DEPARTMENT OF COMPUTER SCIENCE
UNIVERSITY OF COPENHAGEN

CENTRE FOR STOCHASTIC GEOMETRY AND ADVANCED BIOIMAGING

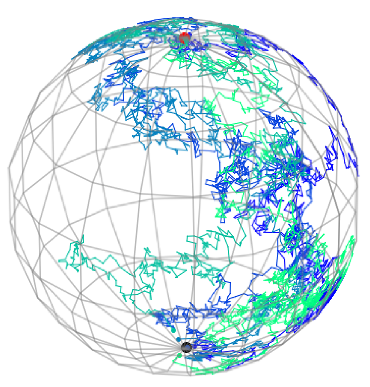
# Simulation of Conditioned Diffusions on Riemannian Manifolds

Mathias Højgaard Jensen — *matje@di.ku.dk*
Stefan Sommer — *sommer@di.ku.dk*

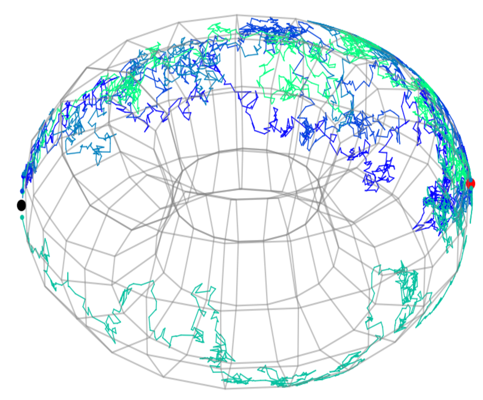
## Summary

- We propose a method for simulating diffusion bridges on general Riemannian manifolds, from $p$ to $v$, over the time interval $[0, T]$.
- The method relies on a guiding scheme dependent on the gradient of the squared distance function, $\nabla_x d(x,p)^2/2$. The bridge process is termed *radial bridge*.
- The radial bridge is applied to estimate the diffusion mean (Hansen et al. 2020) on the sphere, $\mathbb{S}^2$ (see Fig. 5).

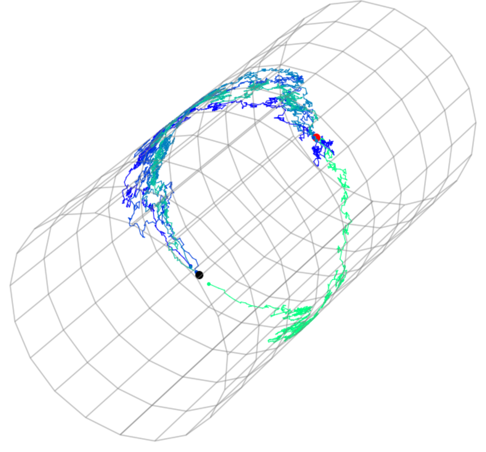
## Simulation of Radial Bridges



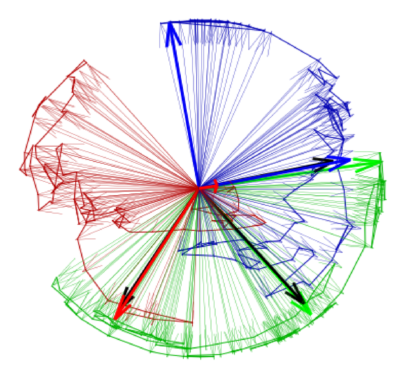
**(a)** $\mathcal{M} = \mathbb{S}^2$. Four simulated paths of a diffusion bridge process from the north pole (red point) to the south pole (black point).



**(b)** $\mathcal{M} = \mathbb{T}^2$. Four sample paths from the simulation scheme of the radial bridge, $X_t$, from $x$ (red point) to $v$ (black point).



**(c)** $\mathcal{M} = \mathbb{S} \times \mathbb{R}$. An example of four sample paths of the radial bridge conditioned to arrive at a point in the cut-locus, $\mathrm{Cut}(x)$, of the initial point $x$.



**(d)** $\mathcal{M} = SO(3)$. The figure illustrates a sample path from the radial bridge on the rotation group, by showing its left action on a basis of $\mathbb{R}^3$. The black arrows indicate the conditioned point.

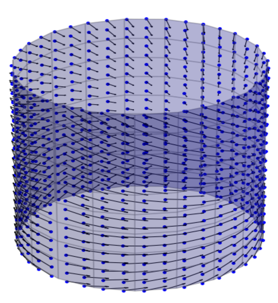
**Figure 1:** The figures show how our simulation scheme applies to different manifolds. The method works in particular across the cut-locus.

## Riemannian Manifolds

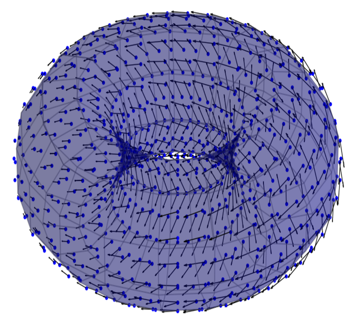
- Let $\mathcal{M}$ denote a $d$-dimensional *Riemannian manifold*, i.e. a smooth topological structure endowed with a smoothly varying inner product on the tangent space, $T_p\mathcal{M}$.
- The inverse of the exponential map $\exp_p \colon T_p\mathcal{M} \to \mathcal{M}$ defines, locally, a distance function on $\mathcal{M}$ by

$$d(x,p) := \|\exp_p^{-1}(x)\|.$$

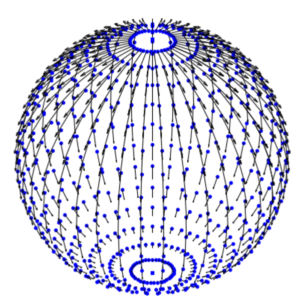
- The gradient of the distance function, $\nabla_x d(x,p)$, is called *radial vector*. The radial vector field is not smooth on the cut-locus (see Fig. 2).



**(a)** Radial vector field on the cylinder, related to the radial bridge, $X_t$, centered at the point $X_T = v$.



**(b)** Radial vector field on the torus, related to the radial bridge, $X_t$, centered at the point $X_T = v$.



**(c)** Squared radial vector field on the 2-sphere centered at the south pole.

**Figure 2:** The figures illustrate the underlying (modified) radial vector field of the cylinder, the torus, and the sphere. The vector field act as a pulling term for the radial bridge process.

## Frame Bundle Stochastics

- The *orthonormal frame bundle* is the disjoint union

$$\mathcal{OM} := \bigsqcup_{p\in\mathcal{M}} \mathcal{OM}_p = \{u \colon \mathbb{R}^d \to T_{\pi(u)}\mathcal{M}\}$$

of fibres over $p \in \mathcal{M}$, where each fibre is the collection of orthonormal basis vectors of the tangent space $T_p\mathcal{M}$ (see Fig. 3).

- The differential, $\pi_*$, of the projection $\pi \colon \mathcal{OM} \to \mathcal{M}$ is an isomorphism when restricted to the horizontal part, $\mathcal{H}_u\mathcal{OM}$, of the tangent space $T_u\mathcal{OM} := \mathcal{V}_u\mathcal{OM} \oplus \mathcal{H}_u\mathcal{OM}$. The horizontal tangent space have globally defined vector fields $H_i(u), i = 1, .., d$.

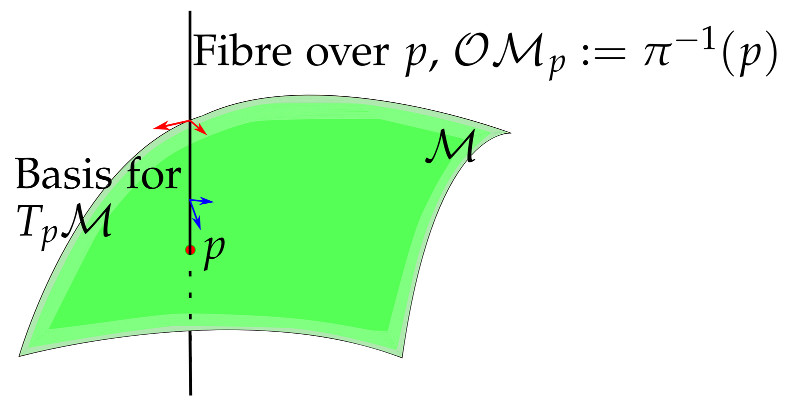



**Figure 3:** Illustration of the frame bundle over $\mathcal{M}$.

- Fixing $u_0 \in \mathcal{OM}$, there is a one-to-one correspondance between stochastic processes on $\mathbb{R}^d$, $\mathcal{M}$, and $\mathcal{OM}$. The solution to the stochastic differential equation

$$dU_t = \sum_i H_i(U_t) \circ dZ_t^i, \qquad X_t = \pi(U_t)$$

provides the one-to-one relation between $Z$, $X$, and $U$.

## Radial Bridge Process

- The *radial bridge* solves the SDE, where $\tilde{d}(u,v) = d(\pi(u), v)$,

$$dU_t = \sum_i H_i(U_t) \circ \left( dZ_t^i + U_t^{-1}\left(\frac{\pi_*\nabla^H \tilde{d}(U_t,v)^2}{2(T-t)}\right)^i dt\right), \qquad X_t = \pi(U_t).$$

- This solution converges to the desired end-point at time $T$ and is equivalent to the desired diffusion on $[0, T)$.
- The non-smoothness of the radial vector field on the cut-locus implies a discontinuity of the guiding term, as seen from Fig. 4.

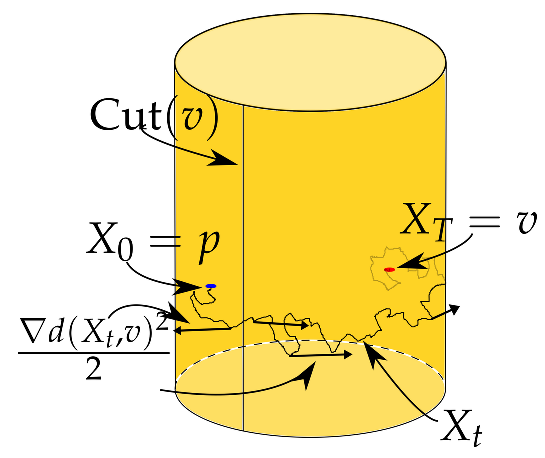
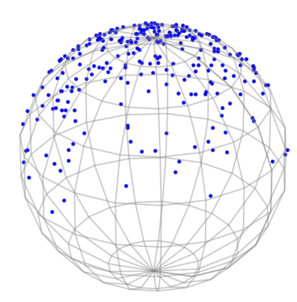
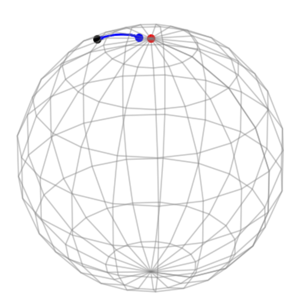



**Figure 4:** One sample path of the radial bridge, $X_t$, from $x$ to $v$, with corresponding pulling term. The drift changes sign when crossing cut-locus.

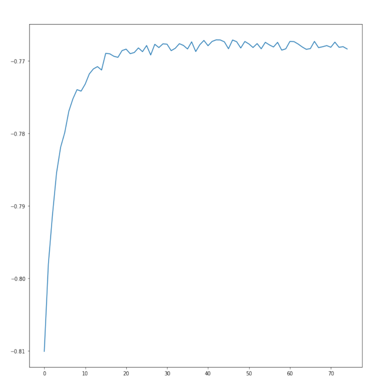
## Application to Maximum Likelihood Estimation



**(a)** Sampled data points on $\mathbb{S}^2$.



**(b)** Convergence to the diffusion mean (blue point) on $\mathbb{S}^2$ from initial guess (black point).



**(c)** Convergence of the likelihood.

**Figure 5:** Bridge simulation can be used for density estimation. To that effect it serves as a method for estimating the diffusion mean on $\mathbb{S}^2$.

## References

*Diffusion mean in geometric spaces*, Hansen, Eltzner, Huckemann, and Sommer (2020).

## Acknowledgements

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