b}(\mathbf{B}_w^{\mathcal{M}})\rangle + \tfrac{1}{2}\langle\mathrm{P}(\mathbf{B}_w^{\mathcal{M}}),\nabla^2\bar{u}(\mathbf{B}_w^{\mathcal{M}})\rangle\}\mathrm{d}w].\end{aligned}$$

In particular, we get that for any $x\in\mathcal{M}$, $\Delta_{\mathcal{M}}u(x) = 2\langle\nabla\bar{u}(x),\bar{b}(x)\rangle + \langle\mathrm{P}(x),\nabla^2\bar{u}(x)\rangle$. Note that $(\mathbf{B}_t^{\mathcal{M}})_{t\in[0,T]}$ (seen as a process on $\mathbb{R}^p$) satisfies the condition (U) in Léonard (2012b), i.e. uniqueness of the trajectories given an initial condition. Therefore applying (Léonard, 2012b, Theorem 2.1), (Cattiaux et al., 2021, Claim 4.5), there exists $\bar{\beta}:\ [0,T]\times\mathbb{R}^p\to\mathbb{R}^p$ such that

$$\mathrm{KL}\left(\mathbb{P}|\mathbb{Q}\right) = \mathrm{KL}\left(\mathbb{P}_0|\mathbb{Q}_0\right) + \tfrac{1}{2}\int_0^T \mathbb{E}[\|\mathrm{P}(\mathbf{X}_t)\bar{\beta}(t,\mathbf{X}_t)\|^2]\mathrm{d}t. \tag{S15}$$

In addition, $\mathbb{P}$ (seen as a process on $\mathbb{R}^p$) satisfies a martingale problem with infinitesimal generator $\bar{\mathcal{A}}:\ [0,T]\times\mathrm{C}_c^2(\mathbb{R}^p)\times\mathbb{R}^p\to\mathbb{R}$ such that for any $t\in[0,T]$, $\bar{u}\in\mathrm{C}_c^2(\mathbb{R}^p)$ and $x\in\mathbb{R}^p$

$$\bar{\mathcal{A}}(t,\bar{u})(x) = \langle\bar{b}(x) + \mathrm{P}(x)\bar{\beta}(t,x),\nabla\bar{u}(x)\rangle + \tfrac{1}{2}\langle\mathrm{P}(x),\nabla^2\bar{u}(x)\rangle.$$

Let $\beta:\ [0,T]\times\mathcal{M}$ such that for any $t\in[0,T]$ and $x\in\mathcal{M}$ we have $\beta(t,x) = \mathrm{P}(x)\bar{\beta}(t,x)$. In particular, we have that for any $x\in\mathcal{M}$, $\beta(t,x)\in\mathrm{T}_x\mathcal{M}$. Let $u\in\mathrm{C}_c^2(\mathcal{M})$ and consider an extension $\bar{u}$ to $\mathrm{C}_c^2(\mathbb{R}^p)$. For any $t\in[0,T]$ and $x\in\mathcal{M}$ we have

$$\begin{aligned}\bar{\mathcal{A}}(t,\bar{u})(x) &= \langle\bar{b}(x) + \mathrm{P}(x)\bar{\beta}(t,x),\nabla\bar{u}(x)\rangle + \tfrac{1}{2}\langle\mathrm{P}(x),\nabla^2\bar{u}(x)\rangle\\ &= \langle\beta(t,x),\nabla\bar{u}(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}}u(x)\\ &= \langle\beta(t,x),\nabla u(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}}u(x).\end{aligned}$$

In particular, we have that $\mathbb{P}$ (seen as a process on $\mathcal{M}$) satisfies a martingale problem with infinitesimal generator $\mathcal{A}: [0,T] \times \mathrm{C}_c^2(\mathcal{M}) \times \mathcal{M} \to \mathbb{R}$ such that for any $t \in [0,T]$, $u \in \mathrm{C}^2(\mathbb{R}^p)$ and $x \in \mathcal{M}$

$$\mathcal{A}(t,\bar{u})(x) = \langle \beta(t,x), \nabla u(x) \rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} u(x).$$

In addition, rewriting (S16) we have

$$\mathrm{KL}\left(\mathbb{P}|\mathbb{Q}\right) = \mathrm{KL}\left(\mathbb{P}_0|\mathbb{Q}_0\right) + \tfrac{1}{2}\int_0^T \mathbb{E}[\|\beta(t,\mathbf{X}_t)\|^2]\mathrm{d}t, \tag{S16}$$

which concludes the proof. □

We also derive the following useful lemma, which will be used in the proof of convergence of RSGM.

Corollary S13. *Assume* **A**1. *Let $\mathbb{P}^1, \mathbb{P}^2$ be a Markov path measure on $\mathrm{C}([0,T], \mathcal{M})$ with $\mathbb{P}_0^1 = \mathbb{P}_0^2$. In addition, assume that there exist $b_1, b_2 \in \mathrm{C}^\infty([0,T], \mathcal{X}(\mathcal{M}))$ such that $(\mathbf{X}_t^1)_{t\in[0,T]}$ and $(\mathbf{X}_t^2)_{t\in[0,T]}$ are associated to $\mathbb{P}^1$ and $\mathbb{P}^2$ respectively and satisfy weakly $\mathrm{d}\mathbf{X}_t^i = b_1(t,\mathbf{X}_t^i)\mathrm{d}t + \mathrm{d}\mathbf{B}_t$ for $i \in \{1,2\}$. Then, we have that*

$$\mathrm{KL}(\mathbb{P}^1|\mathbb{P}^2) = \tfrac{1}{2}\int_0^T \mathbb{E}[\|b_1(t,\mathbf{X}_t^1) - b_2(t,\mathbf{X}_t^1)\|^2]\mathrm{d}t.$$

Proof. Upon, using the Nash embedding theorem (see Gunther, 1991), we can assume that $\mathcal{M}$ is a submanifold of $\mathbb{R}^p$ with $p \in \mathbb{N}$ such that the Riemannian metric on $\mathcal{M}$ is induced by the Euclidean metric on $\mathbb{R}^p$. Since $\mathcal{M}$ is compact, there exists $R > 0$ such that $\mathcal{M} \subset \bar{\mathrm{B}}(0,R)$. Let $\varphi \in \mathrm{C}^\infty(\mathbb{R}^p, [0,1])$ such that for any $x \in \bar{\mathrm{B}}(0,R)$, $\varphi(x) = 1$ and for any $x \in \mathbb{R}^p$ with $\|x\| \geq R+1$, $\varphi(x) = 0$. Consider $\bar{b}_1, \bar{b}_2 \in \mathrm{C}_c^2([0,T] \times \mathbb{R}^p, \mathbb{R}^p)$ such that for any $t \in [0,T]$ and $x \in \mathcal{M}$, $\bar{b}_i(x) = b_i(x)$ with $i \in \{1,2\}$. Consider $(\bar{\mathbf{X}}_t^i)_{t\in[0,T]}$ such that for any $i \in \{1,2\}$

$$\mathrm{d}\bar{\mathbf{X}}_t^i = \varphi(\bar{\mathbf{X}}_t^i)\{\mathrm{P}(\bar{\mathbf{X}}_t^i)\bar{b}^i(t,\bar{\mathbf{X}}_t^i) + \bar{b}(\bar{\mathbf{X}}_t)\}\mathrm{d}t + \varphi(\bar{\mathbf{X}}_t^i)\mathrm{P}(\bar{\mathbf{X}}_t^i)\mathrm{d}\mathbf{B}_t,$$

where $\bar{b} \in \mathrm{C}^\infty(\mathbb{R}^p, \mathbb{R}^p)$ is defined in the proof of Proposition S12. Let $\bar{\mathbf{X}}_0^i \sim \mathbb{P}_0^1$ for any $i \in \{1,2\}$ then for any $i \in \{1,2\}$, $(\bar{\mathbf{X}}_t^i)_{t\in[0,T]}$ (seen as a process on $\mathcal{M}$) is such that $\mathcal{L}((\bar{\mathbf{X}}_t^i)_{t\in[0,T]}) = \mathbb{P}^i$. Indeed, denote $\{\bar{\mathcal{A}}_t^i\}_{t\in[0,T]}$ the generator of $(\bar{\mathbf{X}}_t^i)_{t\in[0,T]}$ for any $i \in \{1,2\}$. Let $f \in \mathrm{C}^\infty(\mathcal{M}, \mathbb{R})$ and $\bar{f} \in \mathrm{C}^\infty(\mathbb{R}^p, \mathbb{R})$ an extension to $\mathbb{R}^p$. We have that for any $i \in \{1,2\}$, $x \in \mathcal{M}$ and $t \in [0,T]$

$$\begin{aligned}\bar{\mathcal{A}}_t^i(\bar{f})(x) &= \langle \bar{b}^i(t,x) + \bar{b}(x), \nabla \bar{f}(x) \rangle + \tfrac{1}{2}\langle \mathrm{P}(x), \nabla^2 \bar{f}(x) \rangle \\ &= \langle b^i(t,x), \nabla f(x) \rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} f(x).\end{aligned}$$

Hence, for any $i \in \{1,2\}$, $(\bar{\mathbf{X}}_t^i)_{t\in[0,T]}$ (seen as a process on $\mathcal{M}$) and $(\mathbf{X}_t^i)_{t\in[0,T]}$ have the same infinitesimal generators. Hence, $\mathcal{L}((\bar{\mathbf{X}}_t^i)_{t\in[0,T]}) = \mathbb{P}^i$ for any $i \in \{1,2\}$. For any $i \in \{1,2\}$, denote $\bar{\mathbb{P}}^i = \mathcal{L}((\bar{\mathbf{X}}_t^i)_{t\in[0,T]})$ (seen as a process on $\mathbb{R}^p$). Note that since for any $x \in \mathbb{R}^p$ with $\|x\| \geq R+1$, $\varphi(x) = 0$ we have that (Liptser and Shiryaev, 2001, Equation (7.137)) is satisfied. In addition, since for any $x \in \mathbb{R}^p$ with $\|x\| \geq R+1$, $\varphi(x) + \|\nabla\varphi(x)\| = 0$, we have that (Liptser and Shiryaev, 2001, Equation (4.110), Equation (4.111)) are satisfied. In addition, letting for any $t \in [0,T]$ and $x \in \mathbb{R}^p$, $\alpha(t,x) = \bar{b}^1(t,x) - \bar{b}^2(t,x) = \mathrm{P}(x)(\bar{b}^1(t,x) - \bar{b}^2(t,x))$, we have that for any $t \in [0,T]$, $\mathrm{P}(x)\alpha(t,x) = \mathrm{P}(x)(\bar{b}^1(t,x) - \bar{b}^2(t,x))$. Therefore, we can apply (Liptser and Shiryaev, 2001, Section 7.6.4) and using that $\mathrm{P}(x)\bar{b}(x) = 0$ for any $x \in \mathcal{M}$ (see the proof of Proposition S12), we have that

$$\begin{aligned}(\mathrm{d}\bar{\mathbb{P}}^1/\mathrm{d}\bar{\mathbb{P}}^2)((\bar{\mathbf{X}}_t^1)_{t\in[0,T]}) &= \exp\,[\textstyle\int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)\mathrm{d}\bar{\mathbf{X}}_t^1 \rangle \\ &\quad - \tfrac{1}{2}\textstyle\int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)(\bar{b}^1(t,\bar{\mathbf{X}}_t^1) + \bar{b}^2(t,\bar{\mathbf{X}}_t^1)) \rangle \mathrm{d}t] \\ &= \exp\,[\textstyle\int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)\{\bar{b}^1(t,\bar{\mathbf{X}}_t^1) + \bar{b}(\bar{\mathbf{X}}_t^1)\} \rangle \mathrm{d}t \\ &\quad + \textstyle\int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)\mathrm{d}\mathbf{B}_t \rangle \\ &\quad - \tfrac{1}{2}\textstyle\int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)(\bar{b}^1(t,\bar{\mathbf{X}}_t^1) + \bar{b}^2(t,\bar{\mathbf{X}}_t^1)) \rangle \mathrm{d}t] \\ &= \exp[\tfrac{1}{2}\textstyle\int_0^T \|\bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1)\|^2 \mathrm{d}t + \int_0^T \langle \bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1), \mathrm{P}(\bar{\mathbf{X}}_t^1)\mathrm{d}\mathbf{B}_t \rangle].\end{aligned}$$

Therefore, we have that

$$\mathrm{KL}(\bar{\mathbb{P}}^1|\bar{\mathbb{P}}^2) = \tfrac{1}{2}\int_0^T \mathbb{E}[\|\bar{b}^1(t,\bar{\mathbf{X}}_t^1) - \bar{b}^2(t,\bar{\mathbf{X}}_t^1)\|^2]\mathrm{d}t.$$

Hence, we get

$$\mathrm{KL}(\bar{\mathbb{P}}^1|\bar{\mathbb{P}}^2) = \tfrac{1}{2}\int_0^T \mathbb{E}[\|b^1(t,\mathbf{X}_t^1) - b^2(t,\mathbf{X}_t^1)\|^2]\mathrm{d}t.$$

which concludes the proof. □

Once Proposition S12 is established, we can obtain the following straightforward extension of Cattiaux et al. (2021, Proposition 4.6).

Proposition S14. *Assume* **A**1. *Let* $\mathbb{Q}$ *be a Brownian motion with* $\mathbb{Q}_0 = p_{\text{ref}}$ *and* $\mathbb{P}$ *a path measure on* $\mathrm{C}([0,T], \mathcal{M})$ *such that* $\mathrm{KL}(\mathbb{P}|\mathbb{Q}) < +\infty$. *Then, there exist* $\beta_{\mathbb{P}}, \beta_{R(\mathbb{P})} : [0,T] \times \mathcal{M} \to$ *such that for any* $t \in [0,T]$ *and* $x \in \mathcal{M}$, $\beta_{\mathbb{P}}(t,x), \beta_{R(\mathbb{P})}(t,x) \in \mathrm{T}_x\mathcal{M}$. *In addition, we have that* $\mathbb{P}$ *and* $R(\mathbb{P})$ *satisfy martingale problems with infinitesimal generator* $\mathcal{A}_{\mathbb{P}}$, *respectively* $\mathcal{A}_{R(\mathbb{P})}$ *where for any* $t \in [0,T]$, $u \in \mathrm{C}^2(\mathcal{M})$ *and* $x \in \mathcal{M}$ *we have*

$$\mathcal{A}_{\mathbb{P}}(t,u)(x) = \langle \beta_{\mathbb{P}}(t,x), \nabla u(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} u(x),$$
$$\mathcal{A}_{R(\mathbb{P})}(t,u)(x) = \langle \beta_{R(\mathbb{P})}(t,x), \nabla u(x)\rangle + \tfrac{1}{2}\Delta_{\mathcal{M}} u(x).$$

Finally, we have that

$$\int_0^T \mathbb{E}[\|\beta_{\mathbb{P}}(t,\mathbf{X}_t)\|^2]\mathrm{d}t + \int_0^T \mathbb{E}[\left\|\beta_{R(\mathbb{P})}(t,\mathbf{X}_{T-t})\right\|^2]\mathrm{d}t < +\infty,$$

where $(\mathbf{X}_t)_{t\in[0,T]}$ *has distribution* $\mathbb{P}$.

Proof. The proof is straightforward upon combining Proposition S12 and the fact that $\mathrm{KL}(\mathbb{P}|\mathbb{Q}) = \mathrm{KL}(R(\mathbb{P})|R(\mathbb{Q})) = \mathrm{KL}(R(\mathbb{P})|\mathbb{Q}) < +\infty$, using that $\mathbb{Q}$ is stationary. □

We conclude this section, with the following application of Theorem S11.

Proposition S15. *For any* $u, v \in \mathrm{C}_c^\infty(\mathcal{M})$, *we have that for almost any* $t \in [0,T]$

$$\mathbb{E}[v(\mathbf{X}_t)(\langle \beta_{\mathbb{P}}(t,\mathbf{X}_t) + \beta_{R(\mathbb{P})}(T-t,\mathbf{X}_t), \nabla u(\mathbf{X}_t)\rangle + \Delta_{\mathcal{M}} u(\mathbf{X}_t)) + \langle \nabla u(\mathbf{X}_t), \nabla v(\mathbf{X}_t)\rangle] = 0. \quad \text{(S17)}$$

Proof. Remark that $\mathrm{C}_c^2(\mathcal{M}) \subset \mathrm{dom}(\Upsilon_{\mathbb{P}})$ and $\mathrm{C}_c^2(\mathcal{M}) \subset \mathrm{dom}(\Upsilon_{R(\mathbb{P})})$. In addition, we have that for any $u, v \in \mathrm{C}_c^2(\mathcal{M})$, $\Upsilon_{\mathbb{P}}(u,v) = \Upsilon_{R(\mathbb{P})}(u,v) = \langle u, v\rangle$. Note that by Proposition S14 and Theorem S11 we have that for any $u, v \in \mathrm{C}_c^\infty(\mathcal{M})$, (S17) holds. □

G.2.3 Concluding the proof

Using Proposition S15 we can now conclude the proof of Theorem 1. First, remark that we can identify $\beta_{\mathbb{P}} = b$. Let $u, v \in \mathrm{C}^\infty(\mathcal{M})$, we have that

$$\mathbb{E}[v(\mathbf{X}_t)\langle b(\mathbf{X}_t) + \beta_{R(\mathbb{P})}(T-t,\mathbf{X}_t), \nabla u(\mathbf{X}_t)\rangle + \Delta_{\mathcal{M}} u(\mathbf{X}_t) v(\mathbf{X}_t) + \langle \nabla u(\mathbf{X}_t), \nabla v(\mathbf{X}_t)\rangle] = 0.$$

Using that for any $t \in [0,T]$, $\mathbb{P}_t$ admits a smooth positive density w.r.t. p_{ref} denoted p_t and the divergence theorem, see (Lee, 2018, p.51), we have that for any $t \in [0,T]$,

$$\begin{aligned}
&\int_{\mathcal{M}} \{\langle \beta_{R(\mathbb{P})}(T-t,x), \nabla u(x)\rangle + \langle b(x), \nabla u(x)\rangle\} v(x) p_t(x) \mathrm{d}p_{\text{ref}}(x) \\
&\qquad = -\int_{\mathcal{M}} \langle \nabla u(x) p_t(x), \nabla v(x)\rangle \mathrm{d}p_{\text{ref}}(x) - \int_{\mathcal{M}} \Delta_{\mathcal{M}} u(x) v(x) p_t(x) \mathrm{d}p_{\text{ref}}(x) \\
&\qquad = \int_{\mathcal{M}} \langle \nabla \log p_t(x), \nabla u(x) v(x) p_t(x) \mathrm{d}p_{\text{ref}}(x).
\end{aligned}$$

Therefore, we get that for any $t \in [0,T]$ and $x \in \mathcal{M}$, $\langle \beta_{R(\mathbb{P})}(T-t,x), \nabla u(x)\rangle = \langle -b(x) + \nabla \log p_t(x), \nabla u(x)\rangle$, which concludes the proof.

H Convergence of RSGM

In this section, we study the convergence of RSGM and prove Theorem 4. We state our main results in App. H.1 and give discretization bounds following the recent work of Cheng et al. (2022) in sec:discr-bounds-grw.

H.1 Main results

In this section, we prove Theorem 4. We start by recalling the sequence considered in RSGM. Let $(Y_k)_{k\in\{0,\dots,N\}}$ be given by $Y_0 \sim p_{\text{ref}}$ and for any $k \in \{0,\dots,N-1\}$

$$Y_{k+1} = \exp_{Y_k}[\gamma \mathbf{s}_{\theta^\star}(T - n\gamma, Y_k) + \sqrt{2} Z_{k+1}],$$

where $\{Z_k\})_{n\in\mathbb{N}}$ is a sequence of independent square integrable random variables with zero mean and identity covariance matrix. For ease of reading, we restate Theorem 4.

Theorem S16. *Assume* **A**1*, that* p_0 *is smooth and positive and that there exists* $\mathtt{M} \geq 0$ *such that for any* $t \in [0,T]$ *and* $x \in \mathcal{M}$*,* $\|\mathbf{s}_{\theta^\star}(t,x) - \nabla \log p_t(x)\| \leq \mathtt{M}$*, with* $\mathbf{s}_{\theta^\star} \in \mathrm{C}([0,T], \mathcal{X}(\mathcal{M}))$*. Then if* $T > 1/2$*, there exists* $C \geq 0$ *independent on* T *such that*

$$\mathbf{W}_1(\mathcal{L}(Y_N), p_0) = C(\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathtt{M} + \mathrm{e}^T \gamma^{1/2}),$$

where $\mathbf{W}_1$ *is the Wasserstein distance of order one on the probability measures on* $\mathcal{M}$*.*

Proof. For any $k \in \{1,\dots,N\}$, denote R_k such that for any $x \in \mathbb{R}^d$, $\mathsf{A} \in \mathcal{B}(\mathbb{R}^d)$ and $k \in \{0,\dots,N-1\}$ we have

$$\mathbb{E}[\mathrm{R}_{k+1}(Y_k, \mathsf{A})] = \mathbb{E}[\mathbb{1}_{\mathsf{A}}(Y_{k+1})].$$

Define for any $k_0, k_1 \in \{1,\dots,N\}$ with $k_1 \geq k_0$ $\mathrm{Q}_{k_0,k_1} = \prod_{\ell=k_0}^{k_1} \mathrm{R}_{k_1+k_0-\ell}$. Finally, for ease of notation, we also define for any $k \in \{1,\dots,N\}$, $\mathrm{Q}_k = \mathrm{Q}_{k+1,N}$. Note that for any $k \in \{1,\dots,N\}$, Y_k has distribution $\pi_\infty \mathrm{Q}_k$, where $\pi_\infty \in \mathcal{P}(\mathcal{M})$ with density w.r.t. the Hausdorff measure p_{ref}. Let $\mathbb{P} \in \mathcal{P}(\mathcal{C})$ be the probability measure associated with $(\mathbf{B}_t)_{t\in[0,T]}$ with $\mathbf{B}_0 \sim \pi_0$, where $\pi_0 \in \mathcal{P}(\mathcal{M})$ admits a density w.r.t. the Hausdorff measure given by p_0. We denote $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$ the process defined by the diffusion $\mathrm{d}\hat{\mathbf{Y}}_t = \mathbf{s}_{\theta^\star}(T-t, \hat{\mathbf{Y}}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t$ and $\hat{\mathbf{Y}}_0 \sim \pi_\infty$. We also denote $\hat{\mathbb{P}}^R \in \mathcal{P}(\mathcal{C})$ the probability measure associated with $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$. First note that using that $\mathbb{P}_0 = \pi_0$ we have for any $\mathsf{A} \in \mathcal{B}(\mathcal{M})$

$$\pi_0 \mathbb{P}_{T|0} (\mathbb{P}^R)_{T|0}(\mathsf{A}) = \mathbb{P}_T (\mathbb{P}^R)_{T|0}(\mathsf{A}) = (\mathbb{P}^R)_0 (\mathbb{P}^R)_{T|0}(\mathsf{A}) = (\mathbb{P}^R)_T(\mathsf{A}) = \pi_0(\mathsf{A}).$$

Hence we have that

$$\pi_0 = \pi_0 \mathbb{P}_{T|0} (\mathbb{P}^R)_{T|0}. \tag{S18}$$

Let $\varphi \in \mathrm{C}(\mathcal{M})$ with is 1-Lipschitz, i.e. for any $x, y \in \mathcal{M}$, $|\varphi(x) - \varphi(y)| \leq d(x,y)$. Since $\mathcal{M}$ is compact, we have that φ is bounded. Using this result, (S18), the data processing theorem (Kullback, 1997, Theorem 4.1) and Pinsker's inequality (Bakry et al., 2014, Equation 5.2.2) we have

$$\begin{aligned}
&|\mathbb{E}[\varphi(Y_N)] - \textstyle\int_{\mathcal{M}} \varphi(x) p_0(x) \mathrm{d}\mu(x)| \\
&\leq |\mathbb{E}[\varphi(\mathbf{B}_0)] - \mathbb{E}[\varphi(\mathbf{Y}_T)]| + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(\mathbf{Y}_T)]||\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]| \\
&\leq \|\varphi\|_\infty \|\pi_0 - \pi_\infty (\mathbb{P}^R)_{T|0}\|_{\mathrm{TV}} + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(\mathbf{Y}_T)]| + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]| \\
&\leq \|\varphi\|_\infty \|\pi_0 \mathbb{P}_{T|0} (\mathbb{P}^R)_{T|0} - \pi_\infty (\mathbb{P}^R)_{T|0}\|_{\mathrm{TV}} + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(\mathbf{Y}_T)]| + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]| \\
&\leq \|\varphi\|_\infty \|\pi_0 \mathbb{P}_{T|0} - \pi_\infty\|_{\mathrm{TV}} + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(\mathbf{Y}_T)]| + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]| \\
&\leq \|\varphi\|_\infty \|\pi_0 \mathbb{P}_{T|0} - \pi_\infty\|_{\mathrm{TV}} + \sqrt{2}\|\varphi\|_\infty \mathrm{KL}^{1/2}(\pi_\infty \mathbb{P}^R_{|0} | \pi_\infty \hat{\mathbb{P}}^R_{|0}) + |\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]|.
\end{aligned}$$

We now control each one of these terms. The first term can be easily controlled using the geometric ergodicity of the Brownian motion on compact manifolds. The second term can be controlled using the Girsanov theory on isometrically embedded manifolds. For the last term, we rely on the convergence of the GRW to its associated diffusion as presented in App. H.2. We now control each one of these terms.

(a) Using Proposition S10, we have that $\|\pi_0 \mathbb{P}_{T|0} - \pi_\infty\|_{\mathrm{TV}} \leq C^{1/2} \mathrm{e}^{\lambda_1/2} \mathrm{e}^{-\lambda_1 T}$ where λ_1 is the first positive eigenvalue of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(\pi_\infty)$. Therefore, we get that

$$\|\varphi\|_\infty \|\pi_0 \mathbb{P}_{T|0} - \pi_\infty\|_{\mathrm{TV}} \leq C^{1/2} \mathrm{e}^{\lambda_1/2} \|\varphi\|_\infty \mathrm{e}^{-\lambda_1 T}.$$

(b) Recall that we have that $\mathbb{P}^R_{|0}$ is associated with the process $\mathrm{d}\mathbf{Y}_t = \nabla \log p_{T-t}(\mathbf{Y}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}^{\mathcal{M}}_t$ and that $\hat{\mathbb{P}}^R_{|0}$ is associated with the process $\mathrm{d}\hat{\mathbf{Y}}_t = \mathbf{s}_{\theta^\star}(T-t, \hat{\mathbf{Y}}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}^{\mathcal{M}}_t$. Using Corollary S13 we have that

$$\mathrm{KL}(\pi_\infty \mathbb{P}^R_{|0} | \pi_\infty \hat{\mathbb{P}}^R_{|0}) = \tfrac{1}{2} \textstyle\int_0^T \mathbb{E}[\|\mathbf{s}_{\theta^\star}(T-t, \mathbf{Y}_t) - \nabla \log p_{T-t}(\mathbf{Y}_t)\|^2] \leq M^2 T.$$

(c) Let us define $\{\bar{\mathbf{Y}}^k\}_{k=0}^N$ such that for any $k \in \{0,\dots,N\}$, $\bar{\mathbf{Y}}^k_0 = \hat{\mathbf{Y}}_0 = Y_0$ and for any $t \in [0, k\gamma]$ we have that $\bar{\mathbf{Y}}^0_t = \hat{\mathbf{Y}}_t$. For any $t \in [k\gamma, T]$, we have that $\bar{\mathbf{Y}}^k_t = Y_{t,k}$, where $Y_{k\gamma,k} = \hat{\mathbf{Y}}_{k\gamma}$ and for any $j \in \{k,\dots,N-1\}$ and $t \in [0,\gamma]$

$$Y_{j\gamma+t,k} = \exp_{Y_{j\gamma,k}}[t\mathbf{s}_{\theta^\star}(T - j\gamma, Y_{j\gamma,k}) + \sqrt{t} E^k_j Z_j],$$

where $\{Z_j\}_{j=0}^{N-1}$ are independent Gaussian random variables with identity covariance matrix and zero mean and E_j^k is a frame of $\mathrm{T}_{Y_{j\gamma,k}}\mathcal{M}$ such that for any $j \in \{k+1,\dots,N-1\}$, $E_j^{k+1} = \Gamma_{Y_{j\gamma,k}}^{Y_{j\gamma,k+1}} E_j^k$ and $\{E_j^0\}_{j=0}^{N-1}$ is such that for any $j \in \{0,\dots,N-1\}$, E_j^0 is a frame of $\mathrm{T}_{Y_{j\gamma}}\mathcal{M}$. One $[0,k\gamma]$, we define $(\hat{\mathbf{Y}}_t^k)_{t\in[0,k\gamma]}$ as follows. For any $k \in \{0,\dots,N-1\}$, we set $(\mathbf{Y}_t^{k+1})_{t\in[0,k\gamma]} = (\mathbf{Y}_t^k)_{t\in[0,k\gamma]}$. For any $k \in \{0,\dots,N-1\}$, we set $(\mathbf{Y}_t)_{k\gamma,(k+1)\gamma}$ as in Proposition S21 (taking the notations of Proposition S21, $X_1^0 = \hat{\mathbf{Y}}_{(k+1)\gamma}^k$ and $\mathbf{X}_\gamma = \hat{\mathbf{Y}}_{k\gamma}^k$). Note that we have $\{\bar{\mathbf{Y}}_{j\gamma,0}^N\}_{j=0}^N = \{Y_j^N\}_{j=0}^N$ and $\{\bar{\mathbf{Y}}_{t,N}\}_{t\in[0,T]} = \{\hat{\mathbf{Y}}_t\}_{t\in[0,T]}$. Therefore, we have that

$$\begin{aligned}|\varphi(\hat{\mathbf{Y}}_T) - \varphi(Y_N)| &= |\varphi(\bar{\mathbf{Y}}_T^0) - \varphi(\bar{\mathbf{Y}}_T^N)| \\ &\le \textstyle\sum_{k=0}^{N-1} |\varphi(\bar{\mathbf{Y}}_T^k) - \varphi(\bar{\mathbf{Y}}_T^{k+1})| \le \|\nabla\varphi\|_\infty \sum_{k=0}^{N-1} d(\bar{\mathbf{Y}}_T^k, \bar{\mathbf{Y}}_T^{k+1}).\end{aligned}$$

In addition, using Proposition S21 and Proposition S22, we have that there exists $C \ge 0$ such that for any $k \in \{0,\dots,N-1\}$

$$\mathbb{E}[d(\bar{\mathbf{Y}}_{k,T}, \bar{\mathbf{Y}}_{k+1,T})] \le C\exp[(N-k)\gamma]\gamma^{3/2}.$$

Therefore, we get that there exists $C \ge 0$ such that

$$|\mathbb{E}[\varphi(\hat{\mathbf{Y}}_T)] - \mathbb{E}[\varphi(Y_N)]| \le C\exp[T]\gamma^{1/2},$$

Therefore, we get that there exists $C \ge 0$ such that for any $\varphi \in \mathrm{C}(\mathcal{M})$ which is 1-Lipschitz, we have

$$\mathbb{E}[\varphi(Y_N)] - \textstyle\int_{\mathcal{M}} \varphi(x)p_0(x)\mathrm{d}p_{\mathrm{ref}}(x) \le C(\mathrm{e}^{\lambda_1/2}\|\varphi\|_\infty \mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\|\varphi\|_\infty \mathtt{M} + \mathrm{e}^T\gamma^{1/2}). \quad \text{(S19)}$$

Let $x_0 \in \mathcal{M}$. Let $\mathrm{Lip}(\mathcal{M})$ the set of Lipschitz functions on $\mathcal{M}$ with Lipschitz constant equal to 1. Let $\mathrm{Lip}(\mathcal{M})_0$ the set of Lipschitz functions on $\mathcal{M}$ with Lipschitz constant equal to 1 and such that for any $\varphi \in \mathrm{Lip}(\mathcal{M})_0$, $\varphi(x_0) = 0$. Note that in this case, we have that $\|\varphi\|_\infty \le \mathrm{diam}(\mathcal{M})$. Using (S19), we have

$$\begin{aligned}\mathbf{W}_1(\mathcal{L}(Y_N), p_0) &= \sup\{\mathbb{E}[\varphi(Y_N)] - \textstyle\int_{\mathcal{M}} \varphi(x)p_0(x)\mathrm{d}p_{\mathrm{ref}}(x) \ : \ \varphi \in \mathrm{Lip}(\mathcal{M})\} \\ &= \sup\{\mathbb{E}[\varphi(Y_N)] - \textstyle\int_{\mathcal{M}} \varphi(x)p_0(x)\mathrm{d}p_{\mathrm{ref}}(x) \ : \ \varphi \in \mathrm{Lip}(\mathcal{M})_0\} \\ &\le C(\mathrm{e}^{\lambda_1/2}\mathrm{diam}(\mathcal{M})\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathrm{diam}(\mathcal{M})\mathtt{M} + \mathrm{e}^T\gamma^{1/2}),\end{aligned}$$

which concludes the proof. □

We now state a result regarding the continuous-time process (i.e. we now longer consider discretization errors). We recall that we denote $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$ the process defined by the diffusion $\mathrm{d}\hat{\mathbf{Y}}_t = \mathbf{s}_{\theta^\star}(T-t, \hat{\mathbf{Y}}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t$ and $\hat{\mathbf{Y}}_0 \sim \pi_\infty$.

Theorem S17. *Assume* **A**1*, that p_0 is smooth and positive and that there exists $\mathtt{M} \ge 0$ such that for any $t \in [0,T]$ and $x \in \mathcal{M}$, $\|\mathbf{s}_{\theta^\star}(t,x) - \nabla \log p_t(x)\| \le \mathtt{M}$, with $\mathbf{s}_{\theta^\star} \in \mathrm{C}([0,T], \mathcal{X}(\mathcal{M}))$. Then if $T > 1/2$, there exists $C \ge 0$ independent on T such that*

$$\|\mathcal{L}(\hat{\mathbf{Y}}_T) - p_0\|_{\mathrm{TV}} = C(\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathtt{M}).$$

Proof. The proof is identical to the one of Theorem S16, except that we do not have to deal with the discretization error. We use that for any $\mu, \nu \in \mathcal{P}(\mathcal{M})$

$$\|\mu - \nu\|_{\mathrm{TV}} = \sup\{\mu[f] - \nu[f] \ : \ f \in \mathrm{C}(\mathcal{M}), \|f\|_\infty \le 1\}.$$

□

The result of Theorem S17 should be compared with the one of (Rozen et al., 2021, Theorem 3). With our result we control a L^1 bound between the density of $\hat{\mathbf{Y}}_T$ and the one of p_0. In (Rozen et al., 2021, Theorem 3) a L^∞ bound between the densities is recovered. It can be shown that $\hat{p}_T = \mathcal{L}(\hat{\mathbf{Y}}_T)$. Let κ be the modulus of continuity of $\hat{p}_T - p_0$, i.e. for any $\varepsilon \ge 0$

$$\kappa(\varepsilon) = \sup\{|\hat{p}_T(x) - p_0(x) - \hat{p}_T(y) + p_0(y)| \ : \ x, y \in \mathcal{M}, \ d(x,y) \le \varepsilon\}.$$

Let $x_0 \in \mathcal{M}$ such that

$$|\hat{p}_T(x_0) - p_0(x_0)| = M = \sup\{|\hat{p}_T(x) - p_0(x)| \,:\, x \in \mathcal{M}\}.$$

For any $x \in \bar{\mathrm{B}}(x_0, \kappa(M/2))$, we have $|\hat{p}_T(x) - p_0(x)| \geq M/2$. Hence, denoting $\mathrm{Vol}_\kappa = \int_{\bar{\mathrm{B}}(x_0,\kappa(M/2))} \mathrm{d}p_{\mathrm{ref}}(x) > 0$, we have

$$(2/\mathrm{Vol}_\kappa) \int_{\mathcal{M}} |\hat{p}_T(x) - p_0(x)| \mathrm{d}p_{\mathrm{ref}}(x) \geq \|\hat{p}_T - p_0\|_\infty \,.$$

Hence, there exists $C \geq 0$ such that for any $T > 1/2$

$$\|\hat{p}_T - p_0\|_\infty \leq C(\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathtt{M}).$$

Therefore, we recover the same guarantees as Theorem S17 (note that $\mathtt{M}$ is not explicitly controlled using network properties in our work, but we could use universal approximation properties as in Rozen et al. (2021) in order to obtain a similar result).

H.2 Discretization bounds for GRW

In this section, we establish discretization bounds for GRW. Our results are a straightforward extension of Cheng et al. (2022) to the case where the drift term in the GRW is time-inhomogeneous.

Since $\mathcal{M}$ is compact, we have that for any $x_1, x_2 \in M$, there exists a minimizing geodesic such that $\gamma \in \mathrm{C}^\infty([0,1], \mathcal{M})$ and $\gamma(0) = x_1$ and $\gamma(1) = x_2$. When this choice is not unique we fix a minimizing geodesic. We denote $\Gamma_{x_1}^{x_2} \,:\, \mathrm{T}_{x_1}\mathcal{M} \to \mathrm{T}_{x_2}\mathcal{M}$ the associated parallel transport. Let $b \in \mathrm{C}^\infty([0,T], \mathcal{X}(\mathcal{M}))$.

We start by introducing a family of GRWs defined on progressively finer grids. Let $\gamma > 0$, $X_0 \in \mathcal{M}$, $E_0 \in \mathrm{F}_{X_0}\mathcal{M}$ (the vector space of frames at X_0) and consider the families $\{E_k^\ell \,:\, k \in \{0,\dots,2^\ell\}, \ \ell \in \mathbb{N}\}$, $\{X_k^\ell \,:\, k \in \{0,\dots,2^\ell\}, \ \ell \in \mathbb{N}\}$ such that $X_0^0 = X_0$, $X_1^0 = \exp_{X_0^0}[\gamma b(0, X_0^0) + \sqrt{\gamma}(\mathbf{B}_1 - \mathbf{B}_0)E_0^0]$ and $E_1^0 = \Gamma_{X_0^0}^{X_1^0} E_0^0$ (note that $E_{2^\ell}^\ell$ is not used in the proof but defined for completeness). In addition, we have that for any $\ell \in \mathbb{N}$ with $\ell \geq 1$, $X_0^\ell = X_0$, $E_0^\ell = E_0$ and for any $k \in \{0,\dots,2^{\ell-1}-1\}$

$$\begin{aligned}
X_{2k+1}^\ell &= \exp_{X_{2k}^\ell}[\gamma_\ell b(2k\gamma_\ell, X_{2k}^\ell) + E_{2k}^\ell(\mathbf{B}_{(2k+1)\gamma_\ell} - \mathbf{B}_{2k\gamma_\ell})],\\
E_{2k+1}^\ell &= \Gamma_{X_{2k}^\ell}^{X_{2k+1}^\ell} E_{2k}^\ell,\\
X_{2k+2}^\ell &= \exp_{X_{2k+1}^\ell}[\gamma_\ell b((2k+1)\gamma_\ell, X_{2k+1}^\ell) + E_{2k+1}^\ell(\mathbf{B}_{(2k+2)\gamma_\ell} - \mathbf{B}_{(2k+1)\gamma_\ell})],\\
E_{2k+2}^\ell &= \Gamma_{X_{k+1}^{\ell-1}}^{X_{2k+2}^\ell} E_{k+1}^{\ell-1},
\end{aligned} \tag{S20}$$

where $\gamma_\ell = \gamma/2^\ell$. For any $\ell \in \mathbb{N}$, we also define $(\mathbf{X}_t^\ell)_{t\in[0,\gamma]}$ such that for any $\ell \in \mathbb{N}$, $k \in \{0,\dots,2^\ell - 1\}$, we have for any $t \in [k\gamma_\ell, (k+1)\gamma_\ell)$, $\mathbf{X}_t^\ell = \exp_{X_k^\ell}[(t - k\gamma_\ell)b(k\gamma_\ell, X_k^\ell) + E_k^\ell(\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})]$. Note that for any $\ell \in \mathbb{N}$ and $k \in \{0,\dots,2^\ell - 1\}$, $\mathbf{X}_{k\gamma_\ell}^\ell = X_k$.

We are going to use the following useful lemma, see (Cheng et al., 2022, Lemma 62).

Lemma S18. *Assume* **A**1. *Then, there exists $C \geq 0$ such that for any $x, y \in \mathcal{M}$, $\gamma : [0,1] \to \mathcal{M}$ minimizing geodesic with $\gamma(0) = x$, $\gamma(1) = y$ and $u \in \mathrm{T}_x\mathcal{M}$, $v \in \mathrm{T}_y\mathcal{M}$ we have*

$$d(\exp_y[v], \exp_x[u])^2 \leq (1 + C\kappa^2 \exp[4\kappa]) d(x,y)^2 + C\exp[4\kappa]\|\Gamma_y^x v - u\|^2 + 2\langle \gamma'(0), \Gamma_y^x v - u\rangle,$$

with $\kappa = \|u\| + \|v\|$.

We are now ready to state the main result of this section.

Proposition S19. *Assume* **A**1. *Then, there exists $C \geq 0$ such that for any $\ell \in \mathbb{N}$*

$$\mathbb{E}[\sup_{t\in[0,\gamma]} d(\mathbf{X}_t^\ell, \mathbf{X}_t^{\ell+1})^2] \leq C\gamma^3 2^{-2\ell}.$$

Proof. Let $\ell \in \mathbb{N}$, $k \in \{0,\dots,2^\ell - 1\}$ and $t \in [k\gamma_\ell, (k+1)\gamma_\ell]$. We define $U_k^t = d(\mathbf{X}_t^\ell, \mathbf{X}_t^{\ell+1})^2$, $U_k = \sup\{U_k^t \,:\, t \in [k\gamma_\ell, (k+1)\gamma_\ell]\}$ and $U_{-1} = 0$. We also introduce for any $j \in \{0,\dots,2^\ell - 1\}$ and for $t \in [k\gamma_\ell, (2k+1)\gamma_{\ell+1})$, $\bar{\mathbf{X}}_t^{\ell+1} = \mathbf{X}_t^{\ell+1}$ and for $t \in [(2k+1)\gamma_{\ell+1}, (k+1)\gamma_\ell)$

$$\bar{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2j}^{\ell+1}}[\gamma_{\ell+1} b(2j\gamma_{\ell+1}, X_{2j}^{\ell+1}) + (t - (2k+1)\gamma_{\ell+1}) b((2j+1)\gamma_{\ell+1}, X_{2j}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{j\gamma_\ell}) E_{2j}^{\ell+1}].$$

Using this result and that for any $a, b \geq 0$, $(a+b)^2 \leq (1+2^{-\ell})a^2 + (1+2^{\ell})b^2$, we have that for any $t \in [k\gamma_\ell, (k+1)\gamma_\ell]$

$$U_{k+1}^t \leq (1+2^{-\ell})d(\mathbf{X}_t^\ell, \bar{\mathbf{X}}_t^{\ell+1})^2 + (1+2^{\ell})d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^{\ell+1})^2. \tag{S21}$$

Note that for $t \in [k\gamma_\ell, (2k+1)\gamma_{\ell+1}]$, the second term in (S21) is zero. We now bound each one of these terms:

(a) First, we assume that $t \in [(k+1)\gamma_\ell, (2k+1)\gamma_{\ell+1}]$. Recall that

$$\bar{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k}^{\ell+1}}[\gamma_{\ell+1} b(k\gamma_\ell, X_{2k}^{\ell+1}) + (t-(2k+1)\gamma_{\ell+1}) b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_{2k}^{\ell+1}],$$
$$\mathbf{X}_t^\ell = \exp_{X_k^\ell}[(t-k\gamma_\ell) b(k\gamma_\ell, X_k^\ell) + (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_k^\ell].$$

Hence, using Lemma S18, we have that

$$\begin{aligned} d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 \leq{}& (1 + C\kappa_k^2 \exp[4\kappa_k]) d(X_k^\ell, X_{2k}^{\ell+1})^2 \\ &+ C\exp[4\kappa_k] \|\Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k - u_k\|^2 + 2\langle w'(0), \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k - u_k\rangle, \end{aligned} \tag{S22}$$

with $w: [0,1] \to \mathcal{M}$ a minimizing geodesic between X_k^ℓ and $X_{2k}^{\ell+1}$

$$\begin{aligned} \kappa_k &= \|u_k\| + \|v_k\|, \\ u_k^1 &= (t-k\gamma_\ell) b(k\gamma_\ell, X_k^\ell), \\ v_k^1 &= \gamma_{\ell+1} b(2k\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (t-(2k+1)\gamma_{\ell+1}) b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}), \\ u_k^2 &= (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_k^\ell, \qquad & v_k^2 &= (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_{2k}^{\ell+1}, \\ u_k &= u_k^1 + u_k^2, & v_k &= v_k^1 + v_k^2. \end{aligned}$$

In particular, since $E_k^\ell = \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} E_{2k}^{\ell+1}$ using (S20), we have that $u_k^2 = \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k^2$. Therefore, combining this result and that $t - (2k+1)\gamma_{\ell+1} + \gamma_{\ell+1} = t - k\gamma_\ell$, we get that

$$\begin{aligned} \|\Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k^1 - u_k^1\| &\leq \gamma_{\ell+1} \|b(k\gamma_\ell, X_k^\ell) - \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} b(k\gamma_\ell, X_{2k}^{\ell+1})\| \\ &\quad + \gamma_{\ell+1} \|b(k\gamma_\ell, X_k^\ell) - \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1})\| \\ &\leq \gamma_\ell \|b(k\gamma_\ell, X_k^\ell) - \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} b(k\gamma_\ell, X_{2k}^{\ell+1})\| + \mathtt{L}_2 \gamma_\ell^2 \\ &\leq \mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) + \mathtt{L}_2 \gamma_\ell^2. \end{aligned}$$

Therefore, we get that $\|u_k - v_k\| \leq \mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) + \mathtt{L}_2 \gamma_\ell^2$. In addition, we have that $\|w'(0)\| \leq d(X_k^\ell, X_{2k}^{\ell+1})$ since w is a minimizing geodesic. Combining these results and (S22) we get that

$$\begin{aligned} d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 \leq{}& (1 + C\kappa_k^2 \exp[4\kappa_k]) d(X_k^\ell, X_{2k}^{\ell+1})^2 \\ &+ C\exp[4\kappa_k](\mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) + \mathtt{L}_2 \gamma_\ell^2)^2 \\ &+ 2(\mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) + \mathtt{L}_2 \gamma_\ell^2) d(X_k^\ell, X_{2k}^{\ell+1}) \\ \leq{}& (1 + C\kappa_k^2 \exp[4\kappa_k] + 2C\exp[4\kappa_k]\mathtt{L}_1^2 \gamma_\ell^2) d(X_k^\ell, X_{2k}^{\ell+1})^2 \\ &+ 2(\mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) + \mathtt{L}_2 \gamma_\ell^2) d(X_k^\ell, X_{2k}^{\ell+1}) + 2\mathtt{L}_2^2 \gamma_\ell^4 \\ \leq{}& (1 + C\kappa_k^2 \exp[4\kappa_k] + 2C\exp[4\kappa_k]\mathtt{L}_1^2 \gamma_\ell^2 + 2\mathtt{L}_1 \gamma_\ell + 4\mathtt{L}_2 \gamma_\ell) d(X_k^\ell, X_{2k}^{\ell+1})^2 + 8\mathtt{L}_2 \gamma_\ell^3, \end{aligned}$$

Hence, there exists $C_1 \geq 0$ (not dependent on k or ℓ) such that

$$(1+2^{-\ell})d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 \leq (1 + C_1\{\kappa_k^2 \exp[4\kappa_k] + \gamma_\ell^2 \exp[4\kappa_k] + 2^{-\ell}\}) d(X_k^\ell, X_{2k}^{\ell+1})^2 + C_1 \gamma_\ell^3.$$

Next, we assume that $t \in [k\gamma_\ell, (2k+1)\gamma_{\ell+1}]$. Recall that

$$\bar{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k}^{\ell+1}}[(t-k\gamma_\ell) b(k\gamma_\ell, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_{2k}^{\ell+1}],$$
$$\mathbf{X}_t^\ell = \exp_{X_k^\ell}[(t-k\gamma_\ell) b(k\gamma_\ell, X_k^\ell) + (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell})E_k^\ell].$$

Hence, using Lemma S18, we have that

$$d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 \leq (1 + C\kappa_k^2 \exp[4\kappa_k]) d(X_k^\ell, X_{2k}^{\ell+1})^2 + C\exp[4\kappa_k] \|\Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k - u_k\|^2 + 2\langle w'(0), \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k - u_k\rangle, \tag{S23}$$

with $w: [0,1] \to \mathcal{M}$ a minimizing geodesic between X_k^ℓ and $X_{2k}^{\ell+1}$

$$\begin{aligned}
\kappa_k &= \|u_k\| + \|v_k\|, \\
u_k^1 &= (t - k\gamma_\ell) b(k\gamma_\ell, X_k^\ell), \\
v_k^1 &= (t - k\gamma_\ell) b(k\gamma_\ell, X_{2k}^{\ell+1}), \\
u_k^2 &= (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell}) E_k^\ell, & v_k^2 &= (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell}) E_{2k}^{\ell+1}, \\
u_k &= u_k^1 + u_k^2, & v_k &= v_k^1 + v_k^2.
\end{aligned}$$

In particular, since $E_k^\ell = \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} E_{2k}^{\ell+1}$ using (S20) and $t - (2k+1)\gamma_{\ell+1} + \gamma_{\ell+1} = t - k\gamma_\ell$, we have that $u_k^2 = \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k^2$. Therefore, we get that

$$\begin{aligned}
\|\Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} v_k^1 - u_k^1\| &\leq \gamma_{\ell+1} \|b(k\gamma_\ell, X_k^\ell) - \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} b(k\gamma_\ell, X_{2k}^{\ell+1})\| \\
&\leq \gamma_\ell \|b(k\gamma_\ell, X_k^\ell) - \Gamma_{X_{2k}^{\ell+1}}^{X_k^\ell} b(k\gamma_\ell, X_{2k}^{\ell+1})\| + \mathtt{L}_2 \gamma_\ell^2 \\
&\leq \mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}).
\end{aligned}$$

Therefore, we get that $\|u_k - v_k\| \leq \mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1})$. In addition, we have that $\|w'(0)\| \leq d(X_k^\ell, X_{2k}^{\ell+1})$ since w is a minimizing geodesic. Combining these results and (S23) we get that

$$\begin{aligned}
d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 &\leq (1 + C\kappa_k^2 \exp[4\kappa_k]) d(X_k^\ell, X_{2k}^{\ell+1})^2 \\
&\quad + C\exp[4\kappa_k] \mathtt{L}_1^2 \gamma_\ell^2 d(X_k^\ell, X_{2k}^{\ell+1})^2 \\
&\quad + 2\mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1}) d(X_k^\ell, X_{2k}^{\ell+1}) \\
&\leq (1 + C\kappa_k^2 \exp[4\kappa_k] + 2C\exp[4\kappa_k] \mathtt{L}_1^2 \gamma_\ell^2) d(X_k^\ell, X_{2k}^{\ell+1})^2 \\
&\quad + 2\mathtt{L}_1 \gamma_\ell d(X_k^\ell, X_{2k}^{\ell+1})^2 + 2\mathtt{L}_2^2 \gamma_\ell^4 \\
&\leq (1 + C\kappa_k^2 \exp[4\kappa_k] + 2C\exp[4\kappa_k] \mathtt{L}_1^2 \gamma_\ell^2 + 2\mathtt{L}_1 \gamma_\ell) d(X_k^\ell, X_{2k}^{\ell+1})^2.
\end{aligned}$$

Hence, there exists $C_1 \geq 0$ (not dependent on k or ℓ) such that for any $t \in [k\gamma_\ell, (k+1)\gamma_\ell]$

$$(1 + 2^{-\ell}) d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^\ell)^2 \leq (1 + C_1\{\kappa_k^2 \exp[4\kappa_k] + \gamma_\ell^2 \exp[4\kappa_k] + 2^{-\ell}\}) d(X_k^\ell, X_{2k}^{\ell+1})^2 + C_1 \gamma_\ell^3. \tag{S24}$$

(b) We recall that if $t \in [k\gamma_\ell, (2k+1)\gamma_{\ell+1}]$ the second term in (S21) is zero. Therefore in what follows, we assume $t \in [(2k+1)\gamma_{\ell+1}, (k+1)\gamma_\ell]$. We introduce

$$\hat{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k+1}^{\ell+1}} [(t - (2k+1)\gamma_{\ell+1}) \Gamma_{X_{2k}^{\ell+1}}^{X_{2k+1}^{\ell+1}} b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}}) E_{2k+1}^{\ell+1}]. \tag{S25}$$

In what follows, we provide an upper-bound for $d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^{\ell+1})$. First, we have that

$$d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^{\ell+1}) \leq d(\bar{\mathbf{X}}_t^{\ell+1}, \hat{\mathbf{X}}_t^{\ell+1}) + d(\hat{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^{\ell+1}).$$

We recall that

$$\bar{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k}^{\ell+1}} [\gamma_{\ell+1} b(2k\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (t - (2k+1)\gamma_{\ell+1}) b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{k\gamma_\ell}) E_{2k}^{\ell+1}]. \tag{S26}$$

Denote a_k, b_k such that

$$\begin{aligned}
a_k &= b(2k\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_{(2k+1)\gamma_{\ell+1}} - \mathbf{B}_{k\gamma_\ell}) E_{2k}^{\ell+1}, \\
b_k &= (t - (2k+1)\gamma_{\ell+1}) b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}}) E_{2k}^{\ell+1}.
\end{aligned}$$

Using (S20), (S25) and (S26) we have that

$$X_{2k+1}^{\ell+1} = \exp_{X_{2k}^{\ell+1}}[a_k], \qquad \hat{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k+1}^{\ell+1}}[\Gamma_{X_{2k}^{\ell+1}}^{X_{2k+1}^{\ell+1}} b_k], \qquad \bar{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k}^{\ell+1}}[a_k + b_k].$$

Using this result and (Sun et al., 2019, Lemma 3), there exists $C_2 \geq 0$ (not dependent on k or ℓ) such that

$$d(\hat{\mathbf{X}}_t^{\ell+1}, \bar{\mathbf{X}}_t^{\ell+1}) \leq C_2(\|a_k\| + \|b_k\|)^3.$$

Using this result and that for any $t \in [0, \gamma]$ and $x \in \mathcal{M}$, $\|b(t,x)\| \leq \mathtt{K}$ we get that there exists $C_3 \geq 0$ (not dependent on k or ℓ) such that

$$d(\hat{\mathbf{X}}_t^{\ell+1}, \bar{\mathbf{X}}_t^{\ell+1})^2 \leq C_3(\gamma_{\ell+1}^6 + \|\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}}\|^6 + \|\mathbf{B}_{(2k+1)\gamma_\ell} - \mathbf{B}_{(k+1)\gamma_\ell}\|^6). \tag{S27}$$

Finally, we recall that

$$\hat{\mathbf{X}}_t^{\ell+1} = \exp_{X_{2k+1}^{\ell+1}}[(t - (2k+1)\gamma_{\ell+1})\Gamma_{X_{2k}^{\ell+1}}^{X_{2k+1}^{\ell+1}} b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}})E_{2k+1}^{\ell+1}],$$
$$\mathbf{X}_t^{\ell+1} = \exp_{X_{2k+1}^{\ell+1}}[(t - (2k+1)\gamma_{\ell+1})b((2k+1)\gamma_{\ell+1}, X_{2k+1}^{\ell+1}) + (\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}})E_{2k+1}^{\ell+1}].$$

Let us define

$$\begin{aligned}
&\tau_k = \|c_k\| + \|d_k\|, \\
&c_k = c_k^1 + c_k^2, \qquad\qquad d_k = d_k^1 + d_k^2, \\
&c_k^1 = (t - (2k+1)\gamma_{\ell+1})b((2k+1)\gamma_{\ell+1}, X_{2k+1}^{\ell+1}), \\
&d_k^1 = (t - (2k+1)\gamma_{\ell+1})\Gamma_{X_{2k}^{\ell+1}}^{X_{2k+1}^{\ell+1}} b((2k+1)\gamma_{\ell+1}, X_{2k}^{\ell+1}), \\
&c_k^2 = d_k^2 = (\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}})E_{2k+1}^{\ell+1}.
\end{aligned} \tag{S28}$$

Using Lemma S18, we get that

$$d(\mathbf{X}_t^{\ell+1}, \hat{\mathbf{X}}_t^{\ell+1})^2 \leq C\exp[4\tau_k]\|c_k - d_k\|^2 \leq C\mathtt{L}_2^2\gamma_{\ell+1}^2\exp[4\tau_k]d(X_{2k+1}^{\ell+1}, X_{2k}^{\ell+1})^2. \tag{S29}$$

In addition, using Lemma S18, we get that

$$d(X_{2k+1}^{\ell+1}, X_{2k}^{\ell+1})^2 \leq \exp[4\|e_k\|]\|e_k\|,$$

with $e_k = \gamma_{\ell+1}b(k\gamma_\ell, X_{2k}^{\ell+1}) + (\mathbf{B}_{(2k+1)\gamma_{\ell+1}} - \mathbf{B}_{k\gamma_\ell})E_{2k}^{\ell+1}$. Combining this result and (S29), we get that

$$d(\mathbf{X}_t^{\ell+1}, \hat{\mathbf{X}}_t^{\ell+1})^2 \leq C_3\gamma_{\ell+1}^2(\gamma_{\ell+1}^2 + \|\mathbf{B}_{(2k+1)\gamma_{\ell+1}} - \mathbf{B}_{k\gamma_\ell}\|^2)\exp[4\tau_k + \|e_k\|]. \tag{S30}$$

Combining (S27) and (S30), there exists C_5 such that

$$\begin{aligned}
d(\bar{\mathbf{X}}_t^{\ell+1}, \mathbf{X}_t^{\ell+1})^2 \leq\ & C_5\gamma_{\ell+1}^2(\gamma_{\ell+1}^2 + \|\mathbf{B}_{(2k+1)\gamma_{\ell+1}} - \mathbf{B}_{k\gamma_\ell}\|^2)\exp[4\tau_k + \|e_k\|] \\
& + C_5(\gamma_{\ell+1}^6 + \|\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}}\|^6 + \|\mathbf{B}_{(2k+1)\gamma_\ell} - \mathbf{B}_{(k+1)\gamma_\ell}\|^6).
\end{aligned} \tag{S31}$$

In what follows, we denote

$$\begin{aligned}
\alpha_k &= C_1\{(\kappa_k^+)^2\exp[4\kappa_k] + \gamma_\ell^2\exp[4\kappa_k^+] + 2^{-\ell}\}. \\
\beta_k &= C_1\gamma_\ell^3 + C_5(1+2^\ell)\gamma_{\ell+1}^2(\gamma_{\ell+1}^2 + \|\mathbf{B}_{(2k+1)\gamma_{\ell+1}} - \mathbf{B}_{k\gamma_\ell}\|^2)\exp[4\tau_k^+ + \|e_k\|] \\
&\quad + C_5(1+2^\ell)\left(\gamma_{\ell+1}^6 + \sup_{t\in[k\gamma_\ell,(k+1)\gamma_\ell]}\{\|\mathbf{B}_t - \mathbf{B}_{(2k+1)\gamma_{\ell+1}}\|^6\} + \|\mathbf{B}_{(2k+1)\gamma_\ell} - \mathbf{B}_{(k+1)\gamma_\ell}\|^6\right),
\end{aligned}$$

with $\tau_k^+ = \sup\{\|c_k\| + \|d_k\| \ :\ t \in [k\gamma_\ell, (k+1)\gamma_\ell]\}$, see (S28). Therefore, using (S21), (S24) and (S31), we get that for any $k \in \{0, \ldots, 2^\ell - 1\}$

$$U_{k+1} \leq (1+\alpha_k)U_k + \beta_k.$$

Let $\{R_k\}_{k=-1}^{2^\ell}$ such that $R_{-1} = 0$ and for any $k \in \{0, \ldots, 2^\ell - 1\}$

$$R_{k+1} = (1+\alpha_k)R_k + \beta_k.$$

Then, for any $k \in \{0, \dots, 2^\ell - 1\}$, we have that $R_{2^\ell - 1} \geq R_k \geq U_k$. Therefore

$$\mathbb{E}[R_{2^\ell}] \geq \mathbb{E}[\sup\{U_k \,:\, k \in \{0, \dots, 2^\ell\}\}] \geq \mathbb{E}[\sup\{d(\mathbf{X}_t^\ell, \mathbf{X}_t^{\ell+1})^2 \,:\, t \in [0, \gamma]\}]. \tag{S32}$$

In addition, using that for any $k \in \{0, \dots, 2^\ell - 1\}$, $\mathbb{E}[\alpha_k | \mathcal{F}_k] = \bar{\alpha}_k$ and $\mathbb{E}[\beta_k | \mathcal{F}_k] = \bar{\beta}_k$ are constant, where $\mathcal{F}_k = \sigma(\{\mathbf{B}_t \,:\, t \in [0, k\gamma_\ell]\})$. Therefore, we get that for any $k \in \{0, \dots, 2^\ell - 1\}$

$$\mathbb{E}[R_{k+1}] = (1 + \bar{\alpha}_k)\mathbb{E}[R_k] + \bar{\beta}_k.$$

Therefore, using the discrete Grönwall lemma we get that for any $k \in \{0, \dots, 2^\ell - 1\}$

$$\mathbb{E}[R_{2^\ell}] \leq \bar{\beta}_{2^\ell - 1} + \exp[\textstyle\sum_{n=0}^{2^\ell - 1} \bar{\alpha}_n] \sum_{j=0}^{2^\ell - 1} \bar{\beta}_j \bar{\alpha}_j.$$

In addition, there exists $C_8 \geq 0$ such that for any $k \in \{0, \dots, 2^\ell\}$, $\bar{\alpha}_k \leq C_8 2^{-\ell}$ and $\bar{\beta}_k \leq C_8 \gamma^3 2^{-2\ell}$. Hence, there exists $C_9 \geq 0$ such that

$$\mathbb{E}[R_{2^\ell}] \leq C_9 \gamma^3 2^{-2\ell},$$

which concludes the proof upon using (S32).

□

Proposition S20. *Assume* **A**1. *Then, there exists* $(\mathbf{X}_t)_{t \in [0,\gamma]}$ *such that* $\lim_{\ell \to +\infty} \sup\{d(\mathbf{X}_t^\ell, \mathbf{X}_t) \,:\, t \in [0, \gamma]\} = 0$ *and* $(\mathbf{X}_t)_{t \in [0,\gamma]}$ *is a weak solution to* $\mathrm{d}\mathbf{X}_t = b(t, \mathbf{X}_t)\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$.

Proof. The proof is a straightforward application of Proposition S19 and (Cheng et al., 2022, A.1 (Step 2 and Step 3), A.2). □

Proposition S21. *Assume* **A**1. *Then, there exists* $C \geq 0$ *such that* $\mathbb{E}\left[d(X_1^0, \mathbf{X}_\gamma)^2 \leq C\gamma^{3/2}\right]$.

Proof. Using Proposition S19, there exists $C \geq 0$ such that for any $\ell \in \mathbb{N}$

$$\mathbb{E}[\sup_{t \in [0,\gamma]} d(\mathbf{X}_t^\ell, \mathbf{X}_t^{\ell+1})] \leq C\gamma^{3/2} 2^{-\ell}.$$

Therefore, combining this result and Proposition S20 we get that for any $\ell \in \mathbb{N}$

$$\mathbb{E}[\sup_{t \in [0,\gamma]} d(\mathbf{X}_t^\ell, \mathbf{X}_t)] \leq 2C\gamma^{3/2},$$

which concludes the proof. □

Finally, we consider the two following processes $(X_k^1, X_k^2)_{k \in \mathbb{N}}$ such that for any $k \in \mathbb{N}$ and $i \in \{1, 2\}$

$$X_{k+1}^i = \exp_{X_k^i}[\gamma b(k\gamma, X_k^i) + \sqrt{\gamma} E_k^i Z_k],$$

where $\{Z_k\}_{k \in \mathbb{N}}$ is a family of independent Gaussian random variables with zero mean and identity covariance matrix, and for any $k \in \mathbb{N}$, E_k^1 is a frame for $\mathrm{T}_{X_k^1}\mathcal{M}$ and $E_k^2 = \Gamma_{X_k^1}^{X_k^2} E_k^1$.

Proposition S22. *Assume* **A**1. *Then, there exists* $C \geq 0$ *such that for any* $k \in \mathbb{N}$

$$\mathbb{E}\left[d(X_k^1, X_k^2)\right] \leq \exp[Ck\gamma]\mathbb{E}\left[d(X_0^1, X_0^2)\right].$$

Proof. Let $k \in \mathbb{N}$. Using Lemma S18, there exists $D \geq 0$ such that

$$\begin{aligned} d(X_{k+1}^1, X_{k+1}^2)^2 \leq{}& (1 + D\kappa_k^2 \exp[4\kappa_k]) d(X_k^1, X_k^2)^2 \\ &+ D\exp[4\kappa_k] \|\Gamma_{X_k^2}^{X_k^1} v_k - u_k\|^2 + 2\langle w'(0), \Gamma_{X_k^2}^{X_k^1} v_k - u_k \rangle, \end{aligned}$$

with $w : [0, 1] \to \mathcal{M}$ a minimizing geodesic between X_k^1 and X_k^2

$$\begin{aligned} \kappa_k &= \|u_k\| + \|v_k\|, \\ u_k^1 &= \gamma b(k\gamma, X_k^1), \\ v_k^1 &= \gamma b(k\gamma, X_k^2), \\ u_k^2 &= \sqrt{\gamma} Z_k E_k^1, & v_k^2 &= \sqrt{\gamma} Z_k E_k^2, \\ u_k &= u_k^1 + u_k^2, & v_k &= v_k^1 + v_k^2. \end{aligned}$$

We have that $\Gamma_{X_k^2}^{X_k^1} v_k^2 = v_k$ and

$$\|\Gamma_{X_k^2}^{X_k^1} v_k^1 - u_k^1\| \leq \mathtt{L}_1 \gamma d(X_k^1, X_k^2).$$

In addition, $\|w'(0)\| \leq d(X_k^1, X_k^2)$. Therefore, we get that

$$d(X_{k+1}^1, X_{k+1}^2)^2 \leq (1 + D\kappa_k^2 \exp[4\kappa_k] + D\gamma^2 \exp[4\kappa_k] + 2\gamma) d(X_k^1, X_k^2)^2.$$

Hence, using that for any $t \geq 0$, $\sqrt{1+t} \leq 1 + t/2$, we have

$$d(X_{k+1}^1, X_{k+1}^2) \leq (1 + D\kappa_k^2 \exp[4\kappa_k] + D\gamma^2 \exp[4\kappa_k] + 2\gamma) d(X_k^1, X_k^2).$$

Therefore, we get that there exists $C \geq 0$ such that

$$\mathbb{E}[d(X_{k+1}^1, X_{k+1}^2)] \leq (1 + C\gamma) \mathbb{E}[d(X_k^1, X_k^2)],$$

which concludes the proof. □

I Proof of Proposition 3

Proof. Let $t \in (0, T]$ and $s_t \in \mathrm{C}^\infty(\mathcal{M})$. Using the divergence theorem (see Lee, 2018, p.51), we have

$$\begin{aligned}
\ell_{t|s}(s_t) = & \int_{\mathcal{M}\times\mathcal{M}} \|\nabla \log p_{t|s}(x_t|x_s)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t) + \int_{\mathcal{M}} \|s_t(x_t)\|^2 \mathrm{d}\mathbb{P}_t(x_t) \\
& -2 \int_{\mathcal{M}\times\mathcal{M}} \langle \nabla \log p_{t|s}(x_t|x_s), s_t(x_t) \rangle_{\mathcal{M}} \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t) \\
= & \int_{\mathcal{M}\times\mathcal{M}} \|\nabla \log p_{t|s}(x_t|x_s)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t) + \int_{\mathcal{M}} \|s_t(x_t)\|^2 \mathrm{d}\mathbb{P}_t(x_t) \\
& -2 \int_{\mathcal{M}\times\mathcal{M}} \langle \nabla \log p_{t|s}(x_t|x_s), s_t(x_t) \rangle_{\mathcal{M}} p_{t|s}(x_t|x_s) p_s(x_s) \mathrm{d}(p_{\text{ref}} \otimes p_{\text{ref}})(x_s, x_t) \\
= & \int_{\mathcal{M}\times\mathcal{M}} \|\nabla \log p_{t|s}(x_t|x_s)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t) + \int_{\mathcal{M}} \|s_t(x_t)\|^2 \mathrm{d}\mathbb{P}_t(x_t) \\
& -2 \int_{\mathcal{M}} \{ \int_{\mathcal{M}} \langle \nabla p_{t|s}(x_t|x_s), s_t(x_t) \rangle_{\mathcal{M}} \mathrm{d}p_{\text{ref}}(x_t) \} p_s(x_s) \mathrm{d}p_{\text{ref}}(x_s) \\
= & \int_{\mathcal{M}\times\mathcal{M}} \|\nabla \log p_{t|s}(x_t|x_s)\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t) + \int_{\mathcal{M}} \|s_t(x_t)\|^2 \mathrm{d}\mathbb{P}_t(x_t) \\
& +2 \int_{\mathcal{M}} \{ \int_{\mathcal{M}} \operatorname{div}(s_t)(x_t) p_{t|s}(x_t|x_s) \mathrm{d}p_{\text{ref}}(x_t) \} p_s(x_s) \mathrm{d}p_{\text{ref}}(x_s),
\end{aligned}$$

which concludes the proof. □

J Comparison with Moser flows

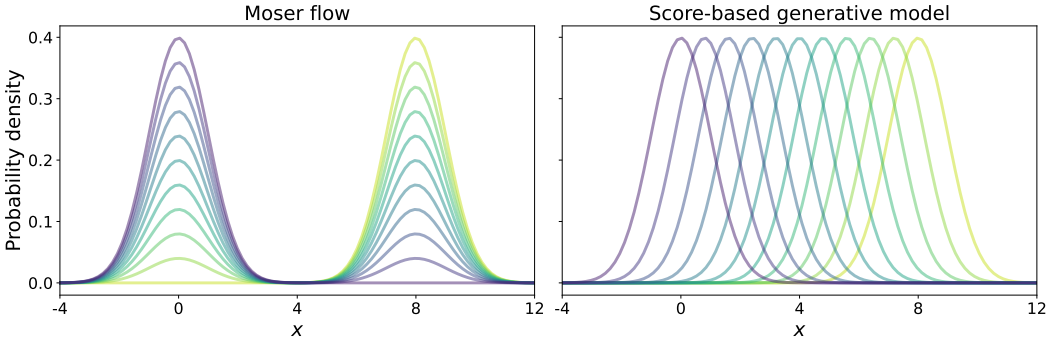
In this section, we compare ourselves with Rozen et al. (2021) in greater details. Rozen et al. (2021) also aims at interpolating between a reference distribution p_{ref} and a target distribution p_0. We assume that we have access to the density p_{ref} and that we know how to sample form p_{ref} (which is often the case if p_{ref} is the uniform distribution on $\mathcal{M}$). Contrary to RSGM, p_{ref} is not necessary the uniform distribution.

We then consider the following interpolation $\hat{p}_t = (1-t)\hat{p}_0 + t\hat{p}_1$, with $\hat{p}_0 = p_{\text{ref}}$ and $\hat{p}_1 = p_0$. Let $(\mathbf{X}_t)_{t\in[0,1]}$ be given by $\mathbf{X}_0 \sim \hat{p}_0$ and $\mathrm{d}\mathbf{X}_t = \mathbf{v}_t(\mathbf{X}_t)\mathrm{d}t$ where for any $t \in [0,1]$, $\mathbf{v}_t = \mathbf{u}/((1-t)\hat{p}_0 + \hat{p}_1)$, with $\operatorname{div}(\mathbf{u}) = \hat{p}_0 - \hat{p}_1$. Using the Fokker-Planck equation, we have that for any $t \in [0,1]$, $\mathbf{X}_t \sim \hat{p}_t$. In Rozen et al. (2021), $\mathbf{u}$ is replaced by a parametric version $\mathbf{u}_\theta$ and the authors optimize the loss

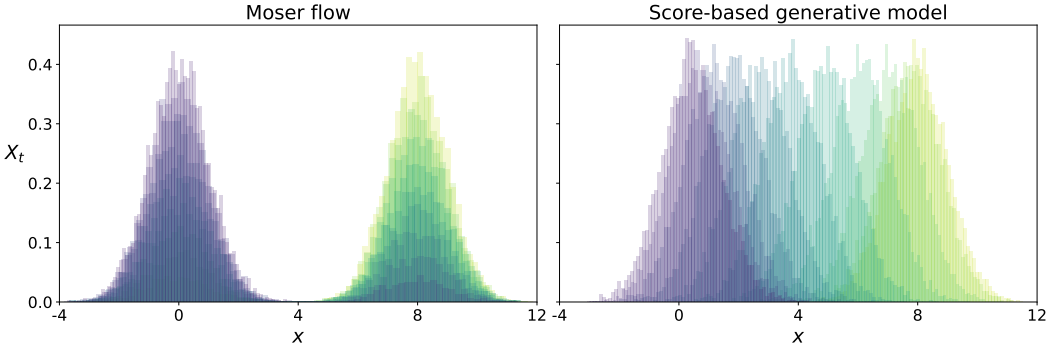
$$\ell(\theta) = \mathbb{E}[(\hat{p}_0 - \operatorname{div}(\mathbf{u}_\theta))^{+,\varepsilon}(\mathbf{X}_1)] + \lambda \int_{\mathcal{M}} (\hat{p}_0 - \operatorname{div}(\mathbf{u}_\theta))^{-,\varepsilon}(x)\mathrm{d}x,$$

with $\lambda, \varepsilon > 0$ and for any $f : \mathcal{M} \to \mathbb{R}$, $f^{+,\varepsilon} = \max(f, \varepsilon)$ and $f^{-,\varepsilon} = \varepsilon - \min(f, \varepsilon)$. Given $\mathbf{u}_\theta$, we then consider $(\mathbf{X}_t^\theta)_{t\in[0,1]}$ such that $\mathrm{d}\mathbf{X}_t^\theta = \mathbf{v}_t^\theta(\mathbf{X}_t^\theta)\mathrm{d}t$, where for any $t \in [0,1]$, $\mathbf{v}_t^\theta = \mathbf{u}_\theta/(\hat{p}_0 + t\operatorname{div}(\mathbf{u}_\theta))$. Note that $\mathbf{u}^\theta$ also enables density estimation using that $\hat{p}_1 = \hat{p}_0 - \operatorname{div}(\mathbf{u}^\theta)$. Density estimation is not directly accessible using RSGM, however in App. K we propose a way to perform such an estimation using Fisher score in a manner akin to Choi et al. (2021).

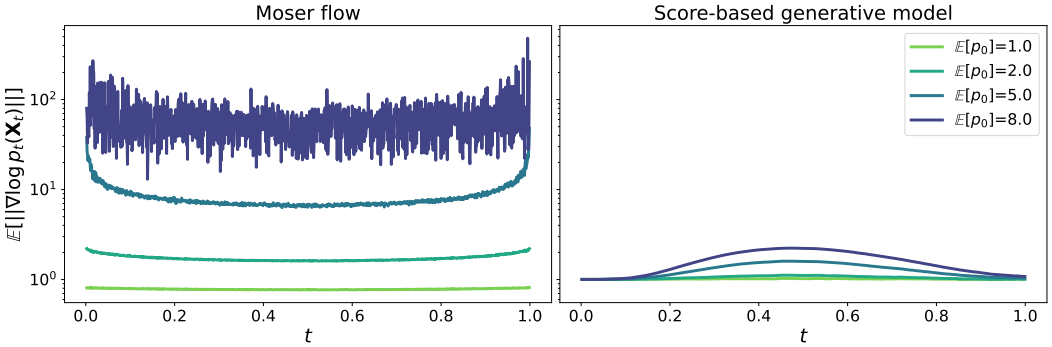
Let $\hat{p}_0 = p_{\text{ref}}$ to be the uniform distribution on $\mathcal{M}$. As RSGM, Moser flow defines a continuous time interpolation between p_0 and p_{ref}. One major difference between the two approaches is that



(a) Interpolated density between the reference $p_{\text{ref}} = \mathrm{N}(0, 1)$ and target $p_0 = \mathrm{N}(8, 1)$ distributions.



(b) Interpolated histograms between the reference $p_{\text{ref}} = \mathrm{N}(0, 1)$ and target $p_0 = \mathrm{N}(8, 1)$ distributions.



(c) Expected norm of the Stein score along trajectories interpolating between reference and target $p_0 = \mathrm{N}(a, 1)$ distributions for different target mean.

Figure S3: The reference distribution is $p_{\text{ref}} = \mathrm{N}(0, 1)$.

Moser flows perform the interpolation in *density space*, i.e. $\hat{p}_t = (1-t)\hat{p}_0 + t\hat{p}_1$ for any $t \in [0, 1]$, whereas RSGM performs the interpolation in *sample space*, i.e. $p_t = \int_{\mathcal{M}} p_0(y) p_{t|0}(y, x) \mathrm{d}p_{\text{ref}}(y)$. Interpolation in the *density space* results in spontaneous creation of density, whereas interpolation in *sample space* corresponds to a displacement of the density, see Figs. S3a and S3b. In that respect, Moser flows can be seen as *vertical displacement* whereas RSGM corresponds to *horizontal displacement*, see Santambrogio (2017). The drawback with the 'spontaneous creation of density' of Moser flows, is that when solving trajectories in *sample space*—for sampling or likelihood evaluation purposes—the Stein score's amplitude can get extremely high in settings where the reference and target distributions have little overlap as shown on Fig. S3c.

K Density estimation with Fisher score

In this section, we show how we can adapt ideas from Choi et al. (2021) for density estimation on $\mathcal{M}$ using the Fisher score. The main idea of using Fisher score is to leverage the following decomposition

for any $x \in \mathcal{M}$

$$\log p_0(x) = \log p_T(x) - \int_0^T \partial_t \log p_t(x) \mathrm{d}t.$$

Assume that an approximation $\hat{\mathrm{s}}_\theta$ of $\partial_t \log p_t$ (the Fisher score) is available then we have that for any $x \in \mathcal{M}$

$$\log p_0(x) \approx \log p_{\text{ref}}(x) - \int_0^T \hat{\mathrm{s}}_\theta(x) \mathrm{d}t.$$

Before turning to our main result, we state the following lemma.

Lemma S23. *Assume* **A**1*. Then, there exists $C, T_0 \geq 0$ such that for any $x \in \mathcal{M}$ and $T \geq T_0$, $|p_T(x) - 1| \leq C \exp[-\lambda_1 T/2]$, where λ_1 is the first non-negative eigenvalue of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(p_{\text{ref}})$.*

Proof. First, using Proposition S10, there exists $C_0 \geq 0$ such that for any $T \geq 1/2$ we have

$$\int_{\mathcal{M}} |p_T(x) - 1| \mathrm{d}p_{\text{ref}}(x) \leq C_0 \mathrm{e}^{-\lambda_1 T}.$$

Using (Grigor'yan, 1999, Corollary 5.5), (Hsu, 1999, Theorem 1.2)and the fact that $\mathcal{M}$ is compact, there exists $C_1, \beta \geq 0$ such that for any $T \geq 1/2$ and $x_0, x_T \in \mathcal{M}$

$$\|\nabla p_{T|0}(x_T|x_0)\| \leq C_1(1 + T^\beta). \tag{S33}$$

In addition, using (Croke, 1980, Proposition 14) we have that there exists $C_2, r_0 > 0$ such that for any $x_0 \in \mathcal{M}$ and $r \in (0, r_0)$

$$\int_{\bar{\mathrm{B}}(x_0,r)} \mathrm{d}p_{\text{ref}}(x) \geq C_2 r^d. \tag{S34}$$

Assume that that $\int_{\mathcal{M}} |p_T(x) - 1| \mathrm{d}p_{\text{ref}}(x) \leq \varepsilon$ and that there exists $x_0 \in \mathcal{M}$ such that $|p_T(x) - 1| > \kappa\varepsilon$ with $\kappa > 0$ and let $T \geq T_0$ with $T_0 = (\kappa\varepsilon/(2C_1))^{1/\beta}$. Then, using (S33) and (S34), we have for any $r \in (0, r_0)$

$$\varepsilon \geq \int_{\bar{\mathrm{B}}(0,r)} |p_T(x) - 1| \geq C_2 r^d (\kappa\varepsilon - C_1(1 + T^\beta) r).$$

Since $\kappa\varepsilon/(2C_1(1 + T^\beta)) \in (0, r_0)$ we have

$$\varepsilon \geq C_2 (\kappa\varepsilon)^{d+1} / (4C_1(1 + T^\beta)).$$

Therefore, we get that

$$\varepsilon \geq C_2 (\kappa\varepsilon)^{d+1} / (4C_1(1 + T^\beta)).$$

Therefore, we get that $\kappa \leq (4C_1(1 + T^\beta)/C_2)^{1/(d+1)} \varepsilon^{-1/(d+1)}$. Therefore, we have that for any $x \in \mathcal{M}$

$$|p_T(x) - 1| \leq (8C_1(1 + T^\beta)/C_2)^{1/(d+1)} \varepsilon^{1-1/(d+1)}. \tag{S35}$$

Let $T_0 \geq 0$ such that for any $T \geq T_0$ we have

$$(8C_1(1 + T^\beta)/C_2)^{1/(d+1)} C_0^{1-1/(d+1)} \mathrm{e}^{-(1-1/(d+1))\lambda_1 T} \leq 2^{1-\beta} C_1.$$

Combining this result and (S36), we get that for any $x \in \mathcal{M}$ and $T \geq 0$

$$|p_T(x) - 1| \leq (8C_1(1 + T^\beta)/C_2)^{1/(d+1)} C_0^{1-1/(d+1)} \mathrm{e}^{-(1-1/(d+1))\lambda_1 T}, \tag{S36}$$

which concludes the proof. □

The following proposition quantifies this approximation.

Proposition S24. *Assume* **A**1 *and that $p_0 \in \mathrm{C}^\infty(\mathcal{M}, (0, +\infty))$. Let $x_0 \in \mathcal{M}$ and assume that for any $t \in [0, T]$, $|\hat{\mathrm{s}}_\theta(t, x_0) - \partial_t \log p_t(x_0)| \leq \mathtt{M}$ with $\mathtt{M} \geq 0$. Then, there exists $C, T_0 \geq 0$ such that for any $T \geq 0$*

$$|\log p_0(x_0) - \int_0^T \hat{\mathrm{s}}_\theta(t, x_0) \mathrm{d}t| \leq C \exp[-\lambda_1 T/2] + \mathtt{M}T.,$$

where λ_1 is the first non-negative eigenvalue of $-\Delta_{\mathcal{M}}$ in $\mathrm{L}^2(p_{\text{ref}})$.

Proof. First using, Lemma S23, there exists $C_0, T_0^{(a)} \geq 0$ such that for any $T \geq T_0^{(a)}$

$$|p_T(x_0) - 1| \leq C_0 \exp[-\lambda_1 T/2].$$

Let $T_0^{(b)} = |\log(C_0)| / \lambda_1$. Using that for any $s \in [1/2, +\infty)$ we have that $|\log(1 + s)| \leq 2\log(2)|s|$ we get that for any $T \geq \max(T_0^{(a)}, T_0^{(b)})$

$$|\log p_T(x_0)| \leq 2\log(2) C_0 \exp[-\lambda_1 T/2],$$

which concludes the proof. □

In practice, we do not have access to $\partial_t \log p_t$. However, following (Choi et al., 2021, Proposition 2), we have the following property.

Proposition S25. *Let $\hat{\mathbf{s}}$ such that for any $t \in [0,T]$ and $x \in \mathcal{M}$, $\hat{\mathbf{s}}(t,x) = \partial_t \log p_t(x)$. Then, we have that $\hat{\mathbf{s}} = \arg\min\{L(\mathbf{s}) \ : \ \mathbf{s} \in \mathrm{C}^\infty([0,T] \times \mathcal{M}, \mathbb{R})\}$, where for any $\mathbf{s} \in \mathrm{C}^\infty([0,T] \times \mathcal{M}, \mathbb{R})$ we have*

$$L(\mathbf{s}) = (1/2)\mathbb{E}[\int_0^T \lambda(t)\mathbf{s}(t,\mathbf{X}_t)\mathrm{d}t] + \mathbb{E}[\int_0^T \lambda(t)\partial_t \mathbf{s}(t,\mathbf{X}_t)\mathrm{d}t] + \mathbb{E}[\int_0^T \partial_t\lambda(t)\partial_t \mathbf{s}(t,\mathbf{X}_t)\mathrm{d}t] + \mathbb{E}[\lambda(0)\mathbf{s}(0,\mathbf{X}_0)] - \mathbb{E}[\lambda(T)\mathbf{s}(T,\mathbf{X}_T)],$$

where $\lambda \in \mathrm{C}^\infty([0,T],\mathbb{R})$ is a weighting function.

Proof. For any $t \in [0,T]$ and $x_t \in \mathcal{M}$ we have

$$\hat{\mathbf{s}}(x_t) = \int_{\mathcal{M}} \partial_t \log p_{t|0}(x_t|x_0) p_{0|t}(x_0|x_t)\mathrm{d}x_0.$$

Hence, since $\mathcal{M}$ is compact and $\hat{\mathbf{s}} \in \mathrm{C}^\infty([0,T] \times \mathcal{M}, \mathbb{R})$, we have that $\hat{\mathbf{s}} = \arg\min\{L_0(\mathbf{s}) \ : \ \mathbf{s} \in \mathrm{C}^\infty([0,T] \times \mathcal{M}, \mathbb{R})\}$ where for any $\mathbf{s} \in \mathrm{C}^\infty([0,T] \times \mathcal{M}, \mathbb{R})$ we have

$$\begin{aligned} L_0(\mathbf{s}) &= \int_0^T \lambda(t) \int_{\mathcal{M}\times\mathcal{M}} (\mathbf{s}(t,x_t) - \partial_t \log p_{t|0}(x_t|x_0))^2 \mathrm{d}p_{0,t}(x_0,x_t)\mathrm{d}t \\ &= \int_0^T \lambda(t) \int_{\mathcal{M}} \mathbf{s}(t,x_t)^2 \mathrm{d}p_t(x_t)\mathrm{d}t - 2\int_0^T \lambda(t) \int_{\mathcal{M}\times\mathcal{M}} \mathbf{s}(t,x_t)\partial_t \log p_{t|0}(x_0,x_t)\mathrm{d}p_{0,t}(x_0,x_t)\mathrm{d}t \\ &\quad + \int_0^T \lambda(t) \int_{\mathcal{M}} \mathrm{d}p_t(x_t)\mathrm{d}t \end{aligned} \tag{S37}$$

In addition, we have that

$$\begin{aligned} &\int_0^T \lambda(t) \int_{\mathcal{M}\times\mathcal{M}} \mathbf{s}(t,x_t)\partial_t \log p_{t|0}(x_t|x_0)\mathrm{d}p_{0,t}(x_0,x_t)\mathrm{d}t \\ &\qquad = \int_0^T \int_{\mathcal{M}\times\mathcal{M}} \lambda(t)\mathbf{s}(t,x_t)\partial_t p_{t|0}(x_t)\mathrm{d}p_0(x_0)\mathrm{d}p_{\mathrm{ref}}(x_t)\mathrm{d}t. \end{aligned}$$

By integration by parts we get

$$\begin{aligned} &\int_0^T \int_{\mathcal{M}\times\mathcal{M}} \lambda(t)\mathbf{s}(t,x_t)\partial_t p_{t|0}(x_t)\mathrm{d}p_0(x_0)\mathrm{d}p_{\mathrm{ref}}(x_t)\mathrm{d}t \\ &\quad = -\int_0^T \int_{\mathcal{M}\times\mathcal{M}} \partial_t(\lambda(t)\mathbf{s}(\cdot,x_t))(t)\mathrm{d}p_{0,t}(x_0,x_t)\mathrm{d}t \\ &\qquad + \lambda(T)\int_{\mathcal{M}} \mathbf{s}(T,x_T)\mathrm{d}p_T(x_T) - \int_{\mathcal{M}} \mathbf{s}(0,x_0)\mathrm{d}p_0(x_0) \\ &\quad = -\int_0^T \int_{\mathcal{M}\times\mathcal{M}} \partial_t\lambda(t)\mathbf{s}(t,x_t)\mathrm{d}p_t(x_t)\mathrm{d}t - \int_0^T \int_{\mathcal{M}\times\mathcal{M}} \lambda(t)\partial_t\mathbf{s}(t,x_t)\mathrm{d}p_t(x_t)\mathrm{d}t \\ &\qquad + \lambda(T)\int_{\mathcal{M}} \mathbf{s}(T,x_T)\mathrm{d}p_T(x_T) - \lambda(0)\int_{\mathcal{M}} \mathbf{s}(0,x_0)\mathrm{d}p_0(x_0) \end{aligned}$$

Combining this result and (S37) we get that

$$\begin{aligned} L_0(\mathbf{s}) &= \int_0^T \lambda(t) \int_{\mathcal{M}\times\mathcal{M}} (\mathbf{s}(t,x_t) - \partial_t \log p_{t|0}(x_t|x_0))^2 \mathrm{d}p_{0,t}(x_0,x_t)\mathrm{d}t \\ &= \int_0^T \lambda(t) \int_{\mathcal{M}} \mathbf{s}(t,x_t)^2 \mathrm{d}p_t(x_t)\mathrm{d}t + 2\int_0^T \int_{\mathcal{M}\times\mathcal{M}} \partial_t\lambda(t)\mathbf{s}(t,x_t)\mathrm{d}p_t(x_t)\mathrm{d}t \\ &\quad + 2\int_0^T \int_{\mathcal{M}\times\mathcal{M}} \lambda(t)\partial_t\mathbf{s}(t,x_t)\mathrm{d}p_t(x_t)\mathrm{d}t - \lambda(T)\int_{\mathcal{M}} \mathbf{s}(T,x_T)\mathrm{d}p_T(x_T) \\ &\quad + \lambda(0)\int_{\mathcal{M}} \mathbf{s}(0,x_0)\mathrm{d}p_0(x_0) + \int_0^T \lambda(t)\int_{\mathcal{M}}^2 \mathrm{d}p_t(x_t)\mathrm{d}t, \end{aligned}$$

which concludes the proof. □

Hence, using Proposition S25, we could estimate jointly the spatial (or Stein) score used in RSGM and the Fisher score considered in this section, see Choi et al. (2021).

L Extensions

L.1 Schrödinger bridge.

For Euclidean SGM, the generative model is given by an approximation of the time-reversal of the noising dynamics $(\mathbf{X}_t)_{t\in[0,T]}$ while the backward dynamics $(\mathbf{Y}_t)_{t\in[0,T]}$ is initialized with the invariant distribution of the noising dynamics (the uniform distribution p_{ref} in case of RSGM). However, in order for the method to yield good results we need $\mathcal{L}(\mathbf{Y}_0) \approx \mathcal{L}(\mathbf{X}_T)$ (see De Bortoli

et al., 2021, Theorem 1). Usually, this requires the number of steps in the backward process to be large in order to keep T large and γ small (where $\gamma > 0$ is the stepsize in the GRW). Another limitation of SGM is that existing methods target an easy-to-sample reference distribution. Hence, classical SGM cannot interpolate between two distributions defined by datasets. To circumvent this problem, one can consider a process whose initial and terminal distribution are pinned down using Schrödinger bridges (Schrödinger, 1932; Léonard, 2012a; Chen et al., 2016; De Bortoli et al., 2021; Vargas et al., 2021).

L.2 Conditional RSGM.

Another extension of interest is conditional sampling. By amortizing SGM with respect to an observation y it is possible to approximately sample from a given posterior distribution. In the Euclidean setting this idea has been successfully applied for several image processing problems such as deblurring, denoising or inpainting (see for instance Kawar et al., 2021a,b; Lee et al., 2021; Sinha et al., 2021; Batzolis et al., 2021; Chung et al., 2021). Similarly, RSGM can be amortized to handle such situations in the case where the underlying posterior distribution is supported on a manifold. Practically, this requires for the score network takes an additional input, i.e $\mathbf{s}_\theta(t, x; y)$.

L.3 Invariant distributions

In what follows, we propose an extension for modelling probability distributions which known invariance. That is, we assume that $p_0(\rho(g)x) = p_0(x)$ for all $g \in G$, with G a group and $\rho : G \to \mathrm{GL}_n(\mathbb{R})$ a representation. Following Köhler et al. (2020), we have that if p_{ref} is invariant w.r.t. G and $\phi : \mathcal{M} \to \mathcal{M}$ is equivariant w.r.t. to G, then the pushforward probability density $p = p_{\text{ref}} \circ \phi^{-1}$ is invariant w.r.t. G.

Let's consider the probability flow ϕ associated with the reverse diffusion (4)—given by $\mathrm{d}\mathbf{Y}_t = \{-b(\mathbf{Y}_t) + \nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \mathrm{d}\mathbf{B}_t^{\mathcal{M}}$— i.e. the solution of the following ODE (see App. C)

$$\mathrm{d}\mathbf{Y}_t = \{-b(\mathbf{Y}_t) + \tfrac{1}{2}\, \nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t.$$

In practice, the Stein score $\nabla \log p_t$ is approximated with the score network $\boldsymbol{s}_\theta(t, \cdot)$. It is sufficient to parametrize the score network so that it is equivariant w.r.t. its second argument —assuming that $\rho(g)$ and the drift b commute (e.g. which is true for a linear drift)—since we then have

$$\left[-b + \tfrac{1}{2}\, \boldsymbol{s}_\theta\left(T - t, \cdot\right)\right](\rho(g)\mathbf{Y}_t) = \rho(g)\left[-b + \tfrac{1}{2}\, \boldsymbol{s}_\theta\left(T - t, \cdot\right)\right](\mathbf{Y}_t).$$

M Stereographic baseline details

In the experiments on the sphere we compare to a Stereographic Score-Based baseline model. This model is an alternative to the RSGM the we propose in order to construct score-based models on manifolds without having to construct the intrinsic approach presented in the paper as Riemannian Score-Based models. They can be applied to more cases than just the sphere.

In general these models work as follows:

1. Project the datapoints from the manifold to Euclidean space through a invertible[11] function $f : \mathcal{M} \to \mathbb{R}^d$.
2. Train a Euclidean score-based generative model on the datapoints projected to Euclidean space, giving a density p_θ on $\mathbb{R}^d$ (where θ are the parameters of the density).
3. Define the density on the manifold as the pushforward of the density in Euclidean space under the inverse of the bijection, $P_{\theta,\mathcal{M}} = f_*^{-1} p_\theta$.

One could also apply these models to the torus. By using the bijection $f : \theta \mapsto \tan(\theta)$ we can project each coordinate onto the real line.

In general we found that these models perform less well than their intrinsic counterparts. In order to map density near the seams of the bijection, it requires the model to send data points off to infinity in

[11] Note that this may not be a bijection. For example for the sphere we use the stereographic projection of the earth onto the plane, which misses out a single point, opposite the projection point.

the Euclidean space. This is numerically challenging and leaves artefacts in the pushforward density on the manifold. In addition, these methods depend on the bijection used to project the data into a Euclidean space and therefore are not intrinsic.

N Experimental details

In what follows we describe the experimental settings used to generate results introduced in Sec. 6. The models and experiments have been implemented in Jax (Bradbury et al., 2018), using a modified version of the Riemannian geometry library Geomstats (Miolane et al., 2020b).

Anonymized code can be found at here[12]. Due to difficulties referencing anonymized repositories, the modified version of geomstats is included as a zip file in the supplementary material. Additionally modified versions of the `submitit` and `hydra-submitit-launcher` packages are not supplied for the same reasons, but the default versions of these will suffice for most users. Full code and all repos will be publicly available after publication.

Models Following Song et al. (2021), the score-based generative models (SGMs) diffusion coefficient is parametrized as $g(t) = \sqrt{\beta(t)}$ with $\beta : \ t \mapsto \beta_{\min} + (\beta_{\max} - \beta_{\min}) \cdot t$.

Architecture The architecture of the score network $\boldsymbol{s}_\theta$ is given by a multilayer perceptron with 5 hidden layers for the Earth and $SO(3)$ experiments, and 3 for the high-dimension experiments with 512 units each. We use sinusoidal activation functions. We decompose the output of the score network on the set of divergence free vector fields as per Sec. 3.4.

Loss Where not specified, SGMs are trained with the sliced score matching (SSM) loss ℓ_t^{im}, relying on the Hutchinson estimator for computing the divergence with Rademacher noise described in Sec. 3.4. We found that training with the denoising score matching (DSM) loss $\ell_{t|0}$ gave similar results. Regarding the weighting function, for DSM loss $\ell_{t|0}$ we use $\lambda_t = \text{Var}[X_t|X_0]$ (where we rely on the closed-form standard deviation available in the Euclidean setting as a proxy for the compact manifold setting), while for the ISM/SSM losses ℓ_t^{im} we use $\lambda_t = g(t)^2 = \beta(t)$.

Optimization All models are trained by the stochastic optimizer Adam (Kingma and Ba, 2015) with parameters $\beta_1 = 0.9$, $\beta_2 = 0.999$, batch-size of 512 data-points. The learning rate is annealed with a linear ramp from 0 to 1000 and from then with a cosine schedule.

Likelihood evaluation and sample drawing We rely on the Dormand-Prince solver (Dormand and Prince, 1980), an adaptive Runge-Kutta 4(5) solver, with absolute and relative tolerance of $1e-5$ to compute approximate numerical solutions of any ODEs. For the rollouts of the SGM SDEs we use a Euler Maruyama predictor and no corrector. Unless stated we use 100 step rollouts.

Hardware Models are trained on a cluster with a mixture of GeForce RTX 1080, 1080 Ti and 2080 Ti GPU cards.

N.1 Sphere

Data We randomly split the datasets intro training, validation and test datasets with $(0.8, 0.1, 0.1)$ proportions. In each case the earth is approximated as a perfect sphere.

Models The mixture of Kent distributions (Peel et al., 2001) were optimised using the EM algorithm and the number of components were selected from a grid search over the range $5, 10, 15, 20, 25, 30, 40, 50, 75, 100$, based on validation set likelihood and 250 EM iterations. The number of components selected were: Volcano 25, Earthquake 50, Flood 100 and Fire 100.

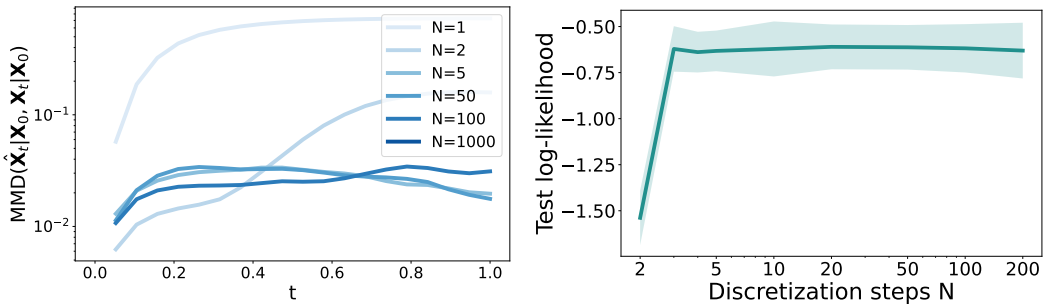
For the stereographic SGM–which is a standard SGM with an Ornstein–Uhlenbeck process followed with the inverse stereographic projection–we found $\beta_{\min} = 0.001$ and $\beta_{\max} = 2$ to work best.

[12] https://anonymous.4open.science/r/rimannian-score-sde

Optimization The score-based models are trained for $600k$ iterations for all datasets but 'Flood' where $300k$ performed best.

Additional experimental results

Approximate forward sampling Standard Euclidean SGMs rely on a Ornstein–Ulhenbeck (OU) forward process (1) which can easily be simulated since $\mathbf{X}_t|\mathbf{X}_0$ is Gaussian. In contrast, for most manifolds one has to rely on an approximate sampling scheme—see Sec. 3.3. First, we directly assess the quality of the approximate samples $\hat{\mathbf{X}}_t|\mathbf{X}_0$ obtained via geodesic random walk (GRW), against 'exact' samples $\mathbf{X}_t|\mathbf{X}_0$ which are obtained by using a high number of discretization steps ($N = 1000$). We report on Fig. S4a the discrepancy between these distributions for different values of discretization steps N, as measured by maximum mean discrepancy (MMD) (Gretton et al., 2012). We see that from $N = 5$ the approximate samples are very closely distributed to the true samples. Then, in order to assess the impact of this approximation on the RSGMs' performance, we report on Fig. S4b the log-likelihood when varying the number of discretization steps N. We similarly observe that apart from very small values of N, the models' performance is very robust to the approximation quality of the forward sampling samples.



(a) Maximum mean discrepancy (MMD) distance between *'exact'* (i.e. approximated with $N = 1000$ steps) $\mathbf{X}_t|\mathbf{X}_0$ and *approximate* $\hat{\mathbf{X}}_t|\mathbf{X}_0$ at for every $t \in [0, 1]$.

(b) Test log-likelihood of trained RSGMs on the Flood dataset while varying the number of discretization steps N when simulating forward sampling $\mathbf{X}_t|\mathbf{X}_0$.

Figure S4: Ablation study on the impact of the forward sampling approximation quality on $\mathbb{S}^2$.

DSM loss $\ell_{t|0}$ On Fig. S5, we show how the test log-likelihood varies with respect to the two hyparameters of the DSM loss, by training RSGMs over a grid of values for τ and J on the Flood dataset. We can see that the Varadhan approximation by itself ($\tau = 1$) yields descent performance, although a wise combination of Varadhan approximation with a truncation of the heat kernel can give even better results. The performance is relatively robust to the choice of such hyperparameters as long as τ and J are high enough.

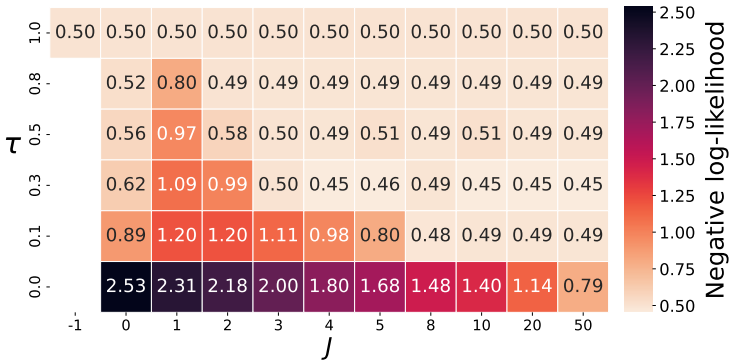


Figure S5: Ablation study on the denoising score matching (DSM) loss $\ell_{t|0}$ when combining the heat kernel truncation and the Varadhan approximation: $\nabla_{x_t} \log p_{t|0}(x_t|x_0) \approx \mathbb{1}(t \leq \tau) \exp_{x_t}^{-1}(x_0) + \mathbb{1}(t > \tau) S_{J,t}(x_0, x_t)$.

N.2 Torus

Data The synthetic data trained on consists of a wrapped Gaussian distribution on $\mathbb{T}^n$ with uniformly chosen random mean and standard deviation of 0.2. Such a distribution is defined by taking the density of a Normal distribution in the tangent space of the manifold at the mean and passing it through the exponential map at the mean.

Architecture To parametrize the vector field on $\mathbb{T}^n$ we use a single filed per dimension pointing in a consistent direction around the ith component in the product, with unit norm.

Models All models were trained with the same 3 layer, 512 units per layer MLP across different dimension sizes.

Optimization The models are optimized for $50k$ iterations. The RSGM models are trained with both the implicit score-matching loss and the sliced score-matching loss.

N.3 Special Orthogonal group

Applications of orthogonal constraints span various fields, such as protein docking with ligands binding pose prediction (Ganea et al., 2022), robotics and Computer vision with rigid body transformation estimation (Barfoot et al., 2011; Prokudin et al., 2018), and medical imaging for data alignment (Hou et al., 2018).

Data We consider the synthetic dataset consisting of samples in $\mathrm{SO}_3(\mathbb{R}^d)$[13] from the mixture distribution with density $p(\mathrm{Q}) = \frac{1}{K}\sum_{k=1}^{K} \mathrm{N}^W(\mathrm{Q}|\mathrm{Q}_k, \sigma_k^2)$ with $K \in \mathbb{N}$, where for any $k \in \{1, \dots, K\}$, we have that $\mathrm{Q} = \mathrm{Q}_k \exp_{\mathrm{Id}}[\sigma_k \hat{z}]$ with $z \sim \mathrm{N}(0, \mathrm{Id}_{\mathbb{R}^3})$ satisfies $Q \sim \mathrm{N}^W(\mathrm{Q}_k, \sigma_k)$ and $(\cdot)^\wedge : \mathbb{R}^3 \to \mathfrak{so}(3)$. For any $k \in \{1, \dots, K\}$, we set $\mathrm{Q}_k \sim \mu$ where μ is the uniform distribution on $\mathrm{SO}_3(\mathbb{R})$ and $\sigma_k^2 \sim \mathrm{IG}(\alpha = 100, \beta = 1)$, where IG is the inverse Gaussian distribution. We choose $K = 32$ mixture components. We showcase a conditional sampling extension of our model—see App. L for more details— by targeting individual mixture components $p(Q|k)$. Our model is trained using the $\ell_{t|0}$ (DSM) loss along with the Varadhan asymptotic approximation, see (8).

Architecture To parametrize the vector field, we rely on the basis of the Lie group, $\mathfrak{so}(n) = \{\mathrm{A} \in \mathrm{M}_d(\mathbb{R}) : \mathrm{A}^\top = -\mathrm{A}\}$ given by $\mathrm{E}_{ij} = \mathrm{U}_{ij} - \mathrm{U}_{ji}$ for $i, j \in \{1, \dots, d\}$ with $i < j$ and $\mathrm{U}_{ij} = (\delta_{ij}(k, \ell))_{1 \le k, \ell \le d}$, which induces a basis on the tangent spaces $\mathrm{T}_{\mathrm{Q}}\mathrm{SO}_d$ for any $\mathrm{Q} \in \mathrm{SO}_d(\mathbb{R})$ given by $\{\mathrm{QE}_{ij}\}_{1 \le i < j \le d}$. This is the divergence-free vector field approach described in Sec. 3.4.

Models We compare our proposed approach against Moser flows (Rozen et al., 2021) and a wrapped-exponential baseline (Falorsi et al., 2019) defined as the pushforward along the transformation $\mathbb{R}^3 \xrightarrow{F_\theta^{-1}} \mathbb{R}^3 \xrightarrow{g} \mathbb{R}^3 \xrightarrow{\wedge} \mathfrak{so}(3) \xrightarrow{\exp} \mathrm{SO}_3(\mathbb{R})$ with F_θ^{-1} denoting the approximate time-reversed diffusion, g denoting the radial operator defined by $g : x \mapsto 2\pi \tanh(\|x\|)x/\|x\|$, $(\cdot)^\wedge : \mathbb{R}^3 \to \mathfrak{so}(n)$ the isomorphism given by the basis on $\mathfrak{so}(3)$ and $\exp$ the matrix exponential. The radial g operator's constant 2π is chosen as the injectivity radius of the group so that the transformation $\tanh \circ \wedge \circ \exp$ is injective (the set of elements with no preimage is then only the cut locus which is known to have measure zero). Henceforth, this wrapped-exponential transformation cannot be bijective, it is either injective *or* surjective depending on the choice of radius in the radial operator g.

Optimization Models are trained for $100k$ iterations. The Riemannian SGM is trained with the Varhadan approximation of the denoising score-matching loss (DSM) Sec. 3.4, and the wrapped-exponential model relies on the exact DSM loss. After a first hyperparameter exploration, a grid search is performed over `learning_rate` $\in [2e-5, 4e-5]$, for SGMs over $\beta_f \in [0.5, 1, 2, 4, 6, 8, 10]$ and for Moser flows over $K \in [1000, 10000]$ and $\lambda_{\min} \in [1, 10, 100]$.

[13] This manifold is 3-dimensional.