Score-based Generative Models on Riemannian manifolds

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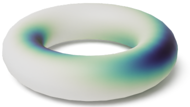
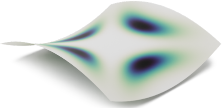
December 15, 2022






Valentin De Bortoli


Émile Mathieu


Michael Hutchinson


James Thornton

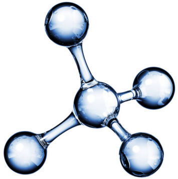

Yee Whye Teh


Arnaud Doucet

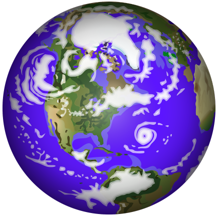
The rise of diffusion models

Figure 1: Images from stable diffusion.

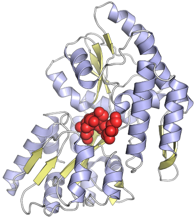
The need for geometric prior



Molecular conformation

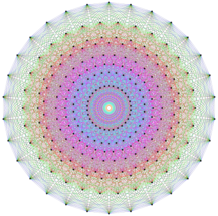


Weather Modelling

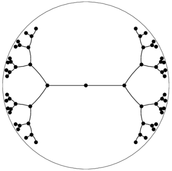


Protein Docking

Robotics



Lie groups



Tree embedding

What are Riemannian manifolds? A smooth manifold $\mathcal{M}$

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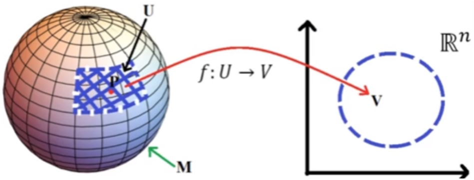

- A smooth **manifold** $\mathcal{M}$ is locally 'similar' (homeomorphic) to $\mathbb{R}^d$.
  - Exists homeomorphic *coordinate charts* (U, ϕ) s.t. $\phi : U \subset \mathcal{M} \rightarrow V \subset \mathbb{R}^d$.
  - Charts are suitably compatible (i.e. compositions are differentiable).

What are Riemannian manifolds? A metric g

A (Riemannian) **metric** $g(x)$ defines a (positive-definite) inner product on $\mathrm{T}\mathcal{M}_x$.

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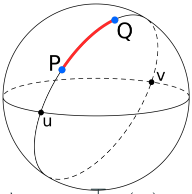
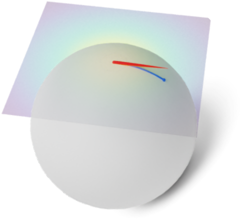


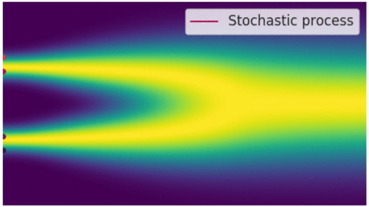


$\langle u, v\rangle_x = u^\top g(x)v$, and $g(x)$ varies smoothly with x.

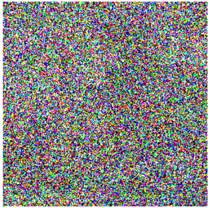
- Gradient $\nabla^{\mathcal{M}} f(x) = g(x)^{-1}\nabla f(x)$ and divergence $\mathrm{div}^{\mathcal{M}}$.
- Geodesic distance: $d^{\mathcal{M}}(x, y) = \inf\{L(\gamma) : \mathrm{C}^1 \text{ curve } \gamma \ s.t.\ \gamma(0) = x \text{ and } \gamma(1) = y\}$.
- Geodesic: argmin $\gamma(t)$ of geodesic distance.
- Exponential map: $\exp_x(tv) = \gamma(t)$ with $\gamma(0) = x$ and $\gamma'(0) = v$.

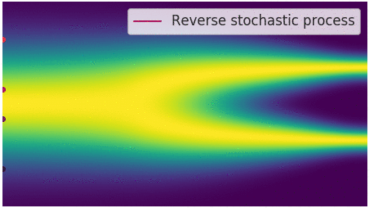
Ingredients of diffusion models

- **Forward process**



- **Backward process**





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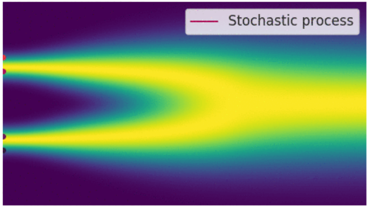

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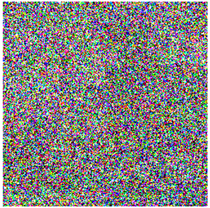

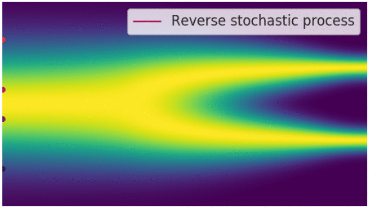

- The main ingredients:
  - Forward noising process
  - Time-reversal formula
  - Score-matching toolbox
  - Discretisation scheme

Video extracted from Yang Song's blog.

Forward processes on manifolds

Stochastic differential equation (SDE):

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

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$$\boxed{\mathrm{d}\mathbf{X}_t = -\nabla_{\mathbf{X}_t} U(\mathbf{X}_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t{}^{\mathcal{M}}}$$

admits **invariant** density: $\mathrm{d}p_{\mathsf{ref}}/\mathrm{dVol}_{\mathcal{M}}(x) \propto \mathrm{e}^{-U(x)}$ (Durmus, 2016, Section 2.4).

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What is this $\mathrm{d}\mathbf{B}_t{}^{\mathcal{M}}$ thing?

Intrinsic view

- Laplace-Beltrami Operator
  $\Delta_{\mathcal{M}} \triangleq \mathrm{div}_{\mathcal{M}} \nabla_{\mathcal{M}}$
- BM has density given by *heat equation*
  $\frac{\partial p_t}{\partial t} = \Delta_{\mathcal{M}} p_t$

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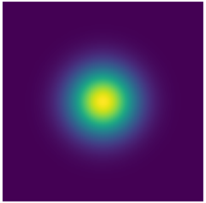
Extrinsic view

- Embed the manifold in $\mathbb{R}^{p>d}$
- Projecting the $\mathbb{R}^p$ BM onto the manifold

Invariant densities

- If $\mathcal{M} = \mathbb{R}^d$ is **Euclidean**
  - $U(x) = \|x\|^2/2$ (Gaussian distribution).
  - $\Rightarrow$ $b(t,x) = -x \Leftrightarrow \boxed{\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t}$ (Ornstein-Uhlenbeck).



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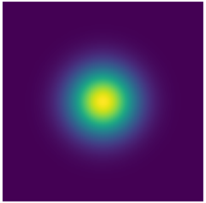
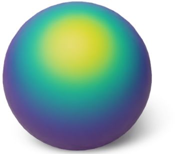


- If is $\mathcal{M}$ **non Euclidean**
  - $U(x) = d_{\mathcal{M}}(x,\mu)^2/(2\gamma^2)$ (*Riemannian* normal).
  - $\Rightarrow$ $b(t,x) = -\exp_x^{-1}(\mu)/\gamma^2$

    $\Leftrightarrow \boxed{\mathrm{d}\mathbf{X}_t = -\exp_{\mathbf{X}_t}^{-1}(\mu)/\gamma^2 \,\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}}$.



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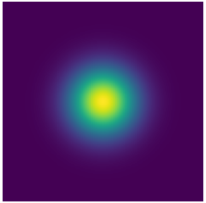

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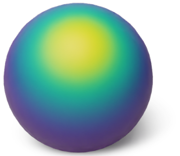

- If $\mathcal{M}$ is **compact**:
  - $U(x) =$ constant (Uniform distribution)
  - $\Rightarrow b(t,x) = \mathbf{0} \Leftrightarrow \boxed{\mathrm{d}\mathbf{X}_t = \mathrm{d}\mathbf{B}_t^{\mathcal{M}}}$ (Brownian motion).

Time reversal process

Theorem 1: Time-reversal diffusion

Let $(\mathbf{X}_t)_{t\in[0,T]}$ associated with the SDE $\mathrm{d}\mathbf{X}_t = b(t,\mathbf{X}_t)\,\mathrm{d}t + \sigma(t)\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}$ and $(\mathbf{Y}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$ the time-reversal. Under mild assumptions on p_0 and on p_t the density of $\mathbb{P}_t = \mathcal{L}(\mathbf{X}_t)$, then $(\mathbf{Y}_t)_{t\in[0,T]}$ is associated with

$$\mathrm{d}\mathbf{Y}_t = \left\{ -b(T-t,\mathbf{Y}_t) + \sigma(T-t)^2\, \nabla \log p_{T-t}(\mathbf{Y}_t) \right\}\mathrm{d}t + \sigma(T-t)\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}. \tag{1}$$

This is an extension of Cattiaux et al. (2021, Theorem 4.9).

Time reversal process

Theorem 2: Time-reversal diffusion

Let $(\mathbf{X}_t)_{t\in[0,T]}$ associated with the SDE $\mathrm{d}\mathbf{X}_t = b(t,\mathbf{X}_t)\,\mathrm{d}t + \sigma(t)\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}$ and $(\mathbf{Y}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$ the time-reversal. Under mild assumptions on p_0 and on p_t the density of $\mathbb{P}_t = \mathcal{L}(\mathbf{X}_t)$, then $(\mathbf{Y}_t)_{t\in[0,T]}$ is associated with

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Time reversal of **Langevin dynamics**:

$$\mathrm{d}\mathbf{Y}_t = \left\{\nabla_{\mathbf{X}_t}U(\mathbf{X}_t) + 2\,\nabla\log p_{T-t}(\mathbf{Y}_t)\right\}\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}. \tag{2}$$

Discretising SDEs: Geodesic Random Walk

- Given a **continuous time dynamics**

$$\boxed{\mathrm{d}\mathbf{X}_t = b(t, \mathbf{X}_t)\,\mathrm{d}t + \sigma(t)\,\mathrm{d}\mathbf{B}_t^{\mathcal{M}}\ .} \tag{3}$$

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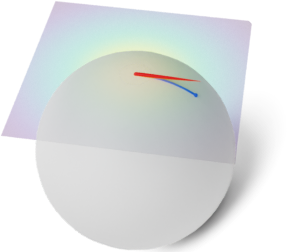
- **Geodesic Random Walk** approximation

$$\boxed{X_{k+1} = \exp_{X_k}[\gamma\, b(k\gamma, X_k) + \sqrt{\gamma}\,\sigma(k\gamma)\, Z_{k+1}]\ .} \tag{4}$$



Score approximation: Denoising score matching (DSM)

Denoising score matching (DSM) on manifolds is *very* similar to the Euclidean case

$$\ell_{t|s}(\mathbf{s}_t) = \int_{\mathcal{M}^2} \left\| \nabla_x \log p_{t|s}(x_t|x_s) - \mathbf{s}_t(x_t) \right\|^2 \mathrm{d}\mathbb{P}_{s,t}(x_s, x_t). \tag{5}$$

However need to evaluate $\nabla_x \log p_{t|s}(x_t|x_s)$.

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- **Sturm–Liouville** decomposition (Chavel, 1984) (assuming compactness)

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

Truncation approximation to DSM

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

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- **Varadhan approximation** to DSM, 1st order taylor expansion

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

Score approximation: Implicit Score Matching (ISM)

We can also avoid the need for $\nabla_{x_t} \log p_{t|0}(x_t|x_0)$ by using **implicit score matching**.

Proposition 1

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

$$\ell_t^{\mathrm{im}}(\mathbf{s}_t) = \int_{\mathcal{M}} \left\{ \frac{1}{2} \left\| \mathbf{s}_t(x_t) \right\|^2 + \mathrm{div}_{\mathcal{M}}(\mathbf{s}_t)(x_t) \right\} \mathrm{d}\mathbb{P}_t(x_t). \tag{9}$$

We need sufficient conditions on $p_{t|s}(x_t|x_s)\boldsymbol{s}(x_t)$, but these are easy to satisfy.

Score approximation: Summary

Loss	Approx	Loss function	Requirements $p_{t\|0}$	Requirements $\exp^{-1}_{\mathbf{X}_t}$	Complexity
$\ell_{t\|0}$ (DSM)	None	$\frac{1}{2}\mathbb{E}\left[\Vert \mathbf{s}(\mathbf{X}_t) - \nabla \log p_{t\|0}(\mathbf{X}_t\|\mathbf{X}_0)\Vert^2\right]$	✓	✗	$\mathcal{O}(1)$
	Truncation	$\frac{1}{2}\mathbb{E}\left[\Vert \mathbf{s}(\mathbf{X}_t) - S_{J,t}(\mathbf{X}_0, \mathbf{X}_t)\Vert^2\right]$	eigen system	✗	$\mathcal{O}(1)$
	Varhadan	$\frac{1}{2}\mathbb{E}\left[\Vert \mathbf{s}(\mathbf{X}_t) - \exp^{-1}_{\mathbf{X}_t}(\mathbf{X}_0)/t\Vert^2\right]$	✗	✓	$\mathcal{O}(1)$
$\ell_{t\|s}$ (DSM)	Varhadan	$\frac{1}{2}\mathbb{E}\left[\Vert \mathbf{s}(\mathbf{X}_t) - \exp^{-1}_{\mathbf{X}_t}(\mathbf{X}_s)/(t-s)\Vert^2\right]$	✗	✓	$\mathcal{O}(1)$
ℓ_t^{im} (ISM)	Deterministic	$\mathbb{E}\left[\frac{1}{2}\Vert \mathbf{s}(\mathbf{X}_t)\Vert^2 + \operatorname{div}_{\mathcal{M}}(\mathbf{s})(\mathbf{X}_t)\right]$	✗	✗	$\mathcal{O}(d)$
	Stochastic	$\mathbb{E}\left[\frac{1}{2}\Vert \mathbf{s}(\mathbf{X}_t)\Vert^2 + \varepsilon^\top \partial\, \mathbf{s}(\mathbf{X}_t)\varepsilon\right]$	✗	✗	$\mathcal{O}(1)$

Table 1: Computational complexity of score matching losses w.r.t. score network passes.

Parametrisation of score network

Approximate **Stein score** $(\nabla \log p_t)_{t\in[0,T]} \approx \mathbf{s}_\theta(t,\cdot)$ and $\mathbf{s}_\theta : [0,T] \to \mathcal{X}(\mathcal{M})$.

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- **Generators** of vector fields:
  - $\mathbf{s}_\theta(t,x) \triangleq \sum_{i=1}^n \mathbf{s}_\theta^i(t,x) E_i(x)$.
  - *Definition*: Smooth vector fields $\{E_i(x)\}_{i=1}^n$ s.t. span $\left(\{E_i(x)\}_{i=1}^n\right) = \mathrm{T}_x\mathcal{M}$.
  - $\mathcal{M}$ is parallelisable $\Leftrightarrow$ there exists generators $\{E_i\}_{i=1}^n$ with $n = d$.

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  - $\mathcal{M}$ is parallelisable $\Leftrightarrow$ there exists generators $\{E_i\}_{i=1}^n$ with $n = d$.
- Examples for several class of manifolds:
  - If $\mathcal{M} = \mathbb{R}^d$, can choose $E_i(x) = e_i$ for $i = 1, \dots, d$.
  - If $\mathcal{M} = G$ is a Lie group, can choose $E_i(g) = g \cdot e_i$ with $\{e_i\}_i$ basis of Lie algebra.
  - If $\mathcal{M} \subset \mathbb{R}^n$ is submersion, can choose $E_i(x) = P_i(x)$ for $i = 1, \dots, n$ with P_i the ith column of the tangent projection matrix operator.

Theoretical guaranties on time-reversal

Theorem 3

Under mild assumption over p_0 and assuming that there exists $\mathtt{M} \geq 0$ such that for any $t \in [0, T]$ and $x \in \mathcal{M}$, $\left\| \mathbf{s}_{\theta^\star}(t, x) - \nabla \log p_t(x) \right\| \leq \mathtt{M}$, 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 s.t.

$$\mathbb{W}_1(\mathcal{L}(Y_N), p_0) = C(\mathrm{e}^{-\lambda_1 T} + \sqrt{T/2}\mathtt{M} + \mathrm{e}^{T} \gamma^{1/2}), \tag{10}$$

where $\mathbb{W}_1$ is the Wasserstein distance of order one.

Experimental results

Prior work

- **Continuous normalising flows** (CNFs) (Mathieu and Nickel, 2020; Falorsi, 2021)

Train drift b_θ by maximising likelihood, solving the following **augmented** ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\mathbf{X}_t \\ \log p(\mathbf{X}_t)\end{bmatrix} = \begin{bmatrix} b_\theta(t,\cdot) \\ -\mathrm{div}\left(b_\theta(t,\cdot)\right)\end{bmatrix}(\mathbf{X}_t)\,. \tag{11}$$

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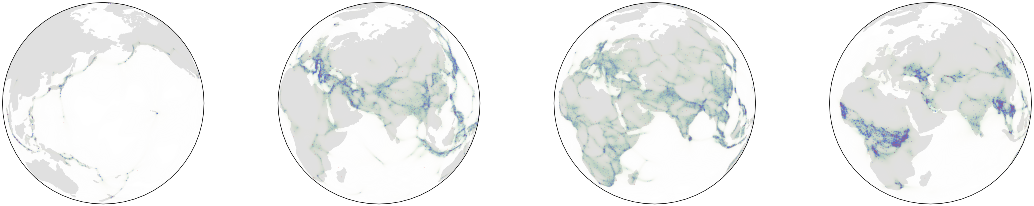
- **Moser flows** (Rozen et al., 2021)
  - Build on CNFs but uses a likelihood estimator which bypass solving an ODE.
  - Require a regularisation term involving an integral over the manifold...
  - Hence scale poorly with the manifold dimension.

Prior work: Summary

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

Table 2: 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.

Earth science data



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

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	$\mathbf{-6.05}_{\pm \mathbf{0.61}}$	$0.14_{\pm 0.23}$	$1.11_{\pm 0.19}$	$\mathbf{-0.80}_{\pm \mathbf{0.54}}$
Moser Flow	$-4.21_{\pm 0.17}$	$\mathbf{-0.16}_{\pm \mathbf{0.06}}$	$\mathbf{0.57}_{\pm \mathbf{0.10}}$	$\mathbf{-1.28}_{\pm \mathbf{0.05}}$
Stereographic Score-Based	$-3.80_{\pm 0.27}$	$\mathbf{-0.19}_{\pm \mathbf{0.05}}$	$\mathbf{0.59}_{\pm \mathbf{0.07}}$	$\mathbf{-1.28}_{\pm \mathbf{0.12}}$
Riemannian Score-Based	$-4.92_{\pm 0.25}$	$\mathbf{-0.19}_{\pm \mathbf{0.07}}$	$\mathbf{0.45}_{\pm \mathbf{0.17}}$	$\mathbf{-1.33}_{\pm \mathbf{0.06}}$
Dataset size	827	6120	4875	12809

High dimensional torus

- We consider a wrapped Gaussian target distribution on $\mathbb{T}^d = \mathbb{S}^1 \times \cdots \times \mathbb{S}^1$.

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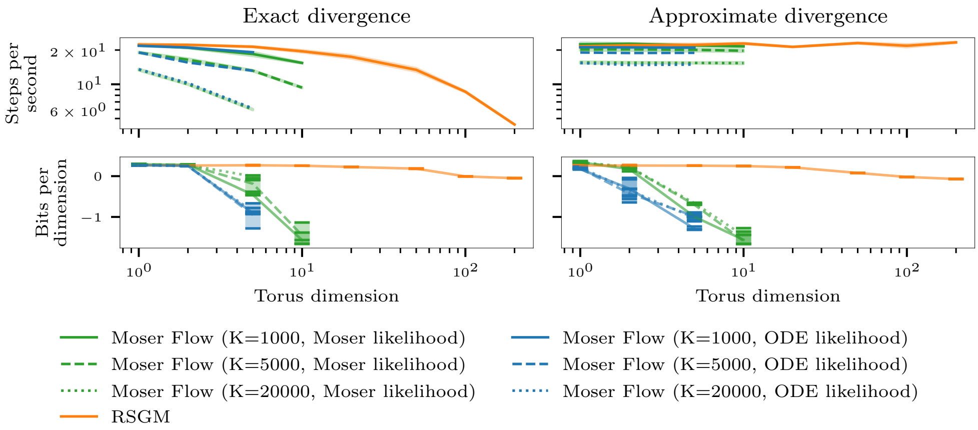

Synthetic data on Lie groups

- We consider a mixture of wrapped Gaussian target distribution on $\mathrm{SO}_3(\mathbb{R}) = \{\mathrm{Q} \in \mathrm{M}_3(\mathbb{R}) \,:\, \mathrm{Q}\mathrm{Q}^\top = I_3,\ \det(\mathrm{Q}) = 1\}$.

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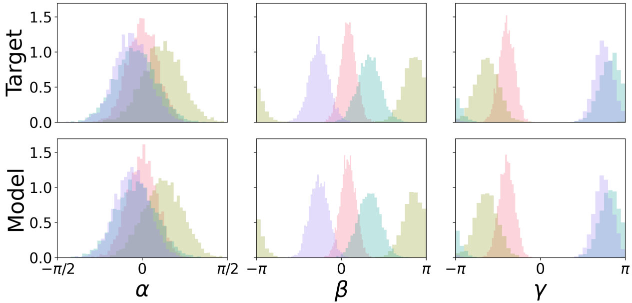


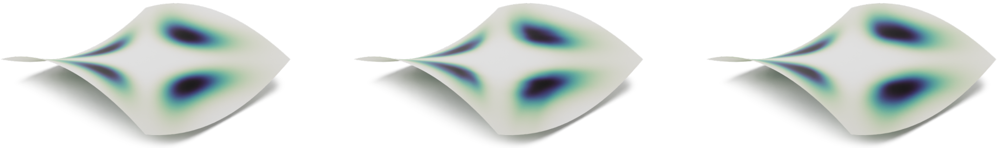
Figure 6: Histograms of $\mathrm{SO}_3(\mathbb{R})$ samples from a target mixture distribution.

Synthetic data on Lie groups (Cont'd)

Method	$M = 16$		$M = 32$		$M = 64$	
	$\log p$	NFE	$\log p$	NFE	$\log p$	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	$\mathbf{0.89_{\pm 0.03}}$	$\mathbf{0.1_{\pm 0.0}}$	$\mathbf{0.20_{\pm 0.03}}$	$\mathbf{0.1_{\pm 0.0}}$	$\mathbf{-0.49_{\pm 0.02}}$	$\mathbf{0.1_{\pm 0.0}}$

Table 4: Log-likelihood and neural function evaluations (NFE) in 10^3.

Hyperbolic experiments



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

Figure 7: Samples from different probability distributions on $\mathbb{H}^2$ coloured w.r.t their density.

Conclusion

- Extension of **diffusion models** to the **Riemannian manifold** setting.

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

Table 5: Differences between SGM on Euclidean spaces and RSGM on manifolds.

- Scalable, flexible, broadly applicable (sphere, $\mathrm{SO}(3)$, hyperbolic space).

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