Riemannian Continuous Normalizing Flows

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Abstract

Normalizing flows have shown great promise for modelling flexible probability distributions in a computationally tractable way. However, whilst data is often naturally described on Riemannian manifolds such as spheres, torii, and hyperbolic spaces, most normalizing flows implicitly assume a flat geometry, making them either misspecified or ill-suited in these situations. To overcome this problem, we introduce Riemannian continuous normalizing flows, a model which admits the parametrization of flexible probability measures on smooth manifolds by defining flows as the solution to ordinary differential equations. We show that this approach can lead to substantial improvements on both synthetic and real-world data when compared to standard flows or previously introduced projected flows.

1 Introduction

Learning well-specified probabilistic models is at the heart of many problems in machine learning and statistics. Much focus has therefore been placed on developing methods for modelling and inferring expressive probability distributions. Normalizing flows (Rezende and Mohamed, 2016) have shown great promise for this task as they provide a general and extensible framework for modelling highly complex and multimodal distributions (Papamakarios et al., 2019).

An orthogonal but equally important aspect of well-specified models is to correctly characterize the geometry which describes the proximity of data points. Riemannian manifolds provide a general framework for this purpose and are a natural approach to model tasks in many scientific fields ranging from earth and climate science to biology and computer vision. For instance, storm trajectories may be modelled as paths on the sphere (Karpatne et al., 2017), the shape of proteins can be parametrized using tori (Hamelryck et al., 2006), cell developmental processes can be described through paths in hyperbolic space (Klimovksaia et al., 2019), and human actions can be recognized in video using matrix manifolds (Lui, 2012). If appropriately chosen, manifold-informed methods can lead to improved sample complexity and generalization, improved fit in the low parameter regime, and guide inference methods to interpretable models. They can also be understood as a geometric prior that encodes a practitioner’s assumption about the data and imposes an inductive bias.

However, conventional normalizing flows are not readily applicable to such manifold-valued data since their implicit Euclidean assumption makes them unaware of the underlying geometry or borders of the manifold. As a result they would yield distributions having some or all of their mass lying

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outside the manifold, rendering them ill-suited or even misspecified so that central concepts like the reverse Kullback-Leibler (KL) divergence would not even be defined.

In this work, we propose a principled way to combine both of these aspects and parametrize flexible probability distributions on Riemannian manifolds. Specifically, we introduce Riemannian continuous normalizing flows in which flows are defined via vector fields on manifolds and computed as the solution to the associated ordinary differential equation (ODE) (see Figure 1 for an illustration). Intuitively, our method operates by first parametrizing a vector field on the manifold with a neural network, then sampling particles from a base distribution, and finally approximating their flow along the vector field using a numerical solver. Both the neural network and the solver are aware of the underlying geometry which ensures that the flow is always located on the manifold – yielding a Riemannian method.

This approach allows us to combine multiple important advantages. One major challenge of normalizing flows lies in designing transformations that enable efficient sampling and density computation. By basing our approach on continuous normalizing flows (CNFs) (Chen et al., 2019; Grathwohl et al., 2018; Salman et al., 2018) we avoid strong structural constraints to be imposed on the flow, as is the case for most discrete normalizing flows. Such unconstrained free-form flows have empirically been shown to be highly expressive (Chen et al., 2020; Grathwohl et al., 2018). Moreover, projected methods require a differentiable mapping from a Euclidean space to the manifold, yet such a function cannot be bijective, which in turn leads to numerical challenges. By taking a Riemannian approach, our method is more versatile since it does not rely on an ad-hoc projection map and simultaneously reduces numerical artefacts that interfere with training. To the best of our knowledge, our method is the first to combine these properties as existing methods for normalizing flows on manifolds are either discrete (Bose et al., 2020; Rezende et al., 2020), projected (Gemici et al., 2016; Falorsi et al., 2019; Bose et al., 2020) or manifold-specific (Sei, 2011; Bose et al., 2020; Rezende et al., 2020).

We empirically demonstrate the advantages of our method on constant curvature manifolds – i.e., the Poincaré disk and the sphere – and show the benefits of the proposed approach compared to non-Riemannian and projected methods for maximum likelihood estimation and reverse KL minimization. We also apply our method to density estimation on earth-sciences data (e.g., locations of earthquakes, floods and wildfires) and show that it yields better generalization performance and faster convergence.

## 2 Continuous Normalizing Flows on Riemannian Manifolds

Normalizing flows operate by pushing a simple base distribution through a series of parametrized invertible maps, referred as the flow. This can yield a highly complex and multimodal distribution which is typically assumed to live in a Euclidean vector space. Here, we propose a principled approach to extend normalizing flows to manifold-valued data, i.e. Riemannian continuous normalizing flows (RCNFs). Following CNFs (Chen et al., 2019; Grathwohl et al., 2018; Salman et al., 2018) we define manifold flows as the solutions to ODEs. The high-level idea is to parametrize flows through the time-evolution of manifold-valued particles $z$ – in particular via their velocity $\dot{z}(t) = \mathbf{f}_\theta(z(t), t)$ where $\mathbf{f}_\theta$ denotes a vector field. Particles are first sampled from a simple base distribution, and then their evolution is integrated by a manifold-aware numerical solver, yielding a new complex multimodal distribution of the particles. This Riemannian and continuous approach has the advantages of allowing almost free-form neural networks and of not requiring any mapping from a Euclidean space which would potentially lead to numerical challenges.

For practical purposes, we focus our theoretical and experimental discussion on constant curvature manifolds (see Table 1). In addition to being widely used in the literature (Nickel and Kiela, 2017; Davidson et al., 2018; Mardia and Jupp, 2000; Hasnat et al., 2017), these manifolds are convenient to work with since most related geometrical quantities are available in closed-form. However, our proposed approach is generic and could be used on a broad class of manifolds such as product

| Geometry   | Model                  | Curvature | Coordinates       | $\sqrt{\det g} = d \text{Vol} / d \text{Leb}_g$ | Compact |
|------------|------------------------|-----------|-------------------|----------------------------------------------|---------|
| Euclidean  | $\mathbb{R}^d$         | $K = 0$   | Cartesian $z$     | 1                                            | No      |
| Hyperbolic | $\mathbb{H}^d_k$       | $K < 0$   | Cartesian $z$     | $(2 \cdot 1 + K \|z\|^2)^d$                   | No      |
| Elliptic   | $\mathbb{S}^d_k$      | $K > 0$   | n-spherical $\varphi$ | $K^{-\frac{d}{2 \cdot (d-1)}} \prod_{i=1}^{d-1} \sin(\varphi)\varphi^{d-i-1}$ | Yes     |
and matrix manifolds like torii and Grassmannians. For a brief overview of relevant concepts in Riemannian geometry please see Appendix A.1 or Lee (2003) for a more thorough introduction.

In the following, we develop the key components which allow us to define continuous normalizing flows that are aware of the underlying Riemannian geometry: flow, likelihood, and vector field.

**Vector flows** Flows in conventional normalizing flows are defined as smooth mappings $\phi : \mathbb{R}^d \to \mathbb{R}^d$ which transform a base distribution $z \sim P_0$ into a complex distribution $P_\theta$. For normalizing flows to be well-behaved and convenient to work with, the flow is required to be bijective and differentiable which introduces significant structural constraints on $\phi$. Continuous normalizing flows overcome this issue by defining the flow $\phi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$ generated by an ordinary differential equation, allowing for unrestricted neural network architectures. Here we show how vector fields can be used to define similar flows $\phi : M \times \mathbb{R} \to M$ on general Riemannian manifolds.

Consider the temporal evolution of a particle $z(t)$ lying on a $d$-dimensional manifold $M$, whose velocity is given by a vector field $f_\theta(z(t), t)$. Intuitively, $f_\theta(z(t), t)$ indicates the direction and speed along which the particle is moving on the manifold’s surface. Classic examples for such vector fields include weathercocks giving wind direction and compasses pointing toward the magnetic north pole of the earth. Formally, let $T_z M$ denote the tangent space at $z$ and $TM = \cap_{x \in M} T_z M$ the associated tangent bundle. Furthermore, let $f_\theta : M \times \mathbb{R} \to TM$ denote a vector field on $M$. The particle’s time-evolution according to $f_\theta$ is then given by the following ODE:

$$\frac{dz(t)}{dt} = f_\theta(z(t), t). \quad (1)$$

To transform a base distribution using this vector field, we are then interested in a particle’s position after time $t$. When starting at an initial position $z(0) = z_0$, the flow operator $\phi : M \times \mathbb{R} \to M$ gives the particle’s position at any time $t$ as $z(t) = \phi(z_0, t)$. Leveraging the fundamental theorem of flows (Lee, 2003), we can show that under mild conditions, this flow is bijective and differentiable. We write $C^1$ for the set of differentiable functions whose derivative are continuous.

**Proposition 1** (Vector flows). Let $M$ be a smooth complete manifold. Furthermore, let $f_\theta$ be a $C^1$-bounded time-dependent vector field. Then there exists a global flow $\phi : M \times \mathbb{R} \to M$ such that for each $t \in \mathbb{R}$, the map $\phi(\cdot, t) : M \to M$ is a $C^1$-diffeomorphism (i.e. $C^1$ bijection with $C^1$ inverse).

*Proof.* See Appendix E.1 for a detailed derivation. \qed

Note that scaling the vector field as $f_\theta^\alpha = \alpha f_\theta$ results in a time-scaled flow $\phi^\alpha(z, t) = \phi(z, \alpha t)$. The integration duration $t$ is therefore arbitrary. Without loss of generality we set $t = 1$ and write $\phi = \phi(\cdot, 1)$. Concerning the evaluation of the flow $\phi$, it generally does not accept a closed-form solution and thus requires to be approximated numerically. To this extent we rely on an explicit Runge-Kutta (RK) integrator of order 4. However, standard integrators used in CNFs generally do not preserve manifold constraints (Hairer, 2006). To overcome this issue we rely on a projective RK4 solver (Hairer, 2011). This solver works by conveniently solving the ODE in the ambient Cartesian coordinates and projecting each step onto the manifold. Projections onto $\mathbb{S}^d$ are computationally cheap since they amount to $l^2$ norm divisions. No projection is required for the Poincaré ball.

**Likelihood** Having a flow at hand, we are now interested in evaluating the likelihood of our pushforward model $P_\theta = \phi_\theta P_0$. Here, the pushforward operator $\#$ indicates that one obtains samples $z \sim \phi_\theta P_0$ as $z = \phi(z_0)$ with $z_0 \sim P_0$. For this purpose, we derive in the following the change in density in terms of the geometry of the manifold and show how to efficiently estimate the likelihood.

**Change in density** In normalizing flows, we can compute the likelihood of a sample via the change in density from the base distribution to the pushforward. Applying the chain rule we get

$$\log p_\theta(z) - \log p_0(z_0) = \log \left| \det \frac{\partial \phi^{-1}(z)}{\partial z} \right| = - \log \left| \det \frac{\partial \phi(z_0)}{\partial z} \right|. \quad (2)$$

In general, computing the Jacobian’s determinant of the flow is challenging since it requires $d$ reverse-mode automatic differentiations to obtain the full Jacobian matrix, and $O(d^3)$ operations to compute its determinant. CNFs side step direct computation of the determinant by leveraging the time-continuity of the flow and re-expressing Equation 2 as the integral of the instantaneous change in log density $\int_0^t \frac{\partial \log p_\theta(z(t))}{\partial t} \, dt$. However, standard CNFs make an implicit Euclidean assumption to
compute this quantity which is violated for general Riemannian manifolds. To overcome this issue we express the instantaneous change in log-density in terms of the determinant of the Jacobian matrix of geodesic hyperplanes $H$ are parametrized by decision boundaries manifolds, and can be seen as computing distances to geodesic distance layer $a$. To inform the neural network about the geometry of the manifold we make use of specific input and output field has a direct impact on the expressiveness of the distribution and is thus crucially important. In order to take into account these geometrical properties we make use of specific input and output.

Estimating the divergence Even though the determinant of Equation 2 has been replaced in Equation 3 by a trace operator with lower computational complexity, we still need to compute the full vector-Jacobian product can be computed through backward auto-differentiation.

Proof. For a detailed derivation of Equation 3 see Appendix C.

Note that in the Euclidean setting $\sqrt{|G(z)|} = 1$ thus the second term of Equation 4 vanishes and we recover the formula from Grathwohl et al. (2018); Chen et al. (2019).

Choice of base distribution $P_0$ The closer the initial base distribution is to the target distribution, the easier the learning task should be. However, it is challenging in practice to incorporate such prior knowledge. We consequently use a uniform distribution on $S^d$ since it is the most "uncertain" distribution. For the Poincaré ball $B^d$, we rely on a standard wrapped Gaussian distribution $N^W$ (Nagano et al., 2019; Mathieu et al., 2019) because it is convenient to work with.

Vector field Finally, we discuss the form of the vector field $f_\theta : \mathcal{M} \times \mathbb{R} \to \mathcal{T} \mathcal{M}$ which generates the flow $\phi$ used to pushforward samples. We parametrize $f_\theta$ via a feed-forward neural network which takes as input manifold-valued particles, and outputs their velocities. The architecture of the vector field has a direct impact on the expressiveness of the distribution and is thus crucially important. In order to take into account these geometrical properties we make use of specific input and output layers that we describe below. The rest of the architecture is based on a multilayer perceptron.

Input layer To inform the neural network about the geometry of the manifold $\mathcal{M}$, we use as first layer a geodesic distance layer (Ganea et al., 2018; Mathieu et al., 2019) which generalizes linear layers to manifolds, and can be seen as computing distances to decision boundaries on $\mathcal{M}$. These boundaries are parametrized by geodesic hyperplanes $H_u$, and the associated neurons $h_w(z) \propto d_M(z, H_w)$, with $d_M$ being the geodesic distance. Horizontally stacking several of these neurons makes a geodesic distance layer. We refer to Appendix E.2 for more details.
Output layer To constrain the neural net to $\mathcal{TM}$, we output vectors in $\mathbb{R}^{d+1}$ when $\mathcal{M} = S^d$, before projecting them to the tangent space i.e. $f_\theta(z) = \text{proj} \mathcal{TM}_\mu \text{neural\_net}(z)$. This is not necessary in $\mathbb{R}^d$ since the ambient space is of equal dimension. Yet, velocities scale as $\|f_\theta(z)\|_2 = |G(z)|^{1/2} \|f_\theta(z)\|_2$, hence we scale the $\text{neural\_net}(z)$ by $|G(z)|^{-1/2}$ s.t. $\|f_\theta(z)\|_2 = \|\text{neural\_net}(z)\|_2$.

Regularity For the flow to be bijective, the vector field $f_\theta$ is required to be $C^1$ and bounded (cf Proposition 1). The boundness and smoothness conditions can be satisfied by relying on bounded smooth non-linearities in $f_\theta$ such as tanh, along with bounded weight and bias at the last layer.

Training In density estimation and inference tasks, one aims to learn a model $P_\theta$ with parameters $\theta$ by minimising a divergence $L(\theta) = D(P_D \| P_\theta)$ w.r.t. a target distribution $P_D$. In our case, the parameters $\theta$ refer to the parameters of the vector field $f_\theta$. We minimize the loss $L(\theta)$ using first-order stochastic optimization, which requires Monte Carlo estimates of loss gradients $\nabla_\theta L(\theta)$. We back-propagate gradients through the explicit solver with $O(1/h)$ memory cost, $h$ being the step size. When the loss $L(\theta)$ is expressed as an expectation over the model $P_\theta$, as in the reverse KL divergence, we rely on the reparametrization trick (Kingma and Welling, 2014; Rezende et al., 2014). In our experiments we will consider both the negative log-likelihood and reverse KL objectives

$$L^{\text{Like}}(\theta) = -E_{z \sim P_D}[\log p_\theta(z)] \text{ and } L^{\text{KL}}(\theta) = D_{\text{KL}}(P_\theta \| P_D) = E_{z \sim P_\theta}[\log p_\theta(z) - \log p_D(z)] \quad (6)$$

Additionally, regularization terms can be added in the hope of improving training and generalization. See Appendix D for a discussion and connections to the dynamical formulation of optimal transport.

3 Related work

Here we discuss previous work that introduced normalizing flows on manifolds. For clarity we split these into projected vs Riemannian methods which we describe below.

Projected methods These methods consist in parametrizing a normalizing flow on $\mathbb{R}^d$ and then pushing-forward the resulting distribution along an invertible map $\psi : \mathbb{R}^d \rightarrow \mathcal{M}$. Yet, the existence of such an invertible map is equivalent to $\mathcal{M}$ being homeomorphic to $\mathbb{R}^d$ (e.g. being “flat”), hence limiting the scope of that approach. Moreover there is no principled way to choose such a map, and different choices lead to different numerical or computational challenges which we discuss below.

Exponential map The first generic projected map that comes to mind in this setting is the exponential map $\exp : T\mu \mathcal{M} \cong \mathbb{R}^d \rightarrow \mathcal{M}$, which parameterizes geodesics starting from $\mu$ with velocity $v \in T\mu \mathcal{M}$. This leads to so called wrapped distributions $P^W_\theta = \exp_{\mu^\theta} P$, with $P$ a probability measure on $\mathbb{R}^d$. This approach has been taken by Falorsi et al. (2019) to parametrize probability distributions on Lie groups. Yet, in compact manifolds – such as spheres or the SO(3) group – computing the density of wrapped distributions requires an infinite summation, which in practice needs to be truncated. This is not the case however on hyperbolic spaces (like the Poincaré ball) since the exponential map is bijective on these manifolds. This approach has been proposed in Bose et al. (2020) where they extend Real-NVP (Dinh et al., 2017) to the hyperboloid model of hyperbolic geometry. In addition to this wrapped Real-NVP, they also introduced a hybrid coupling model which is empirically shown to be more expressive. We note however that the exponential map is believed to be “badly behaved” away from the origin (Dooley and Wildberger, 1993; Al-Mohy and Higham, 2010).

Stereographic map Alternatively to the exponential map, Gemici et al. (2016) proposed to parametrize probability distributions on $S^d$ via the stereographic projection defined as $\rho(z) = z_{2:d} / (1 + z_1)$ with projection point $-\mu_0 = (-1, 0, \ldots, 0)$. Gemici et al. then push a probability measure $P$ defined on $\mathbb{R}^d$ along the inverse of the stereographic map $\rho$, yielding $P^S_\theta = \rho^{-1}_\theta P$. However, the stereographic map $\rho$ is not injective, and projects $-\mu_0$ to $\infty$. This implies that spherical points close to the projection point $-\mu_0$ are mapped far away from the origin of the plane. Modelling probability distributions with mass close to $-\mu_0$ may consequently be numerically challenging since the norm of the Euclidean flow would explode. Similarly, Rezende et al. (2020) introduced flows on hyperspheres and tori by using the inverse tangent function. Although this method is empirically shown to perform well, it similarly suffers from numerical instabilities near singularity points.
Riemannian methods In contrast to projected methods which rely on mapping the manifold to a Euclidean space, Riemannian methods do not. As a consequence they side-step any artefact or numerical instability arising from the manifold’s projection. Early work (Sei, 2011) proposed transformations along geodesics on the hypersphere by evaluating the exponential map at the gradient of a scalar manifold function. Recently, Rezende et al. (2020) introduced ad-hoc discrete Riemannian flows for hyperspheres and torii based on Möbius transformations and spherical splines. We contribute to this line of work by introducing continuous flows on general Riemannian manifolds. In contrast to discrete flows (e.g. Bose et al., 2020; Rezende et al., 2020), time-continuous flows as ours alleviate strong structural constraints on the flow by implicitly parametrizing it as the solution to an ODE (Grathwohl et al., 2018). Additionally, recent and concurrent work (Lou et al., 2020; Falorsi and Forré, 2020) proposed to extend neural ODEs to smooth manifolds.

4 Experimental results

We evaluate the empirical performance of the above-mentioned models on hyperbolic and spherical geometry. We will first demonstrate the advantages of our approach on synthetic datasets which illustrate failure modes of naive and projected methods. We will then show that these advantages also translate to substantial gains on real world datasets. For all projected models (e.g. stereographic and wrapped cf Section 3), the vector field’s architecture is chosen to be a multilayer perceptron as in Grathwohl et al. (2018), whilst the architecture described in Section 2 is used for our Riemannian (continuous normalizing flow) model. For fair comparisons, we also parametrize projected models with a CNF. Also, all models are chosen to have approximately the same number of parameters. All models were implemented in PyTorch (Paszke et al., 2017) and trained by stochastic optimization with Adam (Kingma and Ba, 2015). All 95% confidence intervals are computed over 12 runs. Please refer to Appendix G for full experimental details. We will shortly open-source our code for reproducibility.

Hyperbolic geometry and limits of conventional and wrapped methods First, we aim to show that conventional normalizing flows are ill-suited for modelling target manifold distributions. These are blind to the geometry, so we expect them to behave poorly when the target is located where the manifold behaves most differently from a Euclidean space. We refer to such models as naive and discuss their properties in more detail in Appendix B.1. Second, we wish to inspect the behaviour of wrapped models (see Section 3) when the target is away from the exponential map origin.

To this extent we parametrize a wrapped Gaussian target distribution \( \mathcal{N}^W(\exp_\mu(\alpha \delta x), \Sigma) = \exp_{\mu_\Sigma} \mathcal{N}(\alpha \delta x, \Sigma) \) defined on the Poincaré disk \( \mathbb{B}^2 \) (Nagano et al., 2019; Mathieu et al., 2019).
We neither included the naive model and a wrapped model. The base distribution $P_0$ is a standard Gaussian for the naive and wrapped models, and a standard wrapped Gaussian for the Riemannian model. Models are trained by maximum likelihood until convergence. It can be seen from Figure 4 that the Riemannian model indeed outperforms the naive and wrapped models as we increase the values of $\alpha$—i.e., the closer we move to the boundary of the disk. Figure 2 shows that qualitatively the naive and wrapped models seem to indeed fail to properly fit the target when it is located far from the origin. Additionally, we assess the architectural choice of the vector field used in our Riemannian model. In particular, we conduct an ablation study on the rescaling of the output layer, by training for 10 iterations a rescaled and an unscaled version of our model. Figure 3 shows that the number of function evaluations (NFE) tends to be large and sometimes even dramatically diverges when the vector field’s output is unscaled. In addition to increasing the computational cost, this in turns appears to worsen the convergence’s speed of the model. This further illustrates the benefits of our vector field parameterization.

**Spherical geometry and limits of the stereographic projection model** Next, we evaluate the ability of our model and the stereographic projection model from Section 3 to approximate distributions on the sphere which are located around the projection point $-\mu_0$. We empirically assess this phenomenon by choosing the target distribution to be a Von-Mises Fisher (Downs, 1972) distribution $\text{vMF}(\mu, \kappa)$ located at $\mu = -\mu_0$, and with concentration $\kappa$ (which decreases with the variance). Along with the stereographic projection method, we also consider our Riemannian model from Section 2. We neither included the naive model since it is misspecified here (leading to an undefined reverse KL divergence), nor the wrapped model as computing its density requires an infinite summation (see Section 3). The base distribution $P_0$ is chosen to be a standard Gaussian on $\mathbb{R}^2$ for the stereographic model and a uniform distribution on $\mathbb{S}^2$ for the Riemannian model. The performance of these two models is quantitatively assessed on both the negative log-likelihood and reverse KL criteria.

Figure 5 shows densities of the target distribution along with the base and learned distributions. We observe that the stereographic model fails to push mass close enough to the singularity point $-\mu_0$, as opposed to the Riemannian model which perfectly fits the target. Table 2 shows the negative log-likelihood and reverse KL losses of both models when varying the concentration parameter $\kappa$ of the vMF target. The larger the concentration $\kappa$ is, the closer to the singularity point $-\mu_0$ the target’s mass gets. We observe that the Riemannian model outperforms the stereographic one to fit the target for both objectives, although this performance gap shrinks as the concentration gets smaller. Also, we believe that the gap in performance is particularly large for the log-likelihood objective because it heavily penalizes models that fail to cover the support of the target. When the vMF target is located away from the singularity point, we noted that both models were performing similarly well.

**Density estimation of spherical data** Finally, we aim to measure the expressiveness and modelling capabilities of our method on real world datasets. To this extent, we gathered four earth location datasets, representing respectively volcano eruptions (NOAA, 2020b), earthquakes (NOAA, 2020a), floods (Brakenridge, 2017) and wild fires (EOSDIS, 2020). We approximate the earth’s surface (and thus also these data points) as a perfect sphere. In our experiments, we split datasets randomly into

| Loss   | model $\kappa$  | Stereographic | Riemannian |
|--------|----------------|---------------|------------|
| $L_{\text{Like}}$ | 100    | 92.41±35.75   | -1.80±0.00 |
|        | 50      | 15.94±13.2    | -1.11±0.00 |
|        | 10      | 1.48±0.46     | 0.50±0.00  |
| $L_{\text{KL}}$ | 100    | 1.10±0.14     | 0.02±0.01  |
|        | 50      | 0.47±0.04     | 0.02±0.00  |
|        | 10      | 0.11±0.00     | 0.00±0.00  |

Table 2: Performance of continuous flows on $\mathbb{S}^2$ with $\text{vMF}(\mu = -\mu_0, \kappa = 10)$. When models perfectly fit the target $P_D$, then $L_{\text{like}} = \mathbb{I}[P_D]$, which decreases with $\kappa$, explaining $L_{\text{like}}$’s results for the Riemannian model.
Table 3: Negative test log-likelihood of continuous normalizing flows on $S^2$ datasets.

|                      | Volcano | Earthquake | Flood | Fire  |
|----------------------|---------|------------|-------|-------|
| Stereographic        | -0.54±0.14 | 0.34±0.04 | 0.96±0.05 | -0.50±0.04 |
| Riemannian           | -0.92±0.15 | 0.07±0.06 | 0.75±0.06 | -0.84±0.08 |

Learning curves

Data size

|     | 829  | 6124 | 4877 | 12810 |

Figure 6: Density estimation for earth sciences data. Blue and red dots represent training and testing datapoints, respectively. Heatmaps depict the log-likelihood of the trained models.

training and testing datasets, and fit our Riemannian model and the stereographic projection baseline by maximum likelihood estimation on the training dataset.

We observe from Table 3 that for all datasets, the Riemannian model outperforms its stereographic competitor by a large margin. It can also be seen from the learning curves that the Riemannian model converges faster. Figure 6 shows the learned spherical distributions along with the training and testing datasets. We note that qualitatively the stereographic distribution is generally more diffuse than its Riemannian counterpart. It also appears to allocate some of its mass outside the target support, and to cover less of the data points. Additional figures are shown in Appendix H.

5 Discussion

In this paper we proposed a principled way to parametrize expressive probability distributions on Riemannian manifolds. Specifically, we introduced Riemannian continuous normalizing flows in which flows are defined via vector fields on manifolds and computed as the solution to the associated ODE. We empirically demonstrated that this method can yield substantial improvements when modelling data on constant curvature manifolds compared to conventional or projected flows.
Broader impact

The work presented in this paper focuses on the learning of well-specified probabilistic models for manifold-valued data. Consequently, its applications are especially promising to advance scientific understanding in fields such as earth and climate science, computational biology, and computer vision. As a foundational method, our work inherits the broader ethical aspects and future societal consequences of machine learning in general.

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Appendix
Riemannian Continuous Normalizing Flows

A Constant curvature manifolds

In the following, we provide a brief overview of Riemannian geometry and constant curvature manifolds, specifically the Poincaré ball and the hypersphere models. We will use $||\cdot||$ and $\langle\cdot,\cdot\rangle$ to denote the Euclidean norm and inner product. For norms and inner products on tangent spaces $T_zM$, we write $||\cdot||_z$ and $\langle\cdot,\cdot\rangle_z$ where $z \in M$.

A.1 Review of Riemannian geometry

A real, smooth manifold $M$ is a set of points $z$, which is "locally similar" to a linear space. For every point $z$ of the manifold $M$ is attached a real vector space of the same dimensionality as $M$ called the tangent space $T_zM$. Intuitively, it contains all the possible directions in which one can tangentially pass through $z$. Taking the disjoint union of all tangent spaces yields the tangent bundle $TM = \bigcup_{z \in M} T_zM$. For each point $z$ of the manifold, the metric tensor $g(z)$ defines an inner product on the associated tangent space as $g(z) = \langle\cdot,\cdot\rangle_z : T_zM \times T_zM \to \mathbb{R}$. The matrix representation of the Riemannian metric $G(z)$, is defined such that

$$\forall u, v \in T_zM \times T_zM, \langle u, v \rangle_z = g(z)(u, v) = u^T G(z) v.$$  

A Riemannian manifold is then given as a tuple $(M, g)$ (Petersen, 2006). The metric tensor gives a local notion of angle, length of curves, surface area and volume, from which the Riemannian Continuous Normalizing Flows

A.2 The Poincaré ball model of hyperbolic geometry

In the following, we provide a brief overview of key concepts related to hyperbolic geometry. A $d$-dimensional hyperbolic space is a complete, simply connected, $d$-dimensional Riemannian manifold with constant negative curvature $K$. The Poincaré ball is one model of this geometry, and is formally defined as the Riemannian manifold $\mathbb{H}^d_K = (B^d_K, g_K)$. Here $B^d_K$ denotes the open ball of radius $1/\sqrt{|K|}$, and $g_K$ the metric tensor $g_K(z) = (\Lambda^2 z)^2 g^e(z)$, where $\Lambda^2 z = 2z / \sqrt{1 + K|z|^2}$ and $g^e$ denotes the Euclidean metric tensor, i.e. the usual dot product. The induced invariant measure $Vol$ is absolutely continuous with respect to the Lebesgue measure $Leb$, and its density is given by $dVol_{\mathbb{H}^d_K}(z) = \sqrt{|G(z)|} = (\Lambda^2 z)^d$ for all $z \in \mathbb{H}^d_K$. As motivated by Skopek et al. (2019), the Poincaré ball $\mathbb{H}^d_K$ can conveniently be described through the formalism of gyrovector spaces (Ungar, 2008). These can be seen as an analogy to the way vector spaces are used in Euclidean geometry, but in the non-Euclidean geometry setting. In
particular, the Möbius addition \( \oplus_K \) of \( z, y \) in \( \mathbb{R}^d_K \) is defined as
\[
z \oplus_K y = \frac{(1 - 2K \langle z, y \rangle - K\|y\|^2)z + (1 + K\|z\|^2)y}{1 - 2K \langle z, y \rangle + K^2\|z\|^2\|y\|^2}.
\]
Then the exponential map can be expressed via this Möbius addition as
\[
\exp^K_z(v) = z \oplus_K \left( \tanh \left( \sqrt{-K} \frac{\|v\|}{2} \right) \frac{v}{\sqrt{-K\|v\|}} \right)
\]
where \( x = -z \oplus_K y \) for all \( x, y \in \mathbb{R}^d_K \).

### A.3 The hypersphere model of elliptic geometry

In the following, we discuss key concepts related to positively curved spaces known as elliptic spaces, and in particular to the hypersphere model. The d-sphere, or hypersphere, is a compact submanifold of \( \mathbb{R}^{d+1} \) with positive constant curvature \( K \) whose support is defined by \( S^d_K = \{ z \in \mathbb{R}^{d+1} \mid \langle z, z \rangle = 1/K \} \). It is endowed with the pull-back metric of the ambient Euclidean space.

**Sphere** In the two-dimensional setting \( d = 2 \), we rely on polar coordinates to parametrize the sphere \( S^2 \). These coordinates consist of polar \( \theta \in [0, \pi] \) and azimuth \( \varphi \in [0, 2\pi] \) angles. The ambient Cartesian coordinates are then given by \( \tau(\theta, \varphi) = (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi), \cos(\theta)) \). We have \( \sqrt{G(\theta, \varphi)} = \sin(\theta) \). Applying the generic divergence formula (see Equation 10) yields the celebrated spherical divergence formula
\[
\text{div}(g) = \frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left( \frac{\sin(\theta) g^\theta(\theta, \varphi)}{\sin(\theta)} \right) + \frac{1}{\sin(\theta)} \frac{\partial}{\partial \varphi} (g^\varphi(\theta, \varphi)).
\]

**Hypersphere** For higher dimensions, we can rely on the n-spherical coordinate system in which the coordinates consist of \( d - 1 \) angular coordinates \( \varphi_1, \ldots, \varphi_{d-2} \in [0, \pi] \) and \( \varphi_{d-2} \in [0, 2\pi] \) (Blumenson, 1960). Then we have \( \sqrt{G(\varphi)} = \sin^{d-2}(\varphi_1) \sin^{d-3}(\varphi_2) \ldots \sin(\varphi_{d-2}) \).

Using the ambient cartesian coordinates, the exponential map is given by
\[
\exp^\mu_z(v) = \cos \left( \sqrt{K}\|v\| \right) \mu + \sin \left( \sqrt{K}\|v\| \right) \frac{v}{\sqrt{K\|v\|}}
\]
for all \( z \in S^d_K \) and \( v \in T_z S^d_K \).

### B Probability measures on Riemannian manifolds

In what follows, we discuss core concepts of probability measures on Riemannian manifolds and show how naive methods lead to ill- and mis-specified models on manifolds.

Probability measures and random vectors can intrinsically be defined on Riemannian manifolds so as to model uncertainty on non-flat spaces (Pennec, 2006). The Riemannian metric \( G(z) \) induces an infinitesimal volume element on each tangent space \( \mathcal{T}_z \mathcal{M} \), and thus a measure on the manifold,
\[
d \text{Vol}(z) = \sqrt{|G(z)|} \ d\text{Leb},
\]
with \( \text{Leb} \) the Lebesgue measure. Manifold-valued random variables would naturally be characterized by the Radon-Nikodym derivative of a measure \( \nu \) w.r.t. the Riemannian measure \( \text{Vol} \) (assuming absolute continuity)
\[
p(z) = \frac{d\nu}{d\text{Vol}}(z).
\]

#### B.1 Ambient Euclidean probability distributions

Unfortunately, conventional probabilistic models implicitly assume a flat geometry. This in turn cause these models to either be misspecified or ill-suited to fit manifold distributions. Below we discuss the reasons why.
Let $P_D$ be a target probability measure that we aim to approximate, and which is defined on a $d$-dimensional manifold $M \subseteq \mathbb{R}^D$. Furthermore, we assume it admits a Radon-Nikodym derivative $p_D$ with respect to the manifold invariant measure Vol, denoting $P_D \ll \text{Vol}$ with $\ll$ denoting absolute continuity. Conventional normalizing flows implicitly assume the parametrized probability measure $P_\theta$ to have support on the ambient space $\mathbb{R}^D$ and to be absolutely continuous with respect to the Lebesgue measure $\text{Leb}_{\mathbb{R}^D}$. We denote its density by $p_\theta$.

Next, assume $D = d$, such as for $M = \mathbb{S}^d \subseteq \mathbb{R}^d$. With $z$ the $d$-dimensional Cartesian coordinates, we have $d\text{Vol}_{\mathbb{R}^d}(z) = |G(z)|$. One could then see the manifold-valued target $P_D$ as being a probability measure on $\mathbb{R}^d$ with a density w.r.t. the Lebesgue measure given by

$$\frac{dP_D}{d\text{Leb}_{\mathbb{R}^d}}(z) = p_D(z) \sqrt{|G(z)|} \equiv \hat{p}_D(z).$$

In general $P_D \ll P_\theta$ which implies that the forward Kullback-Leibler divergence, or negative log-likelihood up to constants, is defined and given by

$$\mathcal{L}^{\text{Like}}(\theta) = D_{\text{KL}}(P_D \parallel P_\theta) + \mathbb{E}_{P_D} \left[ \log \left( \frac{\hat{p}_D(z)}{p_\theta(z)} \right) \right] = -\mathbb{E}_{P_\theta} \left[ \log \frac{p_\theta(z)}{\sqrt{|G(z)|}} \right].$$

Minimising $\mathcal{L}^{\text{Like}}(\theta)$ amounts to pushing-forward $P_\theta$’s mass so that empirical observations $z_i \sim P_D$ have a positive likelihood under $P_\theta$. Yet, in general the model $(P_\theta)$ has (most of his) mass outside the manifold’s support which may cause such a naive approach to be ill-suited. More crucially it implies that in general the model’s mass is not covering the full target’s support. In that case, the reverse Kullback-Leibler divergence $D_{\text{KL}}(P_\theta \parallel P_D) = \mathcal{L}^{\text{Like}}(\theta)$ is not even defined.

Next, consider the case where $M$ is a submanifold embedded in $\mathbb{R}^D$ with $D > d$, such as $M = \mathbb{S}^d$ where $D = d + 1$. In this setting the naive model $P_\theta$ is even misspecified since it is defined on a different probability space than the target. In the limit $\text{supp}(P_\theta) \to M$, $P_\theta$ is not defined because we have that $\int_{\text{supp}(P_\theta)} P_\theta \to \infty$. The target does consequently not belong to the model’s class.

### C Instantaneous change of variable

In the following we derive the instantaneous change of density that a manifold-valued random variable induces when its dynamics are governed by an ODE. We show that in the Riemannian setting this instantaneous change of density can be expressed in terms of the manifold’s metric tensor.

**Proof of Proposition 2**

**Proof.** For a time dependant particles $z(t)$, whose dynamics are given by the following ODE

$$\frac{dz(t)}{dt} = f(z(t), t)$$

the change in density is given by the Liouville equation (or Fokker–Planck equation without the diffusion term); $\forall z \in M, \forall t \in [0, T]$

$$\frac{\partial}{\partial t} p(z, t) = -\text{div}(p(z, t)f(z, t))$$

$$= -\left( \frac{\partial}{\partial z} p(z, t), f(z, t) \right)_z \cdot p(z, t) \text{ div}(f(z, t))$$

where the last step was obtained by applying the divergence product rule. By introducing the time dependence in $z(t)$ and differentiating with respect to time we get

$$\frac{\partial}{\partial t} p(z(t), t) = \left( \frac{\partial}{\partial z} p(z(t), t), \frac{\partial}{\partial t} z(t) \right)_{z(t)} + \frac{\partial}{\partial t} p(z(t), t)$$

$$= \left( \frac{\partial}{\partial z} p(z(t), t), f(z(t), t) \right)_{z(t)} - \left( \frac{\partial}{\partial z} p(z(t), t), f(z(t), t) \right)_{z(t)} - p(z(t), t) \text{ div}(f(z(t), t))$$

$$= -p(z(t), t) \text{ div}(f(z(t), t))$$

Hence the evolution of the log density is given by

$$\frac{\partial}{\partial t} \log p(z(t), t) = -\text{div}(f(z(t), t)).$$

$\square$
Divergence computation  For a Riemannian manifold \((\mathcal{M}, g)\), with local coordinates \(z\), the divergence of a vector field \(f\) is given by

\[
\text{div}(f(z, t)) = \frac{1}{\sqrt{G(z)}} \sum_{i=1}^{d} \frac{\partial}{\partial z^i} \left( \sqrt{G(z)} | f^i(z, t) \right)
\]

We note that in Equation 8, \(f\) are the components of the vector field \(f\) with respect to the local unnormalized covariant basis \((e_i)_{i=1}^d = \left( \frac{\partial}{\partial z^i} \right)_{z^{i=1}}\). However it is convenient to work with local basis having unit length vectors. If we write \(\hat{e}_i\) for this normalized basis, and \(\hat{f}^i\) for the components of \(f\) with respect to this normalized basis, we have that

\[
f = \sum_i f^i e_i = \sum_i f^i |e_i|| \hat{e}_i | = \sum_i f^i \sqrt{G_{ii}} \frac{\hat{e}_i}{|\hat{e}_i|} = \sum_i \hat{f}^i \hat{e}_i
\]

using one of the properties of the metric tensor. By dotting both sides of the last equality with the contravariant element \(\hat{e}_i\) we get that \(\hat{f}^i = f^i \sqrt{G_{ii}}\). Substituting in Equation 8 yields

\[
\text{div} \left( \hat{f}(z, t) \right) = \frac{1}{\sqrt{G(z)}} \sum_{i=1}^{d} \frac{\partial}{\partial z^i} \left( \sqrt{G(z)} \hat{f}^i(z, t) \right).
\]

Combining Equations 7 and 10 and we finally get

\[
\frac{\partial \log p(z(t), t)}{\partial t} = -\frac{1}{\sqrt{G(z)}} \sum_{i=1}^{d} \frac{\partial}{\partial z^i} \left( \sqrt{\frac{G(z)}{G_{ii}(z)}} \hat{f}^i(z, t) \right).
\]

We rely on this Equation 11 for practical numerical experiments.

\section{D regularization}

\subsection{\(L^2\)-norm}

Henceforth we motivate the use of an \(L^2\) norm regularization in the context of continuous normalizing flows. We do so by highlighting a connection with the dynamical formulation of optimal transport, and by proving that this formulation still holds in the manifold setting.

\textbf{Monge-Kantorovich mass transfer problem}  Let \((\mathcal{M}, d_M)\) be a metric space, and \(c : \mathcal{M} \times \mathcal{M} \to [0, \infty)\) a measurable map. Given probability measures \(p_0\) and \(p_T\) on \(\mathcal{M}\), Monge’s formulation of the optimal transportation problem is to find a transport map \(\phi^* : \mathcal{M} \to \mathcal{M}\) that realizes the infimum

\[
\inf_{\phi} \int_{\mathcal{M}} c(\phi(z), z) p_0(dz) \text{ s.t. } p_T \# = p_0.
\]

It can be shown that this yields a metric on probability measures, and for \(c = d_M^2\), it is called the \(L^2\) Kantorovich (or Wasserstein) distance

\[
d_W(p_0, p_T)^2 = \inf_{\phi} \int_{\mathcal{M}} d_M(\phi(z), z)^2 p_0(dz).
\]

By reintroducing the time variable in the \(L^2\) Monge-Kantorovich mass transfer problem, the optimal transport map \(\phi^*\) can be reformulated as the generated flow from an optimal vector field \(f\).
We have

\[ \phi \]

This has been observed in the Euclidean setting by Finlay et al. (2020). They empirically showed that additionally regularizing the Frobenius norm of the vector field’s Jacobian helps. In particular, regularizing the vector field with the RHS of Equation 13 would hence tend to make \( \phi \) have constant velocity.

\[ \text{The RHS of Equation (13) can then be approximated with no extra-cost with a Monte Carlo estimator of } f \text{ estimator’s variance perspective.} \]

in the following subsection we remind that this regularization term can also be motivated from an

\[ \text{potential } h \text{ transport map moments and } p \text{ manifold with no boundary and } d \]

\[ \text{Let’s now focus on the setting where } M \text{ is a Riemannian manifold.} \]

\[ \text{Proposition 4 (Optimal map (Ambrosio, 2003)). Assume that } M \text{ is a C}^3 \text{, complete Riemannian manifold with no boundary and } d_M \text{ is the Riemannian distance. If } p_0, p_T \text{ have finite second order moments and } p_0 \text{ is absolutely continuous with respect to } vol_M, \text{ then there exists a unique optimal transport map } \phi \text{ for the Monge-Kantorovich problem with cost } c = d_M^2. \text{ Moreover there exists a potential } h : M \mapsto \mathbb{R} \text{ such that } \]

\[ \phi^*(z) = \exp(-\nabla h(z)) \quad vol_M - a.e.. \]

Proposition 3 has been stated and proved for the case \( M = \mathbb{R}^d \). Below we extend the proof given by Benamou and Brenier (2000) for the manifold setting.

**Proof of Proposition 3.** We follow the same reasoning as the one developed for the Euclidean setting. Let’s first upper bound the Wasserstein distance, and then state the optimal flow which yields equality. We have

\[ \frac{1}{T} \int_0^T \int_M \| f(z, t) \|_z^2 p_0(dz) \, dt = \frac{1}{T} \int_0^T \int_M \| f(\phi(z, t), t) \|_z^2 p_0(dz) \, dt \]

\[ = \frac{1}{T} \int_0^T \int_M \left\| \frac{\partial}{\partial t} \phi(z, t) \right\|_z^2 p_0(dz) \, dt \]

\[ \geq \int_M d_M(\phi(z, T), \phi(z, 0))^2 p_0(dz) \, dt \]

\[ = \int_M d_M(\phi(z, T), z)^2 p_0(dz) \, dt \]

\[ \geq \int_M d_M(\phi(z, z), z)^2 p_0(dz) \, dt \]

\[ = d_W^2(p_0, p_T)^2. \]

Thus, the optimal choice of flow \( \phi \) is given by

\[ \phi(z, t) = \exp \left( \frac{t}{T} \log_\ast(\phi^*(z)) \right), \]

since \( \phi(z, 0) = z, \phi(z, T) = \phi^*(z) \) and

\[ \left\| \frac{\partial}{\partial t} \phi(z, t) \right\|_z = \left\| \frac{\partial}{\partial t} \phi(z, t = 0) \right\|_z = \left\| \log_\ast(\phi^*(z)) \right\|_z = d_M(\phi^*(z), z). \]

Note that the optimal flow from Equation 14 yields integral paths \( \gamma(t) = \phi(z, t) \) that are geodesics and have constant velocity.

**Motivation** Regularizing the vector field with the RHS of Equation 13 would hence tend to make the generated flow \( \phi_T \) closer to the optimal map \( \phi^* \). By doing so, one hopes to increase smoothness of \( f \) and consequently lower the solver NFE given a fixed tolerance.

This has been observed in the Euclidean setting by Finlay et al. (2020). They empirically showed that regularizing the loss of a CNF with the vector field’s \( L^1 \) norm improves training speed. Motivated by the successful use of gradient regularization (Novak et al., 2018; Drucker and Cun, 1992), they showed that additionally regularizing the Frobenius norm of the vector field’s Jacobian helps. In the following subsection we remind that this regularization term can also be motivated from an estimator’s variance perspective.
D.2 Frobenius norm

**Hutchinson’s estimator** Hutchinson’s estimator (Hutchinson, 1990) is a simple way to obtain a stochastic estimate of the trace of a matrix. Given a d-dimensional random vector \( \epsilon \sim p \) such that \( \mathbb{E}[\epsilon] = 0 \) and \( \text{Cov}(\epsilon) = I_d \), we have

\[
\text{tr}(A) = \mathbb{E}_{\epsilon \sim p}[\epsilon^T A \epsilon].
\]

Rademacher and Gaussian distributions have been used in practice. For a Rademacher, the variance is given by (Avron and Toledo, 2011)

\[
\forall \epsilon \sim p[\epsilon^T A \epsilon] = 2 \|A\|_F - 2 \sum_i A_{ii}^2,
\]

whereas for a Gaussian it is given by

\[
\forall \epsilon \sim p[\epsilon^T A \epsilon] = 2 \|A\|_F.
\]

**Divergence computation** As reminded in Appendix C by Equation 9, computing the vector field divergence \( \text{div}(f(z,t)) \) involves the computation of the trace of vector field’s Jacobian \( \text{tr} \left( \frac{\partial}{\partial z} f(z,t) \right) \).

As highlighted in Grathwohl et al. (2018); Salman et al. (2018), one can rely on the Hutchinson’s estimator to estimate this trace with \( A = \frac{\partial}{\partial z} f(z,t) \).

The variance of this estimator thus depends on the Frobenius norm of the vector’s field Jacobian \( \| \frac{\partial}{\partial z} f(z,t) \|_F \), as noted in Grathwohl et al. (2018). Regularizing this Jacobian should then improve training by reducing the variance of the divergence estimator.

E Vector flows and neural architecture

Hereafter we discuss about flows generated by vector fields, and neural architectural choices that we make for their parametrization. Properties of vector fields have direct consequences on the properties of the generated flow and in turn on the associated pushforward probability distributions. In particular we derive sufficient conditions on the flow so that it is *global*, i.e. is a bijection mapping the manifold to itself.

E.1 Existence and uniqueness of a global flow

We start by discussing about vector flows and sufficient conditions on their uniqueness and existence.

**Local flow** First we remind the Fundamental theorem of flows (Lee, 2003) which gives the existence and uniqueness of a smooth local flow.

**Proposition 5** (Fundamental theorem of flows). Let \( M \) be a smooth complete manifold with local coordinates \( z \). Let \( f_0 : M \times \mathbb{R} \mapsto TM \) a \( C^1 \) time-dependent vector field and \( z_0 \in M \). Then there exists an open interval \( I \) with \( 0 \in I \), an open subset \( U \subseteq M \) containing \( z_0 \), and a unique smooth map \( \phi : I \times U \mapsto M \) called local flow which satisfies the following properties. We write \( \phi_t(z) = \phi(z, t) \).

1. \( \frac{\partial}{\partial t} \phi(z, t) = f_0(\phi(z, t), t) \) for all \( z, t \in U \times I \), and \( \phi_0 = \text{id}_M \).
2. For each \( t \in I \), the map \( \phi_t : U \mapsto M \) is a local \( C^1 \)-diffeomorphism.

Note that with such assumptions, the existence and uniqueness of flows \( \phi_t \) are only *local*.

**Global flow** We would like the flow \( \phi \) to be defined for all times and on the whole manifold, i.e. a global flow \( \phi : \mathbb{R} \times M \mapsto M \). Fortunately, if \( M \) is compact (such as n-spheres and torii), then the flow is global (Lee, 2003). We show below that another sufficient condition for the flow to be global is that the vector field be bounded.

**Proposition 6** (Global Flow). Let \( M \) be a smooth complete manifold. Let \( f_0 : \mathbb{R} \times M \mapsto TM \) be a \( C^1 \) bounded time-dependent vector field. Then the domain of the flow \( \phi \) is \( \mathbb{R} \times M \), i.e. the flow is global.

**Corollary 6.1.** For each \( t \in \mathbb{R} \), the map \( \phi_t : M \mapsto M \) is a \( C^1 \)-diffeomorphism.
Proof of Proposition 6. Let \( c > 0 \) s.t. \( \|f\| < c \), and \( z_0 \in \mathcal{M} \) be an initial point. Proposition 5 gives the existence of an open interval \( I = (a, b) \), a neighbourhood \( U \) of \( z_0 \) and a local flow \( \phi : (a, b) \times U \to \mathcal{M} \).

We write \( \gamma = \phi(z_0, \cdot) \). The maximal interval of \( \gamma \) is \( (a, b) \), which means that \( \gamma \) cannot be extended outside \((a, b)\). Suppose that \( b < \infty \).

The integral path \( \gamma \) is Lipschitz continuous on \((a, b)\) since we have
\[
d_M(\gamma(t), \gamma(s)) \leq \int_s^t \|\gamma'(t)\| \, dt = \int_s^t \|f(\gamma(t), t)\| \, dt \leq c |t - s|
\]
for all \( s < t \in (a, b) \).

Let \((t_n)\) be a sequence in \((a, b)\) that converges to \( b \). Then since \((t_n)\) is a convergent sequence, it must also be a Cauchy sequence. Then \( \gamma(t_n) \) is also a Cauchy sequence by Equation 15. Since \( \mathcal{M} \) is geodesically complete, it follows by Hopf-Rinow theorem that \((\mathcal{M}, d_M)\) is complete, hence that \( \gamma(t_n) \) converges to a point \( p \in \mathcal{M} \).

Now suppose that \((s_n)\) is another sequence in \((a, b)\) that converges to \( b \). Then by Equation 15 \( \lim_{n \to \infty} d(\gamma(s_n), \gamma(t_n)) = 0 \), thus \( \gamma(s_n) \) also converges to \( \lim_{n \to \infty} \gamma(t_n) = p \). So for every sequence \((t_n)\) in \((a, b)\) that converges to \( b \), we have that \( \gamma(t_n) \) converges to \( p \). Therefore by the sequential criterion for limits, we have that \( \gamma \) has the limit \( p \) at the point \( b \). Therefore, define \( \gamma(b) = p \) and so \( \gamma \) is continuous at \( b \) which is a contradiction. \( \square \)

E.2 Geodesic distance layer

The expressiveness of CNFs directly depends on the expressiveness of the vector field and consequently on its architecture. Below we detail and motivate the use of a geodesic distance layer, as an input layer for the vector field neural architecture.

Linear layer A linear layer with one neuron can be written in the form \( h_{a,p}(z) = \langle a, z - p \rangle \), with orientation and offset parameters \( a, p \in \mathbb{R}^d \). Stacking \( l \) such neurons \( h \) yields a linear layer with width \( l \). This neuron can be rewritten in the form
\[
h_{a,p}(z) = \text{sign}(\langle a, z - p \rangle) \|a\| d_F(z, H^K_{a,p})
\]
where \( H_{a,p} = \{z \in \mathbb{R}^d \mid \langle a, z - p \rangle = 0\} = p + \|a\|^{-1} \) is the decision hyperplane. The third term is the distance between \( z \) and the decision hyperplane \( H^K_{a,p} \) and the first term refers to the side of \( H^K_{a,p} \) where \( z \) lies.

Poincaré ball Ganea et al. (2018) analogously introduced a neuron \( f^K_{a,p} : \mathbb{E}_K^d \to \mathbb{R}^p \) on the Poincaré ball,
\[
h^K_{a,p}(z) = \text{sign}\left(\langle a, \log^K_{p}(z) \rangle_p\right) \|a\|_p d^K(z, H^K_{a,p})
\]
with \( H^K_{a,p} = \{z \in \mathbb{E}_K^d \mid \langle a, \log^K_{p}(z) \rangle = 0\} = \exp^K_p(\|a\|) \). A closed-formed expression for the distance \( d^K(z, H^K_{a,p}) \) was also derived, \( d^K(z, H^K_{a,p}) = \frac{1}{\|K\|} \sinh^{-1}\left(\frac{\langle \log^K_{p}(z), a \rangle}{\|z - p\|_{\mathbb{E}_K^d}(\|a\|)}\right) \) in the Poincaré ball. To avoid an over-parametrization of the hyperplane, we set \( p = \exp_{\mathbb{E}_K}(a_0) \) and \( a = \Gamma_{p \to a_0}(a_0) \) with \( \Gamma \) parallel transport (under Levi-Civita connection). We observed that the term \( \|a\|_p \) from Equation 16 was sometimes causing numerical instabilities, and that when it was not it also did not improve performance. We consequently removed this scaling term. The hyperplane decision boundary \( H^K_{a,p} \) is called gyroplane and is a semi-hypersphere orthogonal to the Poincaré ball’s boundary.

Hypersphere In hyperspherical geometry, geodesics are great circles which can be parametrized by a vector \( w \in \mathbb{R}^{d+1} \) as \( H_w = \{z \in \mathbb{S}^d \mid \langle w, z \rangle = 0\} \). The geodesic distance between \( z \in \mathbb{S}^d \) and the hyperplane \( H_w \) is then given by
\[
d(z, H_w) = \sin^{-1}\left(\frac{\langle w, z \rangle}{\sqrt{\langle w, w \rangle}}\right).
\]
In a similar fashion, a neuron is now defined by
\[
h_w(z) = \|w\|_2 \sin^{-1}\left(\frac{\langle w, z \rangle}{\sqrt{\langle w, w \rangle}}\right).
\]
**Geodesic distance layer** One can then horizontally-stack \( l \) neurons to make a *geodesic distance* layer \( g : M \rightarrow \mathbb{R}^l \) (Mathieu et al., 2019). Any standard feed-forward neural network can then be vertically-stacked on top of this layer.

**F Extensions**

**F.1 Product of manifolds**

Having described CNFs for complete smooth manifolds in Section 2, we extend these for product manifolds \( M = M_1 \times \cdots \times M_k \). For instance a \( d \)-dimensional torus is defined as \( T^d = S^1 \times \cdots \times S^1 \).

Any density \( p_\theta(z_1, \ldots, z_K) \) can decomposed via the chain rule of probability as

\[
p_\theta(z_1, \ldots, z_K) = \prod_k p_\theta(k | z_1, \ldots, z_{k-1})
\]

where each conditional \( p_\theta(k | z_1, \ldots, z_{k-1}) \) is a density on \( M_k \). As suggested in Rezende et al. (2020), each conditional density can be implemented via a flow \( \phi_k : M_k \rightarrow M_k \) generated by a vector field \( f_k \), whose parameters \( \theta_k \) are a function of \( (z_1, \ldots, z_{k-1}) \). Such a flow \( \phi = \phi_1 \circ \cdots \circ \phi_k \) is called autoregressive (Papamakarios et al., 2018) and conveniently has a lower triangular Jacobian, which determinant can be computed efficiently as the product of the diagonal term.

**G Experimental details**

Below we fully describe the experimental settings used to generate results introduced in Section 4. We will also shortly open-source our code for reproducibility purposes.

**Architecture** The architecture of the vector field \( f_\theta \) is given by a multilayer perceptron (MLP) with 3 hidden layers and 64 hidden units – as in (Grathwohl et al., 2018) – for projected (e.g. stereographic and wrapped cf Section 3) and naive (cf Appendix B.1) models. We rely on tanh activation. For our Riemannian continuous normalizing flow (RCNF), the input layer of the MLP is replaced by a geodesic distance layer (Ganea et al., 2018; Mathieu et al., 2019) (see Appendix E.2).

**Objectives** We consider two objectives, a Monte Carlo (MC) estimator of the negative log-likelihood

\[
\hat{L}_{\text{Like}}(\theta) = -\sum_{i=1}^B \log p_\theta(z_i) \text{ with } z_i \sim P_D
\]

and a MC estimator of the reverse KL divergence

\[
\hat{L}_{\text{KL}}(\theta) = \sum_{i=1}^B \log p_\theta(h_\theta(\epsilon_i)) - \log p_D(h_\theta(\epsilon_i))
\]

with \( z_i \sim P_\theta \) being reparametrized as \( z_i = h_\theta(\epsilon_i) \) and \( \epsilon_i \sim P \).

**Optimization** All models are trained by the stochastic optimizer Adam (Kingma and Ba, 2015) with parameters \( \beta_1 = 0.9, \beta_2 = 0.999 \), batch-size of 400 data-points and a learning rate set to \( 1e^{-3} \). Also, all experiments were performed using the exact divergence estimator.

**G.1 Hyperbolic geometry and limits of conventional and wrapped methods**

In this experiment the target is set to be a wrapped normal on \( \mathbb{B}^2 \) (Nagano et al., 2019; Mathieu et al., 2019) with density \( N^W(\exp_\theta(\alpha \delta x), \Sigma) = \exp_\mu \mathcal{N}(\alpha \delta x, \Sigma) \) with \( \Sigma = \text{diag}(0.3, 1.0) \). The scalar parameter \( \alpha \) allows us to locate the target closer or further away from the origin of the disk. Through this experiment we consider three CNFs:

- **Naive:** \( P^N_\theta = \phi^{B^2}_\theta \mathcal{N}(0, 1) \)
- **Wrapped:** \( P^W_\theta = (\exp_\theta \circ \phi^{B^2}_\theta) \mathcal{N}(0, 1) \)
• **Riemannian:** \( P^R_\theta = \phi^R_\frac{1}{2} N^W(0, 1) \)

with \( \phi^R \) a conventional CNF on \( \mathbb{R}^2 \), \( \phi^S \) our RCNF introduced in Section 2, \( N(0, 1) \) the standard Gaussian and \( N^W(0, 1) \) the standard wrapped normal. For the RCNF we scale the vector field as

\[
 f_\theta(z) = |G(z)|^{-1/2} \text{neural\_net}(z) = \left( \frac{1 - \|z\|^2}{2} \right)^2 \text{neural\_net}(z).
\]

These three models are trained for 1500 iterations, by minimizing the negative log-likelihood (see Figure 4) and the reverse KL divergence (see Figure 7). We rely on the adaptive Runge-Kutta 4(5) solver with absolute and relative tolerance of \( 1e^{-5} \) to numerically approximate the ODE.

### G.2 Spherical geometry

Through the following spherical experiments we consider the two following models

- **Stereographic:** \( P^S_\theta = (\rho^{-1} \circ \phi^S) N(0, 1) \)
- **Riemannian:** \( P^R_\theta = \phi^S S^2 U(S^2) \)

with \( \rho^{-1} \) the inverse of the stereographic projection, \( \phi^S \) a conventional CNF on \( \mathbb{R}^2 \), \( \phi^S \) our RCNF, \( N(0, 1) \) the standard Gaussian and \( U(S^2) \) the uniform distribution on \( S^2 \). For the RCNF we project the output layer of the vector field as

\[
 f_\theta(z) = \text{proj}_{r_s \in S^2} \text{neural\_net}(z) = \frac{\text{neural\_net}(z)}{||\text{neural\_net}(z)||^2}
\]

so as to enforce output vectors to be **tangent**. We observed that training models with an adaptive solver was computationally intensive so we alternatively relied on a fixed-step Runge-Kutta 4(5) solver with 40 steps to numerically approximate the ODE.

**Limits of the stereographic projection model** In this experiment the target is chosen to be a \( \text{vMF}(\mu, \kappa) \) located at \( \mu = -\mu_0 \) with \(-\{\mu_0\} = (-1, 0, \ldots, 0)\). Both models are trained for 3000 iterations by minimizing the negative log-likelihood and the reverse KL divergence.

**Density estimation of spherical data** Finally we consider four earth location datasets, representing respectively volcano eruptions (NOAA, 2020b), earthquakes (NOAA, 2020a), floods (Brakenridge, 2017) and wild fires (EOSDIS, 2020). Models are trained for 1000 epochs by minimizing the negative log-likelihood. We observed that annealing the learning rate such that \( \alpha(t) = 0.98^{(t/300)} \alpha_0 \) with \( \alpha_0 = 1e^{-3} \) helped training convergence.

### H Additional figures

![Figure 7: Reverse KL of CNFs trained to fit a \( \mathcal{N}^W(\exp(\alpha \partial x), \Sigma) \) target on \( S^2 \).](image-url)
Figure 8: Density estimation for earth sciences data with Robinson projection. Blue and red dots represent training and testing datapoints, respectively. Heatmaps depict the log-likelihood of the trained models.