Bridge Simulation on Lie Groups and Homogeneous Spaces with Application to Parameter Estimation

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Abstract. We present three simulation schemes for simulating Brownian bridges on complete and connected Lie groups and homogeneous spaces and use numerical results of the guided processes in the Lie group SO(3) and on the homogeneous spaces $\mathrm{SPD}(3) = \mathrm{GL}_+(3)/\mathrm{SO}(3)$ and $\mathbb{S}^2 = \mathrm{SO}(3)/\mathrm{SO}(2)$ to evaluate our sampling scheme. Brownian motions on Lie groups can be defined via the Laplace-Beltrami of a left- (or right-)invariant Riemannian metric. Given i.i.d. Lie group-valued samples on SO(3) drawn from a Brownian motion with unknown Riemannian metric structure, the underlying Riemannian metric on SO(3) is estimated using an iterative maximum likelihood (MLE) method. Furthermore, the re-sampling technique is applied to yield estimates of the heat kernel on the two-sphere considered as a homogeneous space. Comparing this estimate to the truncated version of the closed-form expression for the heat kernel on $\mathbb{S}^2$ serves as a proof of concept for the validity of the sampling scheme on homogeneous spaces.

Keywords: Brownian Motion, Brownian Bridge Simulation, Lie groups, Homogeneous Spaces, Metric estimation

1 Introduction

In this paper, we consider discrete time observations on Lie groups and homogeneous spaces considered as incomplete observations of a continuous time sample path of a left- (or right-)invariant Brownian motion. In order to handle the discrete time observations and infer properties of the unknown underlying distribution, we derive bridge simulation schemes on Lie groups and homogeneous spaces. To the best of our knowledge, this paper is the first to describe a simulation technique for diffusion bridges in the context of Lie groups.

Simulation of conditioned diffusion processes is a highly non-trivial problem. A common issue is that the transition densities are non-tractable and thus simulating directly from the true distribution is non-feasible. Several papers have described diffusion bridge simulation methods; see, e.g., [2–4,14,15,17] which describes various methods for simulation of multi-dimensional conditioned diffusion processes and their usage for parameter estimation and likelihood inference for stochastic differential equations. These papers introduced a variety of different guiding drift terms which replaced the drift term depending on the intractable transition density. To the best of our knowledge, this paper is the first to describe a simulation technique for diffusion bridges in the context of Lie groups.

The idea of the present paper is based on the method presented in the seminal paper by Delyon and Hu [4]. In here, the authors exchanged the intractable guiding drift term $\nabla_{x=X_t} \log p_{T-t}(x, v)$ in the stochastic differential equation (SDE) for the conditioned diffusion with the guiding drift term in the SDE for a Brownian bridge $(BB_t)_{t\geq 0}$ conditioned at $BB_T = v$.

Geometric statistics and probability on non-linear spaces is still a widely unexplored domain. It can be mentioned as an example that a closed form expression for the transition density of a Brownian motion is only known on a limited amount of geometries. Examples of these geometries include: Euclidean spaces (zero curvature), hyper-spheres (constant positive curvature), and hyperbolic spaces (constant negative curvature). Thompson [20] showed how guiding to the nearest point yielded an approximation of the transition density (heat kernel) of a Brownian motion on Riemannian manifolds. More generally, Thompson obtained an expression of the integrated heat kernel over a submanifold by conditioning a Brownian motion to end up in the submanifold at a fixed positive time.

In this paper, we present three simulation schemes for simulating diffusion bridges on homogeneous spaces. The first scheme builds on the idea of Thompson [20] by conditioning on a submanifold in the Lie group G obtained as a fiber over the point $v \in M = G/K$, for some closed subgroup $K \subseteq G$. The second scheme assumes the homogeneous space has a discrete fiber Γ and therefore the fiber over $v \in M$, $\pi^{-1}(v)$, is discrete. Using the k-nearest-points from the fiber $\pi^{-1}(v)$ to the initial point x_0, we obtain a truncated guiding drift term convergence to a subset of $\pi^{-1}(v)$. The last scheme assumes that the fiber is connected. Sampling k-points in the fiber over v a similar conditioning is obtained.

The paper is organized as follows. In Section 2, we describe some background theory of Lie groups, Brownian motions, and Brownian bridges in Riemannian manifolds. Section 3 presents the theory and results of bridge sampling in Lie groups, while Section 4 introduce bridge sampling on various homogeneous spaces. Numerical experiments on certain Lie groups and homogeneous spaces are presented in 5. Section 5.1 shows in practice the simulation scheme in the Lie group SO(3). A Brownian motion on any nice smooth manifold is intimately connected with its endowed metric through its covariance structure (see Section 2.4). Sampling data points from a Brownian motion with unknown covariance, an estimate of the underlying unknown metric is obtained by means of importance sampling. In Section 5.3, estimates for the heat kernel are visualized on the two-sphere $\mathbb{S}^2$ considered as the homogeneous space SO(3)/SO(2).

The estimate on $\mathbb{S}^2$ is compared to the exact heat kernel on $\mathbb{S}^2$ in case of a bi-invariant metric.

2 Notation and Background

We briefly describe the basics of simulating conditioned diffusion in $\mathbb{R}^n$ as was developed in [4], before reviewing some theory on conditioned diffusion on Riemannian manifolds.

2.1 Conditioned Diffusions in $\mathbb{R}^n$

Suppose a strong solution to an SDE of the form

$$dx_t = b(t, x_t)dt + \sigma(t, x_t)dw_t,$$

where b and σ satisfies certain regularity conditions and where w denote a $\mathbb{R}^n$-valued Brownian motion. In this case x is Markov and its transition density exist. Suppose we define the function

$$h(t, x) = \frac{p_{T-t}(x_t, v)}{p_T(x_0, v)},$$

for some $x_0, v \in \mathbb{R}^n$, then it is easily derived that h is a martingale on $[0, T)$ with $h(0, x_0) = 1$ and Doob's h-transform implies that the SDE of the conditioned diffusion $x|x_T = v$ is given by

$$dy_t = \tilde{b}(t, y_t)dt + \sigma(t, y_t)dw_t$$

where $\tilde{b}(t, y) = b(t, y) + (\sigma\sigma^T)(t, y)\nabla_y \log p_{T-t}(y, v)$. In case that the transition density is intractable, simulation from the exact distribution is in-feasible. Delyon and Hu [4] suggested substituting the latter term in $\tilde{b}$ with a drift term of the form $-(y_t - v)/(T - t)$, which equals the drift term in a Brownian bridge. The guided process obtained by making the above substitution yields a conditioning and one obtain

$$\mathbb{E}[f(x)|x_T = v] = C\mathbb{E}[f(y)\varphi_T], \tag{1}$$

where φ_T is a likelihood function that is tractable and easy to compute, and y is the guided process. Below we generalize this method to manifolds and homogeneous spaces.

2.2 General Lie Group Notation

Throughout, we let G denote a connected Lie Group of dimension d, i.e., a smooth manifold with a group structure such that the group operations $G \times G \ni (x, y) \overset{\mu}{\mapsto} xy \in G$ and $G \ni x \overset{\iota}{\mapsto} x^{-1} \in G$ are smooth maps. If $x \in G$, the left-multiplication map, $L_x y$, defined by $y \mapsto \mu(x, y)$, is a diffeomorphism from G to itself. Similarly, the right-multiplication map $R_x y$ defines a diffeomorphism from G to itself by $y \mapsto \mu(y,x)$. Let $dL_x\colon TG \to TG$ denote the pushforward map given by $(dL_x)_y\colon T_yG \to T_{xy}G$. A vector field V on G is said to be left-invariant if $(dL_x)_yV(y) = V(xy)$. The space of left-invariant vector fields is linearly isomorphic to T_eG, the tangent space at the identity element $e \in G$. By equipping the tangent space T_eG with the Lie bracket we can identify the Lie algebra $\mathfrak{g}$ with T_eG. The group structure of G makes it possible to define an action of G on its Lie algebra $\mathfrak{g}$. The conjugation map $C_x := L_x \circ R_x^{-1}\colon y \mapsto xyx^{-1}$, for $x \in G$, fixes the identity e. Its pushforward map at e, $(dC_x)_e$, is then a linear automorphism of $\mathfrak{g}$. Define $\mathrm{Ad}(x) := (dC_x)_e$, then $\mathrm{Ad}\colon x \mapsto \mathrm{Ad}(x)$ is the adjoint representation of G in $\mathfrak{g}$. The map $G \times \mathfrak{g} \ni (x,v) \mapsto \mathrm{Ad}(x)v \in \mathfrak{g}$ is the adjoint action of G on $\mathfrak{g}$. We denote by $\langle \cdot,\cdot \rangle$ a Riemannian metric on G. The metric is said to be left-invariant if $\langle u,v\rangle_y = \langle (dL_x)_yu, (dL_x)_yv\rangle_{L_x(y)}$, for every $u,v \in T_yG$, i.e., the left-multiplication maps are isometries, for every $x \in G$. In particular, we say that the metric is $\mathrm{Ad}(G)$-invariant if $\langle u,v\rangle_e = \langle \mathrm{Ad}(x)u, \mathrm{Ad}(x)v\rangle_e$, for every $u,v \in \mathfrak{g}$. Note that an $\mathrm{Ad}(G)$-invariant metric on G is equivalent to a bi-invariant (left- and right-invariant) inner product on $\mathfrak{g}$. The differential of the Ad map at the identity yields a linear map $\mathrm{ad}(x) = d/dt\,\mathrm{Ad}(\exp(tx))|_0$. This linear map defines the Lie bracket $[v,w] = \mathrm{ad}(v)w$, $v,w \in \mathfrak{g}$.

A one-parameter subgroup of G is a continuous (Lie) group homomorphism $\gamma\colon (\mathbb{R},+) \to G$. The Lie group exponential map $\exp\colon \mathfrak{g} \to G$ is defined as $\exp(v) = \gamma_v(1)$, for $v \in \mathfrak{g}$, where γ_v is the unique one-parameter subgroup of G whose tangent vector at e is v. For matrix Lie groups the exponential map has the particular form: $\exp(A) = \sum_{k=0}^{\infty} A^k/k!$, for a square matrix A. The resulting matrix $\exp(A)$ is an invertible matrix. Given an invertible matrix B, if there exist a square matrix A such that $B = \exp(A)$, then A is said to be the logarithm of B. In general, the logarithm might not exist and if it does it may fail to be unique. However, the matrix exponential and logarithms can be computed numerically efficient (see [16, Chapter 5] and references therein). Note that we can always find a domain in the Lie algebra $\mathfrak{g}$ where the Lie group exponential map is a diffeomorphism. Therefore, in a neighborhood sufficiently close to the identity the Lie group logarithm exist and is unique. By means of left-translation (or right-translation), the Lie group exponential map can be extended to a map $\exp_g\colon T_gG \to G$, for all $g \in G$, defined by $\exp_g(v) = g\exp(dL_{g^{-1}}v)$. Similarly, the Lie group logarithm at g becomes $\log_g(v) = dL_g\log(g^{-1}v)$.

Example 1. Some common examples of Lie groups include; the n-dimensional Euclidean space $(\mathbb{R}^n,+)$ with the additive group structure, $(\mathbb{R}_+,\cdot)$ the positive real line with a multiplicative group structure, the space of invertible real matrices $\mathrm{GL}(n)$ equipped with a multiplication of matrices forms a Lie group, and the rotation group $\mathrm{SO}(n)$, consisting of real orthogonal matrices with determinant one, equipped with matrix multiplication is a Lie group.

2.3 Homogeneous Spaces

A homogeneous space is a special type of quotient manifold arising as a smooth manifold endowed with a transitive smooth action by a Lie group G. The homogeneous space is called a G-homogeneous space to indicate the Lie group action on it. In fact, all G-homogeneous spaces arise as a quotient manifold G/H, for some closed subgroup $H \subseteq G$. The fact that H is a closed subgroup of the Lie group G makes H into a Lie group. Any homogeneous space is diffeomorphic to the quotient space G/G_x, where G_x is the stabilizer for the point x. The dimension of the G-homogeneous space is equal to $\dim G - \dim H$ the quotient map $\pi\colon G \to G/H$ is a smooth submersion, i.e., the differential of π is surjective at every point. We assume throughout that G acts on itself by left-multiplication.

Example 2. The rotation group $\mathrm{SO}(n)$ acts transitively on $\mathbb{S}^{n-1}$, thus $\mathbb{S}^{n-1}$ is a $\mathrm{SO}(n)$-homogeneous space. Consider for a moment the north-pole. Since any rotations that fix the north-pole are rotations in the xy-plane, we see that the stabilizer or isotropy group is the rotation group $\mathrm{SO}(n-1)$, thus $\mathbb{S}^{n-1} = \mathrm{SO}(n)/\mathrm{SO}(n-1)$.

The set of three-by-three invertible matrices with positive determinant $\mathrm{GL}_+(3)$ acts on the left on the set of covariance matrices, i.e., the symmetric positive definite matrices $\mathrm{SPD}(3)$. The isotropy group is the rotation group $\mathrm{SO}(3)$ and thus $\mathrm{SPD}(3) = \mathrm{GL}_+(3)/\mathrm{SO}(3)$.

A special type of homogeneous space arise when the subgroup is a discrete subgroup of G. Such homogeneous spaces are typically denoted G/Γ. For example, the space $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ defines the n-torus as a homogeneous space.

2.4 Brownian Motion

The Brownian motion is a classical diffusion process defined in $\mathbb{R}^n$ via the Laplace operator. The Brownian motion on Riemannian manifolds and Lie groups can similarly be defined via the generalized Laplacian or Laplace-Beltrami operator. This is described in the sections below.

On Riemannian Manifolds Endowing a smooth manifold M with a Riemannian metric, g, allows us to define the Laplace-Beltrami operator. This operator is the generalization of the Euclidean Laplacian operator to manifolds. The Laplace-Beltrami operator is defined as the gradient's divergence, $\Delta_M f = \mathrm{div}$ grad f. In terms of local coordinates $(x_1, \dots, x_d)$ the expression for the Laplace-Beltrami operator becomes

$$\Delta_M f = \det(g)^{-1/2} \left(\frac{\partial}{\partial x_j} g^{ji} \det(g)^{1/2} \frac{\partial}{\partial x_i} \right) f, \tag{2}$$

where $\det(g)$ denotes the determinant of the Riemannian metric g and g^{ij} are the coefficients of the inverse of g. An application of the product rule implies that (2) can be rewritten as

$$\Delta_M f = a^{ij} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} f + b^j \frac{\partial}{\partial x_j} f, \tag{3}$$

where $a^{ij} = g^{ij}$, $b^k = -g^{ij}\Gamma^k_{ij}$, and Γ denote the Christoffel symbols related to the Riemannian metric. This diffusion operator defines a Brownian motion on the G, valid up to its first exit time of the local coordinate chart, i.e.,

$$N^f(X_t) = f(X_t) - f(X_0) - \frac{1}{2}\int_0^t \Delta_M f(X_s)ds, \tag{4}$$

is a local martingale, for all smooth functions f on G. Equivalently, the stochastic differential equation (SDE) for X in terms of local coordinates is

$$dX^k_t = -\frac{1}{2}g^{ij}(X_t)\Gamma^k_{ij}(X_t)dt + \sigma^k_j(X_t)dB^j_t, \tag{5}$$

for $t < \tau$, where τ is the explosion time of X and $\sigma = \sqrt{g^{-1}}$ the matrix square root of g^{-1}.

On Lie Groups In the case of the Lie group G, the identification of the space of left-invariant vector fields with the Lie algebra $\mathfrak{g}$ allows for a global description of Δ_G. Indeed, let $\{v_1, \dots v_d\}$ be an orthonormal basis of T_eG. Then $V_i(x) = (dL_x)_e v_i$ defines left-invariant vector fields on G and the Laplace-Beltrami operator can be written as (cf. [12, Proposition 2.5])

$$\Delta_G f(e) = \sum_{i=1}^d V_i^2 f(e) - V_0 f(e),$$

where $V_0 = \sum_{i,j=1}^d C^j_{ij} V_j$ and C^k_{ij} denote the structure coefficients given by

$$[V_i, V_j] = C^k_{ij} V_k. \tag{6}$$

By the left-invariance, the formula for the Laplace-Beltrami operator holds globally, i.e., $\Delta_G f(a) = \Delta_G f \circ L_a(e) = (dL_a)_e \Delta_G f(e)$. The corresponding stochastic differential equation (SDE) for the Brownian motion on G, in terms of left-invariant vector fields, then becomes

$$dX_t = -\frac{1}{2}V_0(X_t)dt + V_i(X_t) \circ dB^i_t, \qquad X_0 = e, \tag{7}$$

where $\circ$ denotes integration in the Stratonovich sense. By [12, Proposition 2.6], if the inner product is $\mathrm{Ad}(G)$ invariant, then $V_0 = 0$. The solution of (7) is conservative or non-explosive and is called the left-Brownian motion on G (see [18] and references therein).

2.5 Riemannian Bridges

In this section, we briefly review some classical facts on Brownian bridges on Riemannian manifolds. As Lie groups themselves can be equipped with a Riemannian manifold, the theory carries over *mutatis mutandis*. However, Lie groups' group structure allows the notion of left-invariant (resp. right-invariant) vector fields. The identification of the Lie algebra with the vector space of left-invariant vector fields makes Lie groups parallelizable. The existence of smooth non-vanishing vector fields allows for constructing semimartingales directly on the Lie groups, since the stochastic parallel displacement is ensured by the left-invariant (resp. right-invariant) vector fields.

Brownian Bridges Let $\mathbb{P}_x^t = \mathbb{P}_x|_{\mathcal{F}_t}$ be the measure of a Riemannian Brownian motion, X_t, at some time t started at point x. Suppose p denotes the transition density of the Riemannian Brownian motion. In that case, $d\mathbb{P}_x^t = p_t(x,y)d\operatorname{Vol}(y)$ describes the measure of the Riemannian Brownian motion, where $d\operatorname{Vol}(y)$ is the Riemannian volume measure. Conditioning the Riemannian Brownian motion to hit some point v at time $T > 0$ results in a Riemannian Brownian bridge. Here, $\mathbb{P}_{x,v}^T$ denotes the corresponding probability measure. The two measures are absolutely continuous (equivalent) over the time interval $[0,T)$, however mutually singular at time $t = T$. This is an obvious consequence of the fact that $\mathbb{P}_x(X_T = v) = 0$, whereas $\mathbb{P}_{x,v}^T(X_T = v) = 1$. The corresponding Radon-Nikodym derivative is given by

$$\frac{d\mathbb{P}_{x,v}^T}{d\mathbb{P}_x}\Big|_{\mathcal{F}_s} = \frac{p_{T-s}(X_s,v)}{p_T(x,v)} \qquad \text{for } 0 \leq s < T, \tag{8}$$

which is a martingale for $s < T$. The Radon-Nikodym derivative defines the density for the change of measure and provides the basis for the description of Brownian bridges. In particular, it provides the conditional expectation defined by

$$\mathbb{E}[F(X_t)|X_T = v] = \frac{\mathbb{E}[p_{T-t}(X_t,v)F(X_t)]}{p_T(x,v)}, \tag{9}$$

for any bounded and $\mathcal{F}_s$-measurable random variable $F(X_s)$. (In the case of an empty cut-locus or rather when the exponential map is a covering map, and the underlying manifold is connected, then every point p is a pole. In this case, Truman and Elworthy's *semi-classical Brownian bridges* apply.

As described in Hsu [8], the Brownian bridge on a Riemannian manifold, M, is a nonhomogeneous diffusion on M with an infinitesimal generator

$$\mathcal{L}_s f(z) = \frac{t}{2}\Delta_M f(z) + t\nabla_z \log p_{t(1-s)}(z,v)\cdot\nabla f(z),$$

where Δ_M denotes the Laplacian on M. This infinitesimal generator yields an SDE in the frame bundle, $\mathcal{FM}$, of the lifted M-valued Brownian bridge, $X_t = \pi(U_t)$, in terms the horizontal vector fields (H_i) given by

$$dU_t = H_i(U_t)\circ\Big(dB_t^i + \left(U_t^{-1}\left(\pi_*\left(\nabla_{u|u=U_t}\log\tilde{p}_{T-t}(u,v)\right)\right)\right)^i dt\Big), \qquad U_0 = u_0, \tag{10}$$

where $\tilde{p}_t(u,v) = p_t(\pi(u),v)$ denotes the lift of the transition density, B an $\mathbb{R}^d$-valued Brownian motion, and $\pi_*\colon T\mathcal{FM} \to TM$ is the pushforward of the canonical projection $\pi\colon \mathcal{FM} \to M$. Essentially, the stochastic development approach in the Lie group setting is redundant. The left invariant vector-fields permits a notion of stochastic parallel transport independently of the frame bundle construction.

Bridges to Submanifolds A generalization of Riemannian Brownian bridges can be found in Thompson [20]. There, the author introduces Brownian bridges to submanifolds by considering the transition density on a Riemannian manifold M defined by

$$p_t(x, N) := \int_N p_t(x, y) d\,\mathrm{Vol}_N(y), \tag{11}$$

where $N \subset M$ is a submanifold of M and Vol_N denotes the volume measure on N. The author terms these processes as *Fermi bridges*, having infinitesimal generator given by

$$\tfrac{1}{2}\Delta - \tfrac{r_N}{T-t}\tfrac{\partial}{\partial r_N}, \tag{12}$$

where $r_N(\cdot) := d(\cdot, N) = \inf_{y\in N} d(\cdot, y)$ and $\frac{\partial}{\partial r_N} = \nabla d(\cdot, N)$. The resulting conditional expectation becomes

$$\mathbb{E}[F(X_t)|X_T \in N] = \frac{\mathbb{E}[p_{T-t}(X_t, N)F(X_t)]}{p_T(x, N)}, \tag{13}$$

which holds for all bounded $\mathcal{F}_t$-measurable random variables $F(X_t)$.

3 Simulation of Bridges on Lie Groups

In this section, we consider the task of simulating (7) conditioned to hit $v \in G$, at time $T > 0$. The potentially intractable transition density for the solution of (7) inhibits simulation directly from (10). Instead, we propose to add a guiding term mimicking that of Delyon and Hu [4], i.e., the guiding term becomes the gradient of the distance to v divided by the time to arrival. The SDE for the guided diffusion becomes

$$dY_t = -\frac{1}{2}V_0(Y_t)dt + V_i(Y_t) \circ \left(dB_t^i - \frac{\left(\nabla_{y|_{y=Y_t}} d(y, v)^2\right)^i}{2(T-t)} dt \right), \qquad Y_0 = e, \tag{14}$$

where $d(\cdot, v)$ denotes the Riemannian distance to v. Note that we can always, for convenience, take the initial value to be the identity e. Equation (14) can equivalently be written as

$$dY_t = -\frac{1}{2}V_0(Y_t)dt + V_i(Y_t) \circ \left(dB_t^i - \frac{\mathrm{Log}_{Y_t}(v)^i}{T-t} dt \right), \qquad Y_0 = e,$$

where Log_p is the inverse of the Riemannian exponential map Exp_p. Numerical computations of the Lie group exponential map is often faster than computing the Riemannian exponential map (see [16] and references therein). Therefore, by a change of measures argument the equation above can be expressed in terms of the inverse of the Lie group exponential (this process is denoted Y as well)

$$dY_t = -\frac{1}{2}V_0(Y_t)dt + V_i(Y_t)\circ\left(d\bar{B}_t^i - \tau(Y_t)\frac{\log_{Y_t}(v)^i}{T-t}dt - (1-\tau(Y_t))\,\frac{\mathrm{Log}_{Y_t}(v)^i}{T-t}dt\right) \tag{15}$$

$Y_0 = e$, where $\bar{B}$ is a Brownian motion under a new measure, say $\bar{\mathbb{P}}$, and $\tau(y)$ is a smooth bump function defined in a neighborhood of v where the Lie group logarithm exists and is unique. The measure $\bar{\mathbb{P}}$ can explicitly be expressed as

$$\begin{aligned}\frac{d\bar{\mathbb{P}}}{d\mathbb{P}}|_{\mathcal{F}_t} = \exp\Bigg[&-\int_0^t \left\langle \frac{\tau(Y_s)\left(\log_{Y_s}(v) - \mathrm{Log}_{Y_s}(v)\right)}{T-s}, V(Y_s)dB_s \right\rangle \\ &-\frac{1}{2}\int_0^t \frac{\|\tau(Y_s)\|^2\|\log_{Y_s}(v) - \mathrm{Log}_{Y_s}(v)\|^2}{(T-s)^2}ds\Bigg],\end{aligned} \tag{16}$$

where $\mathbb{P}$ denotes the law of the SDE in (14). A bi-invariant metric on the Lie group implies that the Riemannian exponential map and the Lie group exponential map coincide, and thus the Radon-Nikodym above is identically one. This justifies keeping the Y notation.

Situations where a bi-invariant metric exists, however, are rare. A sufficient condition for the existence of a bi-invariant metric is that the Lie group is compact. In such cases, we can always choose the bi-invariant metric and work with the Lie group exponential and logarithmic map. In the non-compact situation, we restrict ourselves to neighborhoods of $v \in G$ and use the group logarithmic map inside this neighborhood while using the Riemannian logarithm outside.

The result below shows the validity of working with the group logarithm in a small neighborhood. For $v \in \mathfrak{g}$ we define $\tilde{v} = (dL)_e v$ as the corresponding left-invariant vector field. Let $\alpha\colon \mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ be a bi-linear operator which uniquely defines the connection at the identity: $\alpha(v,w) = \nabla_{\tilde{v}}\tilde{w}|_e$. Similar to [16, Chapter 5], we define ad^* as the metric adjoint of the adjoint operator ad: $\langle \mathrm{ad}^*(\tilde{v},\tilde{w}),\tilde{z}\rangle = \langle[\tilde{w},\tilde{z}],\tilde{v}\rangle$.

Proposition 1. *The measures in* (16) *are equivalent, i.e., the Radon-Nikodym derivative is a martingale.*

Proof. If G is compact, there exists a bi-invariant metric such that the Riemannian logarithmic map and the Lie group logarithmic map coincide (see [16, Chapter 5]).

If G is not compact, endowing the Lie group G with a left-invariant metric, the bi-linear form α characterizing the Levi-Civita connection of the left-invariant metric in the Lie algebra is given by

$$\alpha(v,w) = \frac{1}{2}\left([v,w] - \mathrm{ad}^*(v,w) - \mathrm{ad}^*(w,v)\right),$$

where $\mathrm{ad}^*(v,w) := \mathrm{ad}^*(\tilde{v},\tilde{w})|_e$. Whenever $\mathrm{ad}^*(v,v) = 0$, the one-parameter subgroups $\gamma_v(t)$, passing through the identity with tangent vector v, are in fact geodesics wrt. the left-invariant Riemannian metric. In case the Lie group log equals such v's the measures in (16) are equivalent. In such case the Lie group log belongs to the center of $\mathfrak{g}$. This for example holds if the group is abelian.

If G is neither compact nor abelian, we chose a compact neighborhood of $v \in G$ such that the group log is well defined on this compact neighborhood. As the neighborhood is compact there exists constants c and C such that $c\|\mathrm{Log}_y(v)\| \leq \|\log_y(v)\| \leq C\|\mathrm{Log}_y(v)\|$. The triangle inequality then imply

$$\|\tau(Y_s)\|^2\|\log_{Y_s}(v) - \mathrm{Log}_{Y_s}(v)\|^2 \leq (1+3C)\,\|\mathrm{Log}_y(v)\|^2,$$

which in conjunction with Novikov's condition yields the result. □

Radial Process We denote by $r_v(\cdot) := d(\cdot, v)$ the radial process. Due to the singularities of the radial process on $\mathrm{Cut}(v) \cup \{v\}$, the usual Itô's formula only applies on subsets away from the cut-locus. The extension beyond the cut-locus of a Brownian motion's radial process was due to Kendall [10]. Barden and Le [1,11] generalized the result to M-semimartingales. The radial process of the Brownian motion (7) is given by

$$r_v(X_t) = r_v(X_0)^2 + \int_0^t \langle \nabla r_v(X_s), V(X_s)dB_s\rangle + \frac{1}{2}\int_0^t \Delta_G r_v(X_s)ds - L_s^v(X), \tag{17}$$

where L^v is the geometric local time of the cut-locus $\mathrm{Cut}(v)$, which is non-decreasing continuous random functional increasing only when X is in $\mathrm{Cut}(v)$ (see [1,10,11]). Let $W_t := \int_0^t \left\langle \frac{\partial}{\partial r}, V_i(X_s)\right\rangle dB_s^i$, which is the local-martingale part in the above equation. The quadratic variation of W_t satisfies $d[W,W]_t = dt$, by the orthonormality of $\{V_1, \dots, V_d\}$, thus W_t is a Brownian motion by Levy's characterization theorem. From the stochastic integration by parts formula and (17), the squared radial process of X satisfies

$$r_v(X_t)^2 = r_v(X_0)^2 + 2\int_0^t r_v(X_s)dW_s + \int_0^t r_v(X_s)\Delta_G r_v(X_s)ds - 2\int_0^t r(X_s)dL_s^v, \tag{18}$$

where dL_s^v is the random measure associated to $L_s^v(X)$.

Similarly, we obtain an expression for the squared radial process of Y. Using the shorthand notation $r_t := r_v(Y_t)$ the radial process then becomes

$$r_t^2 = r_0^2 + 2\int_0^t r_s dW_s + \int_0^t \frac{1}{2}\Delta_G r_s^2 ds - \int_0^t \frac{r_s^2}{T-s}ds - 2\int_0^t r_s dL_s^v. \tag{19}$$

Imposing a growth condition on the radial process yields an L^2-bound on the radial process of the guided diffusion, [20]. So assume there exist constants $\nu \geq 1$ and $\lambda \in \mathbb{R}$ such that $\frac{1}{2}\Delta_G r_v^2 \leq \nu + \lambda r_v^2$ on $D\setminus \mathrm{Cut}(v)$, for every regular domain $D \subseteq G$. Then (19) satisfies

$$\mathbb{E}[1_{t<\tau_D} r_v(Y_t)^2] \leq \left(r_v^2(e) + \nu t\left(\frac{t}{T-t}\right)\right)\left(\frac{T-t}{t}\right)^2 e^{\lambda t}, \tag{20}$$

where τ_D is the first exit time of Y from the domain D.

Girsanov Change of Measure Let B be the Brownian motion in $\mathbb{R}^d$ defined on the filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_s), \mathbb{P})$ and X the solution of (7). The process $\frac{\nabla r_v(X_t)^2}{2(T-t)}$ is an adapted process. As X is non-explosive, we see that

$$\int_0^t \left\| \frac{\nabla r_v(X_s)^2}{2(T-s)} \right\|^2 ds = \int_0^t \frac{r_v(X_s)^2}{(T-s)^2} ds \leq C, \tag{21}$$

for every $0 \leq t < T$, almost surely, and for some fixed constant $C > 0$. Define a new measure $\mathbb{Q}$ by

$$Z_t := \frac{d\mathbb{Q}}{d\mathbb{P}}\bigg|_{\mathcal{F}_t}(X) = \exp\left[-\int_0^t \left\langle \frac{\nabla r_v(X_s)^2}{2(T-s)}, V(X_t)dB_s \right\rangle - \frac{1}{2}\int_0^t \frac{r_v(X_s)^2}{(T-s)^2} ds \right]. \tag{22}$$

From (21), the process Z_t is a martingale, for $t \in [0,T)$, and $\mathbb{Q}_t$ defines a probability measure on each $\mathcal{F}_t$ absolutely continuous with respect to $\mathbb{P}$. By Girsanov's theorem (see e.g. [7, Theorem 8.1.2]), we get a new process b_s which is a Brownian motion under the probability measure $\mathbb{Q}$. Moreover, under the probability $\mathbb{Q}$, equation (7) becomes

$$dY_t = -\frac{1}{2}V_0(Y_t)dt + V_i(Y_t) \circ \left(db_t^i - \frac{r_v(Y_t)}{T-t} \left(\frac{\partial}{\partial r} \right)_v^i dt \right), \tag{23}$$

where $\left(\frac{\partial}{\partial r}\right)^i$ is the i'th component of the unit radial vector field in the direction of v. The squared radial vector field is smooth away from $\mathrm{Cut}(v)$ and thus we set it to zero on $\mathrm{Cut}(v)$. Away from $\mathrm{Cut}(v)$, the squared radial vector field is $2\,\mathrm{Log}_v$, which is the inverse exponential at v. The added drift term acts as a guiding term, which pulls the process towards v at time $T > 0$.

From (22), we see that $\mathbb{E}[f(Y_t)] = \mathbb{E}[f(X_t)Z_t]$. Using (18) and the identity $\Delta_G r_v = \frac{d-1}{r_v} + \frac{\partial}{\partial r_v}\log \Theta_v$ (see e.g. [19]), we equivalently write $\mathbb{E}[f(Y_t)\varphi_t] = \mathbb{E}[f(X_t)\psi_t]$, with

$$\psi_t := \exp\left[\frac{-r(X_t)^2}{2(T-t)} \right] \qquad \varphi_{t,v} := \exp\left[\int_0^t \frac{r_v(Y_s)^2}{T-s} \left(dA_s^v + dL_s^v \right) \right], \tag{24}$$

where $dA_s^v = \frac{\partial}{\partial r_v} \log \Theta_v^{-1/2}(Y_s)ds$ is a random measure supported on $G \setminus \mathrm{Cut}(v)$ and Θ_v is the Jacobian determinant of Exp_v.

Delyon and Hu in Lie Groups This section generalizes the result of Delyon and Hu [4, Theorem 5] to the Lie group setting. It is possible to modify the result to incorporate a generalization of [4, Theorem 6]. The results in the remaining part of this section are modified from the Riemmanian setting in [9]to the Lie group setting presented here.

Theorem 1. *Let X be the solution of* (7)*. The SDE* (14) *yields a strong solution on* $[0,T)$ *and satisfies* $\lim_{t\uparrow T} Y_t = v$ *almost surely. Moreover, the conditional expectation of X given $X_T = v$ is*

$$\mathbb{E}[f(X)|X_T = v] = C\mathbb{E}\left[f(Y)\varphi_{T,v} \right], \tag{25}$$

for every $\mathcal{F}_t$-measurable non-negative function f on G, $t < T$, where φ_t is given in (24).

Proof. The result is a consequence of the change of measure together with Lemma 1, Lemma 2, and Lemma 3. □

Lemma 1. *The solution of SDE* (14) *satisfies* $\lim_{t\to T} Y_t = v$ *almost surely.*

Proof. Let $\{D_n\}_{n=1}^{\infty}$ be an exhaustion of G, that is, the sequence consists of open, relatively compact subsets of M such that $\bar{D}_n \subseteq D_{n+1}$ and $G = \bigcup_{n=1}^{\infty} D_n$. Furthermore, let τ_{D_n} denote the first exit time of Y from D_n, then from (20) we have that the sequence $\left(\mathbb{E}[1_{\{t<\tau_{D_n}\}} r_v^2(Y_t)]\right)_{n=1}^{\infty}$ is non-decreasing and bounded, hence from the monotone convergence theorem, it has a limit which is bounded by the right-hand side of (20). Applying Jensen's inequality to the left-hand side of (20)

$$\mathbb{E}[r_v(Y_t)] \leq \left(r_v^2(e) + \nu t\left(\frac{t}{T-t}\right)\right)^{\frac{1}{2}}\left(\frac{T-t}{t}\right)e^{\frac{\lambda t}{2}}.$$

Since obviously $\mathbb{E}[r_v(Y_T)] = r_v(Y_T)\mathbb{Q}(r_v(Y_T) \neq 0)$, by Fatou's lemma

$$\mathbb{E}[r_v(Y_T)] \leq \liminf_{t\to T} \mathbb{E}[r(Y_t)] = 0,$$

we conclude that $r(Y_t) \to 0$, $\mathbb{Q}$-almost surely. □

Lemma 2. *Let $0 < t_1 < t_2 < \cdots < t_N < T$ and h be a continuous bounded function function on G^N. With ψ_t as in* (24)*, then*

$$\lim_{t\to T} \frac{\mathbb{E}\left[h\left(X_{t_1}, X_{t_2}, \ldots, X_{t_N}\right)\psi_t\right]}{\mathbb{E}[\psi_t]} = \mathbb{E}\left[h\left(X_{t_1}, X_{t_2}, \ldots, X_{t_N}\right)|X_T = v\right]. \quad (26)$$

Proof. The proof is similar to that of [4, Lemma 7]. Let (U, ϕ) be a normal chart centered at $v \in G$. First, since the cut locus of any complete connected manifold has (volume) measure zero, we can integrate indifferently in any normal chart. For any $t \in (t_N, T)$ we have

$$\mathbb{E}[h(x_{t_1}, ..., x_{t_N})\psi_t] = \int_G \Phi_h(t, z)e^{-\frac{r_v(z)^2}{2(T-t)}}\, d\operatorname{Vol}(z) \quad (27)$$

where $d\operatorname{Vol}(z) = \sqrt{\det(A(z))}dz$ denotes the volume measure on G, dz the Lebesgue measure, and A the metric tensor. Moreover,

$$\Phi_h(t, z) = \int_{G^N} h(z_1, ..., z_N)p_{t_1}(u, z_1)\cdots p_{t-t_N}(z_N, z)d\operatorname{Vol}(z_1)\cdots d\operatorname{Vol}(z_N),$$

and of course $\Phi_1(t, z) = p_t(e, z)$. Using the normal chart and applying the change of variable $x = (T-t)^{1/2}y$ we get

$$(T-t)^{-\frac{d}{2}}\mathbb{E}[h(x_{t_1}, ..., x_{t_N})\psi_t] \overset{t\to T}{\to} \Phi_h(T, v)\det(A(v))^{\frac{d}{2}} \int_{\phi(G)} e^{-\frac{r_v(\phi^{-1}(y))^2}{2}}dy.$$

The conclusion follows from Bayes' formula. □

On simply connected spaces, we have the following L_1-convergence of φ.

Lemma 3. *Suppose G is simply connected. With $\varphi_{t,v}$ as defined above then $\varphi_{t,v} \overset{L_1}{\to} \varphi_{T,v}$.*

Proof. Note that for each $t \in [0,T)$ we have $\mathbb{E}^{\mathbb{Q}}[\varphi_t] < \infty$ as well as $\varphi_t \to \varphi_T$ almost surely by Lemma 1. The result then follows from the uniform integrability of $\{\varphi_t \colon t \in [0,T)\}$, which can be found in Appendix C.2 in [19]. □

4 Simulation of Bridges in Homogeneous Spaces

Consider the homogeneous space $M = G/K$, where K is a Lie subgroup of the Lie group G and let $\pi \colon G \to M$ denote the canonical projection. Suppose that G acts on M on the left and that g_t is a process in G. As described in Liao [12], we obtain an induced process in M induced by the process g_t in G. For any $x \in M$, the induced process $x_t = g_t x$ defines the one-point motion of g_t in M, with initial value x. Using one-point motions, we define conditioned processes in the homogeneous space M. Throughout this section, let $\hat{X} = \pi(X)$ and $\hat{Y} = \pi(Y)$ denote the one-point motions of respectively X and Y as defined above.

4.1 Guided Diffusions on Homogeneous Space as Guided Diffusions in Lie Groups

To simulate bridges on homogeneous spaces, we develop simulation schemes on the top space, that is, bridge simulation schemes on the Lie group G, which we then project onto the homogeneous space M. We will be considering two different schemes. Let $v \in M$.

1. Whenever $\pi^{-1}(v)$ is closed, find closest point $\bar{v}$ in fiber above v and iterative update $\bar{v}$ at each time step.
2. Sample k-points in fiber above $v \in M$ and consider the bridge X in G conditioned on $X_T \in \{\bar{v}_1, \dots, \bar{v}_k\}$.

We make the following assumptions throughout on the Markov transition density $p_t^G(\cdot,\cdot)$.

Assumption 1. *1. The Markov transition density is symmetric, i.e.,*

$$p_t^G(x,y) = p_t^G(y,x).$$

2. The Chapman-Kolmogorov equation is satisfied, i.e.,

$$p_{t+s}^G(x,y) = \int_G p_t^G(x,z) p_s^G(z,y) d\,\mathrm{Vol}_G(z).$$

3. For any bounded continuous function f on G and every fixed $y \in G$

$$\lim_{t\downarrow 0} \int_G p_t^G(x,y) f(x) d\,\mathrm{Vol}_G(x) = f(y).$$

4.2 Guiding to Nearest Point

This section addresses the approach outlined in the previous section when guiding to a closed embedded manifold $N \subseteq G$. Considering the one-point motion of the guided process Y towards $N := \pi^{-1}(v)$ yields a conditioning in the homogeneous space M.

Lemma 4. *Let $v \in M$ and $\pi \colon G \to M$ be the canonical projection with $N = \pi^{-1}(v)$ being the fiber over v and let $e \in G$ denote the identity element. Furthermore, define Y as the process with infinitesimal generator* (12) *and Δ_G being the Laplace-Beltrami operator on G. Then N is a submanifold of G and Y is the Fermi bridge from $Y_0 = e$ to N at time T.*

Proof. The result follows from standard differential geometry and [20]. □

We reinvigorate the fact that the one-point motion, $X_t = g_t x$, of a Brownian motion g_t in G, started at $g_0 = e$, is only a Brownian motion in M under certain regularity conditions (see [12, Proposition 2.7]). In case of a bi-invariant metric, a Brownian motion on G maps to a Brownian motion in M through its one-point motion. In the general case, one-point processes might not even preserve the Markov property. A numerical example is provided below which show how we can obtain anisotropic distribution on the homogeneous space from a non-invariant metric on the top space.

The Riemannian volume measure Vol_G on G decomposes into a product measure consisting of the volume measure on fibers in G, e.g. $\pi^{-1}(z)$, and the volume measure on its horizontal complement, i.e., $d\,\mathrm{Vol}_G = d\,\mathrm{Vol}_{\pi^{-1}(z)}\, d\,\mathrm{Vol}_{|H}(z)$, where $d\,\mathrm{Vol}_{|H}$ is the horizontal restriction of the volume measure in G.

Assume that we have an induced volume measure defined on the homogeneous space M. This is, for example, the case when the metric on G is bi-invariant.

Theorem 2. *Let $x \in M$. The Fermi bridge Y_t converges almost surely to N and the one-point motion $\hat{Y}_t = Y_t x$ is a diffusion bridge starting at $x \in M$ converging almost surely to v.*

Proof. Since the Fermi bridge converges almost surely to N (cf. [20]), it converges in the horizontal direction. Hence the one-point motion converges almost surely in M to $\pi(N) = v \in M$. □

Suppose endowing both G and $M := G/K$ with sigma algebras making them into two measurable spaces. Suppose further that the sigma algebras $\sigma(G)$ and $\sigma(M)$ on G and M, respectively, are the Borel-sigma algebras of all open sets. This assumption is, of course, dependent on the metric. If the metric space is non-separable, then Borel algebra is too big for anything sensible to be said. Let $\pi \colon G \to M$ be the smooth submersion onto the homogeneous space M. Then π is a measurable map and if μ is a measure on G the pushforward of μ by π, defined by $\pi_*\mu(B) = \mu\left(\pi^{-1}(B)\right)$, for all $B \in \sigma(M)$, is a measure on M. Then we have the following result.

Given an initial value $x_0 \in G$ for the process X_t, we can, by left-translation, assume that the process starts at the identity in G, i.e., $x_0 = e$. This alleviates the dependency on the distribution of the initial value in the quotient space.

Theorem 3. *With the assumptions above, let $p_T^G(x_0,)$ denote the transition density of a diffusion process X_t on G initiated at $x_0 \in G$. The density $p_T^G(x_0,)$ pushes forward to a transition density $p_T^M(\hat{x}_0,)$ of the diffusion process $\hat{X}_t = \pi(X_t)$ on M, initiated from $\hat{x}_0 = \pi(x_0)$.*

Proof. Let $N_z := \pi^{-1}(z)$ be the fiber over z, for any $z \in M$, then $N_v \subseteq G$ is a submanifold of G by Lemma 4. Also, let $\mathbb{P}$ be the corresponding probability measure defined by $\mathbb{P}(B) = \int_B p_T(u, x) d\,\mathrm{Vol}_G(x)$, then we see that for any Borel measurable set $B \subseteq M$

$$\begin{aligned}
\mathbb{P}\left(X_T \in \pi^{-1}(B)\right) &= \int_{\pi^{-1}(B)} p_T^G(x_0, y) d\,\mathrm{Vol}_G(y) \\
&= \int_B \int_{N_z} p_T^G(x_0, y) d\,\mathrm{Vol}_{N_z}(y) d\,\mathrm{Vol}_{|H}(z) \\
&= \int_B \int_{N_z} p_T^G(x_0, y) d\,\mathrm{Vol}_{N_z}(y) d\,\mathrm{Vol}_M(z) \\
&= \int_B p_T^G\left(x_0, N_z\right) d\,\mathrm{Vol}_M(z),
\end{aligned}$$

where the third equality follows by assumption and the last equality by (11). Since $\hat{X}_T \in B$ if and only of $X_T \in \pi^{-1}(B)$, we see that $p_T^G\left(x_0, \pi^{-1}(\cdot)\right)$ is the transition density for $\hat{X}_t$ which is exactly the pushforward $\pi_* p_T^G(x_0, \cdot) := p_T^M(\hat{x}_0, \cdot)$. □

Note that the above is equivalent to $\pi P(f) = P(f \circ \pi)$, for any measurable function f on M.

Lemma 5. *Let X be a Markov process on G, started at $x_0 \in G$, with density $p_t^G(x_0, \cdot)$ satisfying the conditions in Assumption 1. The conditional expectation on M satisfies*

$$\mathbb{E}[f(\hat{X}) | \hat{X}_T = v] = \mathbb{E}\left[f(\hat{X}) \frac{p_{T-t}^M(\hat{X}_t, v)}{p_T^M(\hat{x}_0, v)}\right], \tag{28}$$

for all bounded, continuous, and non-negative measurable f on M. Furthermore,

$$\mathbb{E}[\tilde{f}(X) | X_T \in N] = \mathbb{E}[f(\hat{X}) | \hat{X}_T = v],$$

where $\tilde{f} = f \circ \pi$.

Proof. For the first part note that $\frac{p_{T-t}^M(\hat{X}_t, v)}{p_T^M(\hat{x}_0, v)}$ imply a conditioning. For the second part, let f be a bounded, continuous, and non-negative measurable function on

M, and let $\tilde{f} = f \circ \pi$. Then it follows directly from [19] and Theorem 3

$$\begin{aligned}\mathbb{E}[\tilde{f}(X_t)|X_T \in N] =&\mathbb{E}\left[f(\pi(X_t))\frac{p^G_{T-t}(X_t, N)}{p^G_T(x_0, N)}\right]\\ =&\mathbb{E}\left[f(\pi(X_t))\frac{p^G_{T-t}(X_t, \pi^{-1}(v))}{p^G_T(x_0, \pi^{-1}(v))}\right]\\ =&\mathbb{E}\left[f(\pi(X_t))\frac{\pi_* p^G_{T-t}(X_t, v)}{\pi_* p^G_T(x_0, v)}\right]\\ =&\mathbb{E}\left[f(\hat{X}_t)\frac{p^M_{T-t}(\hat{X}_t, v)}{p^M_T(\hat{x}_0, v)}\right].\end{aligned}$$

□

We summarize the main theorem of this section, namely, how to simulate guided bridges on homogeneous spaces. Let $\hat{X}_t$ be a process in M arising as the one-point process of a Markov process X_t in G.

Theorem 4. *The projection $\hat{X}_t$ of the G-valued Markov X_t onto M started at $x \in M$ conditioned on $\hat{X}_T = v$, for any $v \in M$, is identical in law to the process $\hat{Y}_t := \pi(Y_t)$, where $g \overset{\pi}{\mapsto} g \cdot x$ and Y_t is the Fermi bridge on G conditioned at $Y_T \in N$. Moreover, the conditional expectation of $\hat{X}$ given $\hat{X}_T = v$ is*

$$\mathbb{E}[f(\hat{X})|\hat{X}_T = v] = C\mathbb{E}\left[f(\hat{Y})\varphi_T\right], \tag{29}$$

for every $\mathcal{F}_t$-measurable non-negative function f on G, $t < T$, where φ_t is given in (24)*.*

Proof. Note that for any bounded, continuous, and non-negative measurable function $\tilde{f}$ on G we have [9]

$$\mathbb{E}\left[\tilde{f}(X)|X_T \in \pi^{-1}(v)\right] = C\mathbb{E}\left[\tilde{f}(Y)\varphi_{T,N}\right].$$

Let f be any bounded, continuous, and non-negative measurable function on M. For any such f on M, let $\tilde{f} = f \circ \pi$. Then by Lemma 5,

$$\mathbb{E}\left[f(\hat{X})|\hat{X}_T = v\right] = \mathbb{E}\left[f \circ \pi(X)|X_T \in \pi^{-1}(v)\right]$$

the conclusion follows. □

4.3 Guiding to *k*-Points in Fiber

For certain homogeneous spaces, the fiber $N = \pi^{-1}(v)$ is a discrete subgroup in G. In this case, the volume measure Vol_N in (11) is the counting measure and we can write the density as

$$p^G_t(x, N) = \sum_{v \in N} p^G_t(x, v).$$

From a numerical perspective, when the discrete subgroup is large restricting to a smaller finite subgroup $N_k \subseteq N$ of k-nearest-points of the initial starting point may speed up computation-time.

Recall the Radon-Nikodym derivative given in (13), which in the case of a discrete subgroup N takes the form

$$\frac{d\mathbb{P}^T_{x,N}}{d\mathbb{P}^T_x}\Big|_{\mathcal{F}_s} = \frac{p^G_{T-s}(X_s, N)}{p^G_T(x, N)} = \sum_{v\in N} \frac{p^G_{T-s}(X_s, v)}{\sum_{v\in N} p^G_T(x, v)}, \tag{30}$$

for $0 \leq s < T$. Suppose that $N_k := \{v_1, \ldots, v_k\} \subseteq N$. By Theorem 5.2.1 in Thompson [19], the heat kernel to v_i, $p_t(x, v_i)$, has the following expression

$$p^G_T(x, v_i) = q_T(x, v_i) \lim_{t\uparrow T} \mathbb{E}\left[\varphi_t\right], \tag{31}$$

where φ_t is defined in (24) and $q_t(\cdot, v_i)$ is the Euclidean normal density

$$q_t(x, v_i) = (2\pi t)^{-\frac{(d-n)}{2}} \exp\left[-\frac{r^2_{v_i}(x)}{2t}\right]. \tag{32}$$

From (30) and (31), we can see that the Radon-Nikodym derivative is equal to

$$\sum_{i=1}^k \frac{p^G_{T-s}(x, v_i)}{\sum_{j=1}^k p^G_T(x_0, v_j)} = \sum_{i=1}^k \frac{c_j q_{T-s}(x, v_i)}{\sum_{j=1}^k c_j q_T(x_0, v_j)}, \tag{33}$$

where c_i are the constants $\lim_{t\uparrow T} \mathbb{E}[\varphi_{t,v_i}]$, with subscript v_i to indicate its dependence on the conditioning point. From the arguments above, the conditional expectation is equal to

$$\begin{aligned}
\mathbb{E}_{\mathbb{P}}[F(X_t)|X_T \in N_k] &= \frac{\mathbb{E}_{\mathbb{P}}[p^G_{T-t}(X_t, N_k)F(X_t)]}{p^G_T(x_0, N_k)} \\
&= \sum_{i=1}^k \frac{\mathbb{E}_{\mathbb{P}}[p^G_{T-t}(X_t, v_i)F(X_t)]}{\sum_{j=1}^k p^G_T(x_0, v_k)} \\
&= \sum_{i=1}^k c_i \frac{\mathbb{E}_{\mathbb{P}}\left[\exp\left[-\frac{r^2_{v_i}(X_t)}{2(T-t)}\right] F(X_t)\right]}{\sum_{j=1}^k c_j \exp\left[-\frac{r^2_{v_j}(x_0)}{2(T-t)}\right]} = \mathbb{E}_{\mathbb{Q}}\left[F(Y_t)\right].
\end{aligned}$$

Let $h(s, X_s)$ be the function defined by the right hand side of (33). It is a classical argument following Chapman-Kolmogorov that $h(s, X_s)$ is a martingale on $[0,T)$, namely, for $s<t$

$$\begin{aligned}\mathbb{E}_{\mathbb{P}}\left[h(t,X_t)|\mathcal{F}_s\right] =&\mathbb{E}_{\mathbb{P}}\left[h(t,X_t)|X_s\right]\\ =&\int h(t,z)p^G_{t-s}(X_s,z)d\operatorname{Vol}_G(z)\\ =&\sum_{i=1}^k \frac{\int p^G_{T-t}(z,v_i)p^G_{t-s}(X_s,z)d\operatorname{Vol}_G(z)}{\sum_{j=1}^k p^G_T(x_0,v_j)}\\ =&\sum_{i=1}^k \frac{p_{T-s}(X_s,v_i)}{\sum_{j=1}^k p_T(x_0,v_j)} = h(s,X_s),\end{aligned}$$

where we have assumed that X is a Markov process and clearly $h(0,x)=1$. Then it is easily seen that

$$\nabla_{x_{|x=X_t}}\log h(t,x) = -\sum_{i=1}^k c_i \frac{q_{T-t}(X_t,v_i)}{\sum_{j=1}^k c_j q_T(x_0,v_j)}\frac{\nabla_{x_{|x=X_t}} r^2_{v_i}(x)}{2(T-t)} \tag{34}$$

which from Doob's h-transform yields an SDE of the form

$$dY_t = -\frac{1}{2}V_0(Y_t)dt + V_i(Y_t)\circ\left(dB^i_t - \sum_{i=1}^k c_i\frac{q_{T-t}(Y_t,v_i)}{\sum_{j=1}^k c_j q_T(y_0,v_j)}\frac{\nabla_{y_{|y=Y_t}} r^2_{v_i}(y)}{2(T-t)}dt\right), \tag{35}$$

where $Y_0=y_0=e$. Combining the above arguments, we have the following result.

Theorem 5. *Let Y be the solution of the SDE* (35)*, then Y converges almost surely to N_k as $t\uparrow T$ and the conditional expectation is given as*

$$\mathbb{E}_{\mathbb{Q}}\left[F(Y)\right] = \sum_{i=1}^k c_i\frac{\mathbb{E}_{\mathbb{P}}\left[\exp\left[-\frac{r^2_{v_i}(Y_t)}{2(T-t)}\right]F(Y)\right]}{\sum_{j=1}^k c_j\exp\left[-\frac{r^2_{v_j}(x_0)}{2(T-t)}\right]} = \mathbb{E}_{\mathbb{P}}\left[F(X)|X_T\in N_k\right].$$

Remark 1. Choosing which k-points to condition on introduce a certain bias. An argument could be to choose the k-points closest to the initial value $y_0\in G$ and somehow obtain a truncated version of the true bridge process. However, if the fiber is connected and continuous such a choice is not feasible.

Consider now the case where N is a continuous, connected, and compact fiber (Compactness assumption so we get the existence of a uniform distribution on N). Suppose we sample k-points in N uniformly at random.

Theorem 6. *Let X be a Markov process defined on $(\Omega,\mathcal{F},\mathbb{P})$ with values in G, $X_0=x_0$, and let $p^G_t(\cdot,\cdot)$ be its transition density defined by $\mathbb{P}(X_T\in du|X_t=x)=p^G_{T-t}(x,u)d\operatorname{Vol}_G(u)$. Assume $0\le t<T$ and $X_T\sim f\cdot\operatorname{Vol}_N$ (e.g., uniform distribution on fiber over v) under the probability measure $\mathbb{P}_{x_0}$ started at x_0.*

The conditional law of X_t given $X_T = v$, $\mathbb{P}^T_{x_0,v}$, has density wrt. the reference measure $d\,\mathrm{Vol}_G$ given by

$$\frac{p^G_{T-t}(y,v)p^G_t(y,x_0)}{p^G_T(x_0,v)}, \tag{36}$$

and the simultaneous distribution of (X_t, X_T) has density given by

$$\frac{\mathbb{P}(X_t \in dx, X_T \in du)}{d\,\mathrm{Vol}_N(u)d\,\mathrm{Vol}_G(x)} = f(u)\frac{p^G_{T-t}(y,u)p^G_t(y,x)}{p^G_T(x_0,u)}. \tag{37}$$

Furthermore, if we define the h-function as

$$h(t,X_t) = \frac{\int f(u)\frac{p^G_{T-t}(X_t,u)}{p^G_T(x_0,u)}d\,\mathrm{Vol}_N(u)}{\int_N f(y)d\,\mathrm{Vol}_N(y)}, \tag{38}$$

then for any non-negative measurable functional F we have

$$\begin{aligned}\mathbb{E}_{\mathbb{Q}}[F(X)] =&\mathbb{E}_{\mathbb{P}}[h(t,X_t)F(X)]\\ &= \int \mathbb{E}_{\mathbb{P}}[F(X)|X_T = u]\frac{f(u)}{\int_N f(y)d\,\mathrm{Vol}_N(y)}d\,\mathrm{Vol}_N(u).\end{aligned}$$

The conditional distribution of X_t given X_T has density

$$k_t(x,u) = \frac{f(u)}{\int_N f(y)d\,\mathrm{Vol}_N(y)}\frac{p^G_{T-t}(y,u)p^G_t(y,x)}{p^G_T(x_0,u)}, \tag{39}$$

with respect to the volume measure Vol_N. If the distribution $X_T(\mathbb{P})$ has full mass in the fiber N, i.e., $X_T(\mathbb{P})(N) = \int_N f dVol = 1$ the term above simplifies.

Proof. The fact that (36) is the conditional density wrt. $d\,\mathrm{Vol}_G$ the volume measure on G follows from (8), since $\mathbb{P}^t_x = p_t(x,y)d\,\mathrm{Vol}_G(y)$ and therefore

$$d\mathbb{P}^T_{x_0,v}(X_t) = \frac{p^G_{T-t}(y,v)p^G_t(x_0,y)}{p^G_T(x_0,v)}d\,\mathrm{Vol}_G(y).$$

Hence (37) follows.

For the second part take h as defined in (38). Without loss of generality assume that $X_T(\mathbb{P})(N) = 1$. Note that h is a martingale with $h(0,X_0) = 1$, since X is a Markov process and

$$\begin{aligned}\mathbb{E}[h(t,X_t)|X_s] &= \int p^G_{t-s}(X_s,x)h(t,x)d\,\mathrm{Vol}_G(x)\\ &= \int p^G_{t-s}(X_s,x)\int f(u)\frac{p^G_{T-t}(x,u)}{p^G_T(x_0,u)}d\,\mathrm{Vol}_N(u)d\,\mathrm{Vol}_G(x)\\ &= \int f(u)\frac{p^G_{T-s}(X_s,u)}{p^G_T(x_0,u)}d\,\mathrm{Vol}_N(u) = h(s,X_s)\end{aligned}$$

together with

$$\mathbb{E}[h(t,X_t)] = \int f(u)\frac{p_T^G(x_0,u)}{p_T^G(x_0,u)}d\,\mathrm{Vol}_N(u) = 1.$$

Since $\lim_{t\downarrow 0}\int p_t^G(x,y)f(y)d\,\mathrm{Vol}_G(y) = f(x)$, for any bounded continuous function f, Fatou's lemma ensures that $\mathbb{E}[h(T,X_T)] = 1$

$$\begin{aligned}
1 =& \limsup_{t\uparrow T}\mathbb{E}[h(t,X_t)] \\
\leq& \mathbb{E}\left[\limsup_{t\uparrow T} h(t,X_t)\right] \\
=& \int_G \limsup_{t\uparrow T}\int f(u)\frac{p_{T-t}^G(x,u)}{p_T^G(x_0,u)}d\,\mathrm{Vol}_N(u)d\,\mathrm{Vol}_G(x) \\
=& \int_G \frac{f(x)}{p_T^G(x_0,x)}d\,\mathrm{Vol}_G(x) \\
=& \int_G \liminf_{t\uparrow T}\int f(u)\frac{p_{T-t}^G(x,u)}{p_T^G(x_0,u)}d\,\mathrm{Vol}_N(u)d\,\mathrm{Vol}_G(x) \\
\leq& \liminf_{t\uparrow T}\mathbb{E}[h(t,X_t)] = 1.
\end{aligned}$$

Hence h is a true martingale on $[0,T]$ and thus defines a new probability measure $\mathbb{Q}$ on $\mathcal{F}$ by $\frac{d\mathbb{Q}}{d\mathbb{P}}|_{\mathcal{F}_t}(X) = h(t,X_t)$.

For the second part of the proof, assume, temporarily, that F is a measurable function such that

$$\begin{aligned}
\mathbb{E}_{\mathbb{P}}[h(t,X_t)F(X_t)] &= \int p_t^G(x_0,x)h(t,x)F(x)d\,\mathrm{Vol}_G(x) \\
&= \int\int \frac{p_{T-t}^G(x,u)p_t^G(x_0,x)}{p_T^G(x_0,u)}F(x)d\,\mathrm{Vol}_G(x)f(u)d\,\mathrm{Vol}_N(u) \\
&= \int\int F(x)d\mathbb{P}_{x_0,u}^T(x)f(u)d\,\mathrm{Vol}_N(u) \\
&= \int \mathbb{E}_{\mathbb{P}}[F(X_t)|X_T = u]f(u)d\,\mathrm{Vol}_N(u).
\end{aligned}$$

In order to conclude, we need to show that for any finite distribution $(X_{t_1},\ldots,X_{t_n})$

$$\mathbb{E}_{\mathbb{P}}[h(t,X_t)F(X_{t_1},\ldots,X_{t_n})] = \int \mathbb{E}_{\mathbb{P}}[F(X_{t_1},\ldots,X_{t_n})|X_T = u]f(u)d\,\mathrm{Vol}_N(u).$$

Therefore, let $0 < t_1 < \cdots < t_n < T$ and $t \in (t_n, T)$. Define Φ_F similar to how it was defined in Lemma 2. Then

$$\begin{aligned}\mathbb{E}_{\mathbb{P}}[h(t,X_t)F(X_{t_1},\ldots,X_{t_n})] &= \int_G h(t,x)\Phi_F(t,x)d\,\mathrm{Vol}_G(x)\\ &= \int f(u)\int F(z)P(z,x,u)d\,\mathrm{Vol}(z)d\,\mathrm{Vol}(x)d\,\mathrm{Vol}(u)\\ &= \int \mathbb{E}_{\mathbb{P}}[F(X_{t_1},\ldots,X_{t_n})|X_T=u]f(u)d\,\mathrm{Vol}_N(u),\end{aligned}$$

where $z = (z_1, \ldots, z_n)$ and $d\,\mathrm{Vol}(z) = d\,\mathrm{Vol}(z_1)\ldots d\,\mathrm{Vol}(z_n)$ and where

$$P(z,x,u) = \frac{p^G_{t_1}(x_0,z_1)\ldots p^G_{t-t_n}(z_n,x)p^G_{T-t}(x,u)}{p^G_T(x_0,u)}.$$

□

The next result uses the type of conditioning found in van der Meulen and Schauer [13]. By imposing noise on the conditioning point they showed that the endpoint is tilted to have a given density. We adapt here this type of conditioning by imposing noise in the on the conditioning point.

Theorem 7. *Let X be a Markov process defined on $(\Omega, \mathcal{F}, \mathbb{P})$ with values in G, $X_0 = x_0$, and let $p^G_t(\cdot,\cdot)$ be its transition density defined by $\mathbb{P}(X_T \in du|X_t = x) = p^G_{T-t}(x,u)d\,\mathrm{Vol}_G(u)$. Assume $0 \le t < T$ and $X_T \sim f \cdot \mathrm{Vol}_N$ (e.g., uniform distribution on fiber over v). The simultaneous distribution of (X_t, X_T) has density given by*

$$\frac{\mathbb{P}(X_t \in dx, X_T \in du)}{d\,\mathrm{Vol}_N(u)d\,\mathrm{Vol}_G(x)} = f(u)p^G_{T-t}(x,u) \tag{40}$$

Furthermore, the conditional distribution of X_t given X_T has density

$$k_t(x,u) = \frac{f(u)p^G_{T-t}(x,u)}{\int_N f(y)p^G_T(x_0,y)d\,\mathrm{Vol}_N(y)}. \tag{41}$$

(NB. σ-finite measures exists on any connected locally compact Lie group)

Proof. The first part is a direct consequence of standard measure theory. For the second part define

$$Z_t = h(t,X_t) = \frac{\int f(u)p^G_{T-t}(X_t,u)d\,\mathrm{Vol}_N(u)}{\int f(u)p^G_T(x_0,u)d\,\mathrm{Vol}_N(u)}. \tag{42}$$

Then, for $0 \le s < t$

$$
\begin{aligned}
\mathbb{E}^{\mathbb{P}}[Z_t|\mathcal{F}_s] = \mathbb{E}^{\mathbb{P}}[h(t,X_t)|X_s] &= \int \frac{\int f(u) p^G_{T-t}(x,u) d\operatorname{Vol}_N(u)}{\int f(u) p^G_T(x_0,u) d\operatorname{Vol}_N(u)} p_{t-s}(X_s,x) d\operatorname{Vol}_G(x) \\
&= \frac{\int f(u) \int p^G_{T-t}(x,u) p_{t-s}(X_s,x) d\operatorname{Vol}_G(x) d\operatorname{Vol}_N(u)}{\int f(u) p^G_T(x_0,u) d\operatorname{Vol}_N(u)} \\
&= \frac{\int f(u) p^G_{T-s}(X_s,u) d\operatorname{Vol}_N(u)}{\int f(u) p^G_T(x_0,u) d\operatorname{Vol}_N(u)} \\
&= Z_s,
\end{aligned}
$$

and we see that Z is a local martingale with $Z_0 = 1$. Defining $\mathbb{Q}_t = Z_t \cdot \mathbb{P}$, we see from the abstract Bayes formula

$$
\begin{aligned}
\mathbb{E}^{\mathbb{Q}}[F(X_t)|X_s] &= \frac{\mathbb{E}^{\mathbb{P}}[Z_t F(X_t)|X_s]}{Z_s} \\
&= \frac{\int F(x) p^G_{t-s}(X_s,x) \frac{\int f(u) p^G_{T-t}(x,u) d\operatorname{Vol}_N(u)}{\int f(u) p^G_T(x_0,u) d\operatorname{Vol}_N(u)} d\operatorname{Vol}_G(x)}{\frac{\int f(u) p^G_{T-s}(X_s,u) d\operatorname{Vol}_N(u)}{\int f(u) p^G_T(x_0,u) d\operatorname{Vol}_N(u)}} \\
&= \frac{\int F(x) p^G_{t-s}(X_s,x) \int f(u) p^G_{T-t}(x,u) d\operatorname{Vol}_N(u) d\operatorname{Vol}_G(x)}{\int f(u) p^G_{T-s}(X_s,u) d\operatorname{Vol}_N(u)} \\
&= \int \int \frac{F(x) p^G_{t-s}(X_s,x) p^G_{T-t}(x,u)}{p^G_{T-s}(X_s,u)} d\operatorname{Vol}_G(x) k_u(X_s) d\operatorname{Vol}_N(u) \\
&= \int \mathbb{E}^{\mathbb{P}}\left[F(X_t)|\mathcal{F}_s, X_T = u\right] k_u(X_s) d\operatorname{Vol}_N(u),
\end{aligned}
$$

where exactly

$$
k_t(X_s,u) = \frac{f(u) p^G_{T-s}(X_s,u)}{\int f(u) p^G_{T-s}(X_s,u) d\operatorname{Vol}_N(u)}.
$$

□

We note that the density $k_u(x)$ is proportional to the expression

$$
k_T(x_0,u) = \frac{f(u) p^G_T(x,u)}{\int_N f(y) p^G_T(x_0,y) d\operatorname{Vol}_N(y)} \propto f(u) q_T(x_0,u) \lim_{t\uparrow T} \mathbb{E}[\varphi_{t,u}]. \tag{43}
$$

Assume that the constants c_i exist. We can obtain unbiased estimates of the constants c_i via simulation of sample paths of the guided process. Let $y^i_t = Y_t(\omega_i)$ be realizations of the guided bridge process. We can then use the unbiased estimator

$$
\bar{\varphi}_{T,v_i}(y) = \frac{1}{m} \sum_{n=1}^{m} \exp\left[\int_0^T \frac{r_{v_i}(y^n_s)}{T-s} \left(dA^{v_i}_s + dL^{v_i}_s\right)\right] \tag{44}
$$

to approximate the constants $c_i = \mathbb{E}[\varphi_{T,v_i}]$.

Algorithm 1: Stochastic Metropolis-Hastings Algorithm

```
// Initialization
```
Choose initial point $e \in G$ and $v_1 \in N$ closest to e. Simulate a guided bridge process to v_1 and obtain an unbiased estimate of $\mathbb{E}[\varphi_{T,v_1}]$.
```
// Main loop
```
while *k points not reached* **do**
```
    // Step 1:
```
    Propose u from the proposal density $f(v_i, u)$ (e.g. uniform density in N centered at v_i or normal density in N centered at v_i) and sample estimator for $\mathbb{E}[\varphi_{T,u}]$
```
    // Step 2:
```
    Calculate the acceptance ratio $g(u, v_i) = \min\left\{1, \frac{f(u,v_i)q_T(x_0,u)\bar{\varphi}_{T,u}}{f(v_i,u)q_T(x_0,v_i)\bar{\varphi}_{T,v_i}}\right\}$ (Note that if f is symmetric it cancels out in the acceptance probability)
```
    // Step 3
```
    Accept with probability $\mathrm{g}(u, v_i)$ and set $v_{i+1} = u$ as well as $c_{i+1} = \bar{\varphi}_{T,v_{i+1}}$ otherwise do nothing.

end
```
// Output:
```
$\{(v_1, c_1), \ldots, (v_k, c_k)\}$

Proof. By repeated use of the tower property and Markov property

$$\begin{aligned}\mathbb{E}[g(X_T)F(X)] =& \mathbb{E}\left[g(X_T)\mathbb{E}[F(X)|X_T]\right]\\ =& \mathbb{E}\left[F(X)\mathbb{E}[g(X_T)|X_s]\right],\end{aligned}$$

for any $\mathcal{F}_s$-measurable functional F and $\mathcal{F}_T$-measurable function g. From the Markov property it follows that

$$\begin{aligned}\mathbb{E}\left[F(X)\mathbb{E}[g(X_T)|X_s]\right] =& \mathbb{E}\left[F(X)\int_G g(v)p^G_{T-s}(X_s, v)d\,\mathrm{Vol}_G(v)\right]\\ =& \int_G \mathbb{E}[F(X)p^G_{T-s}(X_s, v)]g(v)d\,\mathrm{Vol}_G(v).\end{aligned}$$

Using the fact that $X_T(\mathbb{P})(v) = f(v)d\,\mathrm{Vol}_G(v)$, where $f(v) \equiv 0$ for any $v \in G\backslash N$,

$$\begin{aligned}\mathbb{E}\left[g(X_T)\mathbb{E}[F(X)|X_T]\right] &= \int_G g(v)\mathbb{E}[F(X)|X_T = v]dX_T(\mathbb{P})(v)\\ &= \int_G \mathbb{E}[F(X)|X_T = v]f(v)g(v)d\,\mathrm{Vol}_G(v).\end{aligned}$$

From this we see that for any non-negative measurable function g

$$\int_G \mathbb{E}[F(X)p^G_{T-s}(X_s, v)]g(v)d\,\mathrm{Vol}_G(v) = \int_G \mathbb{E}[F(X)|X_T = v]f(v)g(v)d\,\mathrm{Vol}_G(v),$$

which implies that almost everywhere, for any $F \in \mathcal{F}_s$,

$$\mathbb{E}[F(X)|X_T = v] = \frac{\mathbb{E}[F(X)p^G_{T-s}(X_s, v)]}{f(v)}.$$

□

5 Numerical Experiments

In this section, we present numerical results of bridge sampling on specific Lie groups and homogeneous spaces. The specific Lie groups in question are the three-dimensional rotation group SO(3) and the general linear group of invertible matrices with positive determinant $\mathrm{GL}_+(3)$.

The rotation group SO(3) is a Lie group with Lie algebra $\mathfrak{so}(3)$, consisting of skew-symmetric matrices. The Lie group SO(3) is well-studied group, where closed form expressions of the Lie group exponential and logarithmic map are available. Furthermore, the structure coefficients of SO(3) are particularly simple to work with. Exploiting the bridge sampling scheme described above, we show below how to estimate the underlying true metric on SO(3) via an iterative MLE method.

The space of covariance matrices, i.e., the symmetric positive definite matrices SPD(n), is an example of a non-linear space in which geometric data appear in many applications. The space SPD(3) can be obtained as the homogeneous space $\mathrm{GL}_+(3)/\mathrm{SO}(3)$, where GL_+ is the space of invertible matrices with positive determinant.

Lastly, considering the two-sphere $\mathbb{S}^2$ as the homogeneous space SO(3)/SO(2), we verify that the bridge sampling scheme on this homogeneous space yields admissible heat kernel estimates on $\mathbb{S}^2$.

Numerical Simulations The Euler-Heun scheme leads to approximation of the Stratonovich integral. With a time discretization $t_1, \dots, t_k$, $t_k - t_{k-1} = \Delta t$ and corresponding noise $\Delta B_{t_i} \sim N(0, \Delta t)$, the numerical approximation of the Brownian motion (7) takes the form

$$x_{t_{k+1}} = x_{t_k} - \frac{1}{2}\sum_{j,i} C^j_{ij} V_i(x_{t_k})\Delta t + \frac{v_{t_{k+1}} + V_i(v_{t_{k+1}} + x_{t_k})\Delta B^i_{t_k}}{2} \tag{45}$$

where $v_{t_{k+1}} = V_i(x_{t_k})\Delta B^i_{t_k}$ is only used as an intermediate value in integration. Adding the logarithmic term in (23) to (45) we obtain a numerical approximation of a guided diffusion (14).

5.1 Importance Sampling and Metric Estimation on SO(3)

This section takes G to be the special orthogonal group of rotation matrices, SO(3), a compact connected matrix Lie group. In the context of matrix Lie groups, computing left-invariant vector fields is straightforward.

The Lie algebra of the rotation group SO(3) is the space of three-by-three skew symmetric matrices, $\mathfrak{so}(3)$. The exponential map $\exp\colon \mathfrak{so}(3) \to \mathrm{SO}(3)$ is a well-defined surjective map which coincide with usual matrix exponential e^A.

With $a \in \mathbb{R}^3$, we can express any element $A \in \mathfrak{so}(3)$ in terms of the standard basis $\{e_1, e_2, e_3\}$ of $\mathbb{R}^3$ as

$$A = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}.$$

Let $\theta = \|a\|_2$ and assume that $\theta \neq 0$. By Rodrigues' formula the matrix Lie group exponential map $\exp\colon \mathfrak{so}(3) \to \mathrm{SO}(3)$ is given by

$$R := e^A = I + \frac{\sin(\theta)}{\theta} A + \frac{(1 - \cos(\theta))}{\theta^2} A^2$$

and the corresponding inverse matrix Lie group exponential map $\log\colon \mathrm{SO}(3) \to \mathfrak{so}(3)$

$$\log(R) = \frac{\sin^{-1}(\theta)}{2\theta}(R - R^T).$$

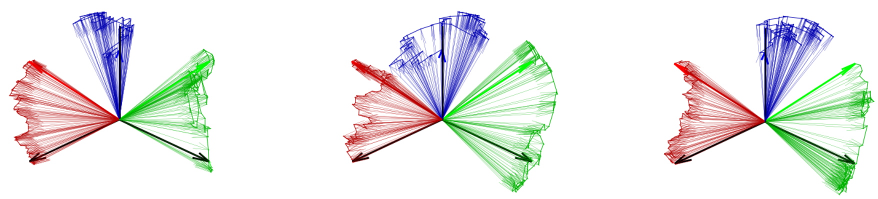
The rotation group SO(3) is semi-simple, hence there exist a bi-invariant inner product. In this case, the Riemannian exponential map Exp coincide with the Lie group exponential map exp and thus the Riemannian distance function $d(R, I)^2 = \|\mathrm{Log}_I(R)\|^2$, from the rotation R to the identity I, satisfies $\nabla_R d(R, I)^2 = 2\log(R)$.

The structure coefficients of $\mathfrak{so}(3)$ are particularly simple. Let $A_i = A$ with $a_j = 1$ if $i = j$ and zero otherwise. In this case, $\{A_1, A_2, A_3\}$ defines a basis of $\mathfrak{so}(3)$. The structure coefficients satisfy the relation $[A_i, A_j] = C_{ij}^k A_k = \epsilon^{ijk} A_k$, where ϵ^{ijk} denotes the Levi-Civita symbols. The Levi-Civita symbols are defined as $+1$, for (i, j, k) an even permutation of $(1, 2, 3)$, -1 for every odd permutation, and zero otherwise.

Numerical Bridge Sampling Algorithm on SO(3) Utilizing the simple expressions for the structure coefficients and the Lie group logarithmic map, we can explicitly write up the numerical approximation of the guided bridge processes (Brownian bridge) on SO(3) as

$$x_{t_{k+1}} = x_{t_k} - \frac{1}{2}\sum_{j,i} \epsilon^{ijj} V_i(x_{t_k})\Delta t + \frac{v_{t_{k+1}} + V_i(v_{t_{k+1}} + x_{t_k})\left(\Delta B_{t_k}^i - \frac{\log(x_k)}{T - t_k}\Delta t\right)}{2}, \tag{46}$$

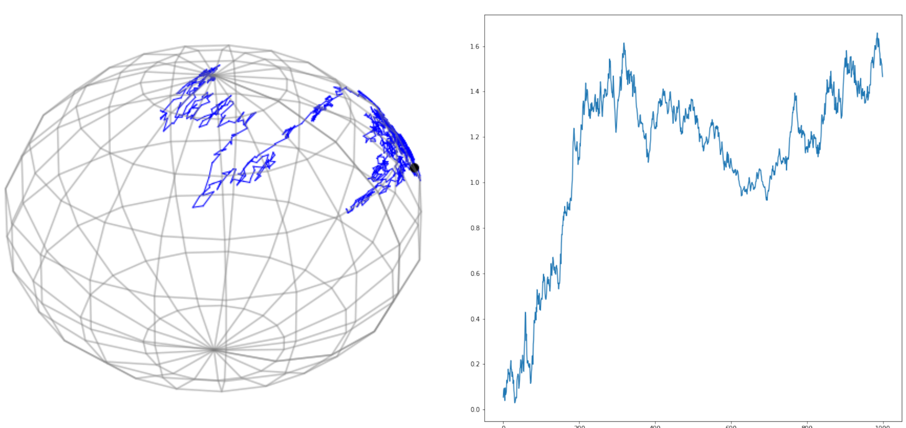
where in this case we have $v_{t_{k+1}} = V_i(x_{t_k})\left(\Delta B_{t_k}^i - \frac{\log(x_k)}{T - t_k}\Delta t\right)$. Figure 1 illustrates the numerical approximation by showcasing three different sample paths from the guided diffusion conditioned to hit the rotation represented by the black vectors.



(a) (b) (c)

Fig. 1: Three sample paths $(a) - (c)$ of the guided diffusion process on SO(3) visualized by its action on the basis vectors $\{e_1, e_2, e_3\}$ (red, green, blue) arrows of $\mathbb{R}^3$ (rotated view). The sample paths are conditioned to hit the rotation represented by the black vectors.

Another way of visualizing the guided bridge on the rotation group SO(3) is through the angle-axis representation. Figure 2 represents a guided process on SO(3) by presenting the axis representation on $\mathbb{S}^2$ and its corresponding angle of rotation.



(a) The axis representation of the rotation matrices corresponding to the axis around which the rotation happens.

(b) The angle-representation of the rotation around the "fixed" rotation axis.

Fig. 2: Angle-axis representation of a guided bridge process on the rotation group SO(3)

Metric Estimation on SO(3) In the d-dimensional Euclidean case, importance sampling yields the estimate [15]

$$p_T(u,v) = \left(\frac{\det\left(A(T,v)\right)}{2\pi T}\right)^{\frac{d}{2}} e^{-\frac{\|u-v\|_A^2}{2T}}\mathbb{E}[\varphi_{v,T}],$$

where $\|x\|_A = x^T A(0,u)x$. Thus, from the output of the importance sampling we get an estimate of the transition density. Similar to the Euclidean case, we obtain an expression for the heat kernel $p_T(e,v)$ as $p_T(e,v) = q(T,e)\mathbb{E}\left[\varphi_{v,T}\right]$, where

$$\begin{aligned} q(T,e) &= \left(\frac{\det A(v)}{2\pi T}\right)^{\frac{3}{2}} \exp\left(-\frac{d(e,v)^2}{2T}\right) \\ &= \left(\frac{\det A(T,v)}{2\pi T}\right)^{\frac{3}{2}} \exp\left(-\frac{\|\mathrm{Log}_v(e)\|_A^2}{2T}\right), \end{aligned} \tag{47}$$

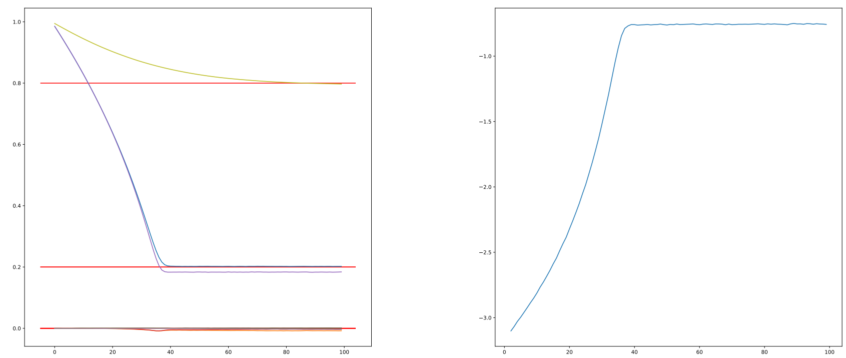
where the equality holds almost everywhere and $A \in \mathrm{Sym}^+(\mathfrak{g})$ denotes the metric $A(e) := A(0,e)$. The Log_v map in (47) is the Riemannian inverse exponential map.

Figure 3 illustrates how importance sampling on SO(3) leads to a metric estimation of the underlying unknown metric, which generated the Brownian motion. We sampled 128 points as endpoints of a Brownian motion from the metric $\mathrm{diag}(0.2, 0.2, 0.8)$, and used 20 time steps to sample 4 bridges per observation. An iterative MLE method using gradient descent with a learning rate of 0.2, and initial guess of the metric being $\mathrm{diag}(1, 1, 1)$ yielded a convergence to the true metric. Note that in iteration the logarithmic map changes.

5.2 Diffusion-Mean Estimation on SPD(3)

The space of symmetric positive definite (SPD) matrices is an essential class of matrices arising as geometric data in many applications. For example, in diffusion tensor imaging, SPD(3) matrices are used to model the anisotropic diffusion of water molecules in each voxel. The SPD matrices constitute a smooth incomplete manifold when endowed with the Euclidean metric of matrices (Pennec et al. [16]). The space of SPD(3) matrices can be regarded as the homogeneous space $\mathrm{GL}_+(3)/\mathrm{SO}(3)$ of invertible matrices with positive determinants being rotationally invariant to three-dimensional rotations.

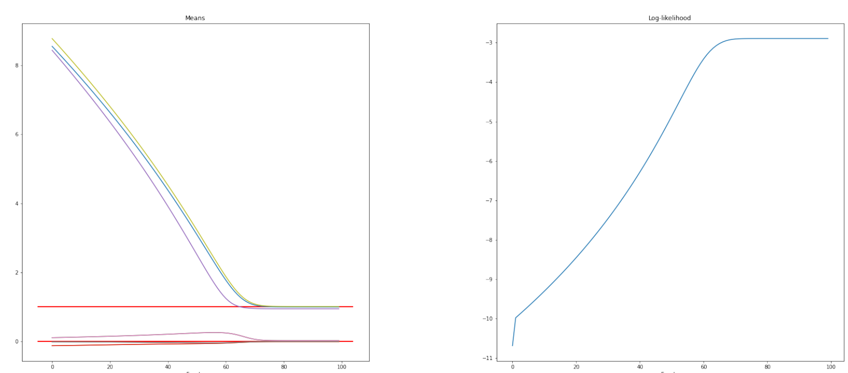
In this section, the bridge sampling scheme derived above allow us to obtain an estimate of the diffusion-mean [5, 6] on SPD(3), by sampling guided bridge processes in the space of invertible matrices with positive determinants $\mathrm{GL}_+(3)$. This sampling method provides an estimate of the density on $\mathrm{GL}_+(3)$ which projects to a density in SPD(3). Exploiting the resulting density in SPD(3), an iterative MLE method then yield a convergence to the diffusion mean.



(a) Estimation of the unknown underlying metric using bridge sampling. Here the true metric is the diagonal matrix diag$(0.2, 0.2, 0.8)$.

(b) The iterative log-likelihood.

Fig. 3: The importance sampling technique applies to metric estimation on the Lie group SO(3). Sampling a Brownian motion from an underlying unknown metric, we obtain convergence to the true underlying metric using an iterative MLE method. Here we sampled 4 guided bridges per observation, starting from the metric diag$(1, 1, 1)$, providing a relatively smooth iterative likelihood in 3b.



(a) Convergence of the diffusion mean on SPD(3).

(b) Iterative log-likelihood for the diffusion mean.

Fig. 4: Given 64 data points in SPD(3), simulating three bridges per observation in $\mathrm{GL}_+(3)$, conditioned on the fibers, we obtain convergence of the diffusion-mean using the iterative MLE with a learning rate of 0.75. The true mean is the identity matrix illustrated by the red lines in (a). The yellow, blue, and purple lines visualize the diagonal elements in the SPD(3) matrix, while the remaining lines represent the off-diagonal.

Algorithm 2: Parameter Estimation: Iterative MLE.

```
// Initialization
```
Given n data points $\{v_1, \ldots, v_n\}$.
```
// Specify initial parameters θ_0 = (g_0, A) and a learning rate η.
```
for $k = 1$ *to* K **do**

  for $j = 1$ *to* n **do**

    Sample m bridges conditioned on v_j to get estimate for $\mathbb{E}[\varphi_{v_j,T}] \approx \frac{1}{m}\sum_{i=1}^{m} \varphi_{v_j,T}^i$

  end

  $\ell_{\theta_{k-1}}(v_1, \ldots, v_n) = \prod_{j=1}^{n} \left(\frac{\det A(T,v_j)}{2\pi T}\right)^{3/2} e^{-\frac{\|\mathrm{Log}_{v_j}(e)\|_A^2}{2T}} \frac{1}{m}\sum_{i=1}^{m} \varphi_{v_j,T}^i$

  ```
  // Compute the gradient
  ```
  $v_{k-1} = \nabla_{\theta_{k-1}} \log \ell_{\theta_{k-1}}(v_1, \ldots, v_n)$

  ```
  // Update the parameters
  ```
  $\theta_k = \theta_{k-1} - \eta v_k$

end

```
// Return final parameters θ_K
```

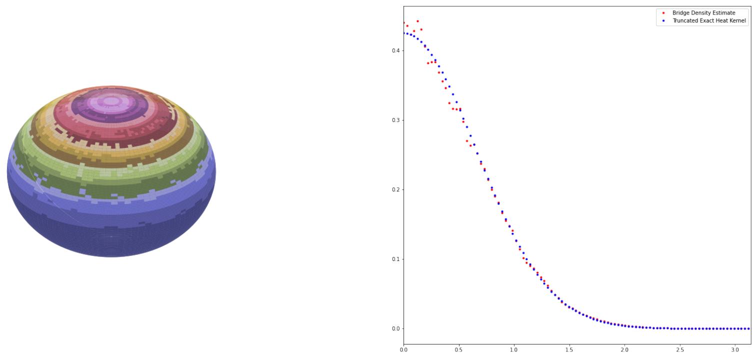
Fig. 4 visualize the MLE approach to estimating the diffusion mean. As SPD(3) matrices are six-dimensional, we only need six parameters (three in the diagonal and three in the off-diagonal) to estimate the diffusion mean.

5.3 Density Estimation on $\mathbb{S}^2 := \mathrm{SO}(3)/\mathrm{SO}(2)$

Bi-invariant Metric A simulation scheme on specific homogeneous spaces was introduced in Section 4.2 by using guided bridges in the top space conditioned to arrive in the fiber at time T. The two-sphere $\mathbb{S}^2$ can be considered as the homogeneous space SO(3)/SO(2) of three-dimensional rotations, identifying the subgroup of two-dimensional rotations as a single point. Conditioning on the fiber SO(2) in SO(3), we obtain guided bridges on $\mathbb{S}^2$.

Comparing the estimated heat kernel on $\mathbb{S}^2$, obtained from bridge samples in SO(3), with the truncated version of the exact heat kernel, as described by Zhao and Song [21], the bridge estimated density offers a good approximation of the (truncated) exact density. Fig. 5 shows the relation between the estimated heat kernel and the truncated exact heat kernel.

Non-invariant Metric Changing the metric structure on SO(3) results in an anisotropic distribution on $\mathbb{S}^2$, arising as the pushforward measure from SO(3). Fig. 6 illustrate the anisotropic distributions on $\mathbb{S}^2$ induced by a left-invariant metric on SO(3) for $T = 0.5, 1.0, 1.5$, and 2.0, respectively.



(a) The estimated heat kernel on $\mathbb{S}^2$ obtained from bridge sampling in SO(3) for $T = 0.5$.

(b) The estimated heat kernel, for $T = 0.5$, on $\mathbb{S}^2$ along a geodesic from the north pole to the south pole against the truncated exact heat kernel, where $T = 0.4$.

Fig. 5: From 128 sample points on $\mathbb{S}^2$, sampling guided bridges in SO(3) conditioned on the fibers over the sample points, an estimate of the heat kernel on $\mathbb{S}^2$ is obtained.

Fig. 6: Anisotropic distributions on $\mathbb{S}^2$ arising from a non-invariant metric on SO(3), for $T = 0.5, 1.0, 1.5$, and 2.0, respectively. The density estimates are based on 512 sample points on SO(3). For each sample point and end-time, three guided bridge processes were sampled in SO(3) yielding estimates of the densities in SO(3), which projected to anisotropic densities in $\mathbb{S}^2$.

References

1. Barden, D., Le, H.: Some consequences of the nature of the distance function on the cut locus in a riemannian manifold. Journal of the LMS (1997)
2. Bladt, M., Finch, S., Sørensen, M.: Simulation of multivariate diffusion bridges. Journal of the Royal Statistical Society: Series B: Statistical Methodology pp. 343–369 (2016)
3. Bladt, M., Sørensen, M.: Simple simulation of diffusion bridges with application to likelihood inference for diffusions. Bernoulli **20**(2), 645–675 (2014)
4. Delyon, B., Hu, Y.: Simulation of conditioned diffusion and application to parameter estimation. Stochastic Processes and their Applications (2006)
5. Hansen, P., Eltzner, B., Huckemann, S.F., Sommer, S.: Diffusion means in geometric spaces. arXiv preprint arXiv:2105.12061 (2021)

6. Hansen, P., Eltzner, B., Sommer, S.: Diffusion means and heat kernel on manifolds. Geometric Science of Information (2021)
7. Hsu, E.P.: Stochastic analysis on manifolds, vol. 38. AMS (2002)
8. Hsu, P.: Brownian bridges on riemannian manifolds. Probability theory and related fields **84**(1), 103–118 (1990)
9. Jensen, M.H., Sommer, S.: Simulation of conditioned semimartingales on riemannian manifolds. arXiv preprint arXiv:2105.13190 (2021)
10. Kendall, W.S.: The radial part of brownian motion on a manifold: a semimartingale property. The Annals of Probability **15**(4), 1491–1500 (1987)
11. Le, H., Barden, D.: Itô correction terms for the radial parts of semimartingales on manifolds. Probability theory and related fields **101**(1), 133–146 (1995)
12. Liao, M.: Lévy processes in Lie groups, vol. 162. Cambridge university press (2004)
13. van der Meulen, F., Schauer, M.: Bayesian estimation of incompletely observed diffusions. Stochastics **90**(5), 641–662 (2018)
14. van der Meulen, F., Schauer, M., et al.: Bayesian estimation of discretely observed multi-dimensional diffusion processes using guided proposals. Electronic Journal of Statistics **11**(1), 2358–2396 (2017)
15. Papaspiliopoulos, O., Roberts, G.: Importance sampling techniques for estimation of diffusion models. Statistical methods for stochastic differential equations (2012)
16. Pennec, X., Sommer, S., Fletcher, T.: Riemannian Geometric Statistics in Medical Image Analysis. Academic Press (2019)
17. Schauer, M., Van Der Meulen, F., Van Zanten, H., et al.: Guided proposals for simulating multi-dimensional diffusion bridges. Bernoulli **23**(4A), 2917–2950 (2017)
18. Shigekawa, I.: Transformations of the brownian motion on a riemannian symmetric space. Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete (1984)
19. Thompson, J.: Submanifold bridge processes. Ph.D. thesis, University of Warwick (2015)
20. Thompson, J.: Brownian bridges to submanifolds. Potential Analysis **49**(4) (2018)
21. Zhao, C., Song, J.S.: Exact heat kernel on a hypersphere and its applications in kernel svm. Frontiers in Applied Mathematics and Statistics **4**, 1 (2018)