Vector-valued Gaussian Processes on Riemannian Manifolds

Michael Hutchinson*[1], Alexander Terenin*[2,3], Viacheslav Borovitskiy*[4], So Takao*[5], Yee Whye Teh[1], Marc Peter Deisenroth[5]

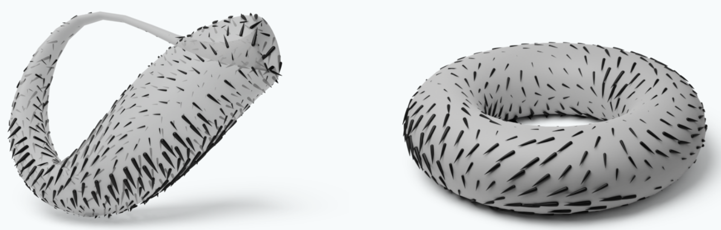
*Equal contribution, [1]University of Oxford, [2]University of Cambridge, [3]Imperial College London, [4]St. Petersburg State University, [5]University College London

Abstract

Gaussian processes are machine learning models capable of learning unknown functions in a way that represents uncertainty, thereby facilitating construction of optimal decision-making systems. Motivated by a desire to deploy Gaussian processes in novel areas of science, a rapidly-growing line of research has focused on constructively extending these models to handle non-Euclidean domains, including Riemannian manifolds, such as spheres and tori. We propose techniques that generalize this class to model vector fields on Riemannian manifolds, which are important in a number of application areas in the physical sciences. To do so, we present a general recipe for constructing gauge independent kernels, which induce Gaussian vector fields, i.e. vector-valued Gaussian processes coherent with geometry, from scalar-valued Riemannian kernels. We extend standard Gaussian process training methods, such as variational inference, to this setting. This enables vector-valued Gaussian processes on Riemannian manifolds to be trained using standard methods and makes them accessible to machine learning practitioners.

Vector Fields on Manifolds

Manifold X	smooth geometric space where rules of calculus apply
Tangent space $T_x X$	vector space of all directions one can move at $x \in X$
Tangent bundle TX	manifold obtained by gluing together all tangent spaces
Cotangent bundle T^*X	similar, but glue together *dual spaces* of tangent spaces
Vector field f	$f : X \to TX$ s.t. arrow $f(x) \in TX$ matches point $x \in X$



Gaussian Vector Fields and Cross-covariance Kernels

A vector field is a map $f : X \to TX$ between manifolds: range is *not* a vector space.

$\implies$ need an appropriate notion of Gaussianity for bundles

Definition. A random vector field f is *Gaussian* if for any points $x_1, \ldots, x_n \in X$ on the manifold, the vectors $f(x_1), .., f(x_n) \in T_{x_1}X \oplus .. \oplus T_{x_n}X$ attached to them are jointly Gaussian, where $\oplus$ is the vector direct sum.

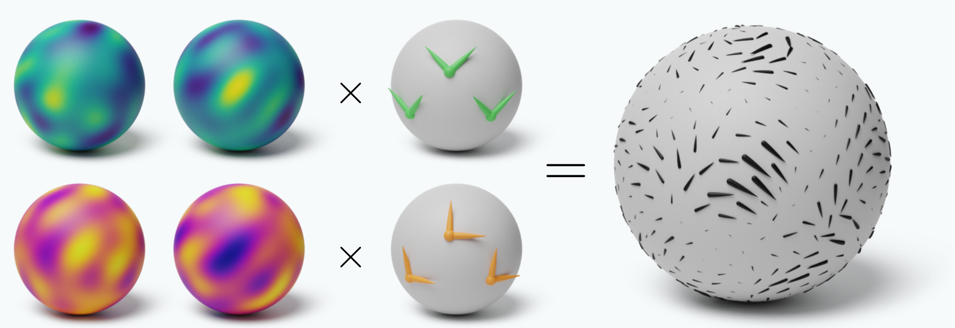
Provides an appropriate notion of finite-dimensional marginals

Definition. We say that a scalar-valued function $k : T^*X \times T^*X \to \mathbb{R}$ is a *cross-covariance kernel* if it satisfies the following key properties.

1. Symmetry: for all $\alpha, \beta \in T^*X$, $k(\alpha, \beta) = k(\beta, \alpha)$ holds.
2. Fiberwise bilinearity: for any $x, x' \in X$, we have $k(\lambda\alpha_x + \mu\beta_x, \gamma_{x'}) = \lambda k(\alpha_x, \gamma_{x'}) + \mu k(\beta_x, \gamma_{x'})$ for any $\alpha_x, \beta_x \in T^*_x X$, $\gamma_{x'} \in T^*_{x'} X$ and $\lambda, \mu \in \mathbb{R}$.
3. Positive definiteness: for any covectors $\alpha_1, .., \alpha_n \in T^*X$, we have that $\sum_{i=1}^n \sum_{j=1}^n k(\alpha_i, \alpha_j) \geq 0$.

Theorem. Every Gaussian random vector field admits and is uniquely determined by a mean vector field and a cross-covariance kernel.

Equivariant Matrix-valued Kernels

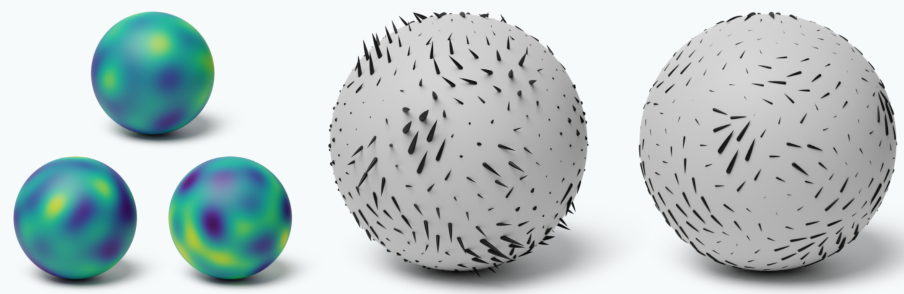


Frame: simultaneous systems of coordinates chosen in all tangent spaces

Proposition. Every cross-covariance kernel can be represented in a frame as an equivariant matrix-valued kernel.

Different frames $\rightsquigarrow$ different representations as matrices

Projected Kernels



Idea: construct Gaussian vector field by the following steps.

(1) Embed scalar-valued Gaussian processes into a higher-dim. space $\mathbb{R}^{d'}$.

(2) Assemble them into a vector-valued Gaussian process $\boldsymbol{f} : X \to \mathbb{R}^{d'}$,

(3) Project onto the tangent spaces to obtain a tangential vector field.

Scalar-valued Riemannian kernels [1]: basic building block

In a frame F, this procedure defines a *projected kernel*:

$$\mathbf{K}_F(x, x') = \mathbf{P}_x \boldsymbol{\kappa}(x, x') \mathbf{P}_{x'}^T.$$

$\boldsymbol{\kappa}$: vector-valued kernel from manifold into $\mathbb{R}^{d'}$

$\mathbf{P}_x$: projection matrix between $T_x X$ and the Euclidean tangent space

Different frames $\rightsquigarrow$ different projection matrices $\rightsquigarrow$ different $\mathbf{K}_F$

Proposition. All cross-covariance kernels can be written as projected kernels.

Train by choosing a frame and working with matrix-valued kernels using standard techniques such as inducing points and variational inference

Dynamics Modelling: pendulum with friction

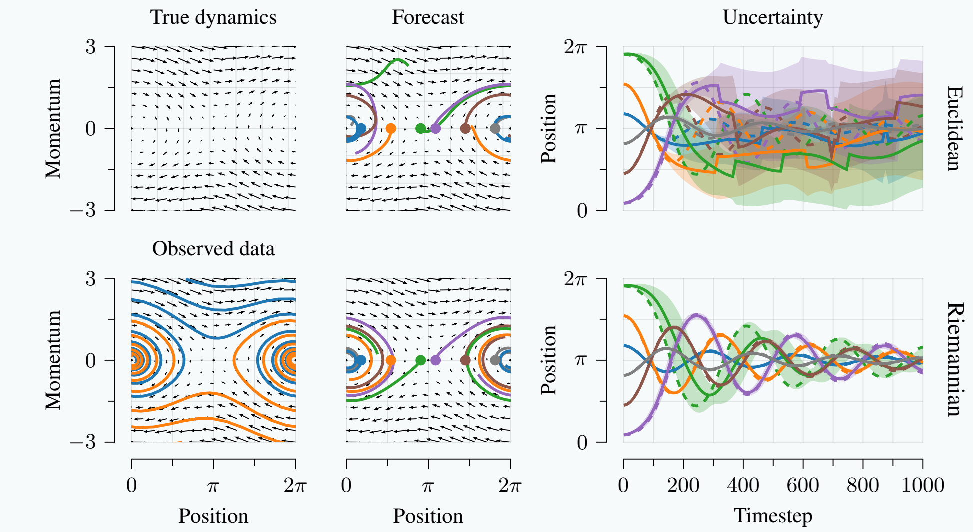


Figure 1: An ideal pendulum with pivot friction has a state space that is a cylinder, $[0, 2\pi] \times \mathbb{R}$. Taking into account the geometry ensures no discontinuity at 2π, and facilitates stable long term predictions.

Weather Modelling

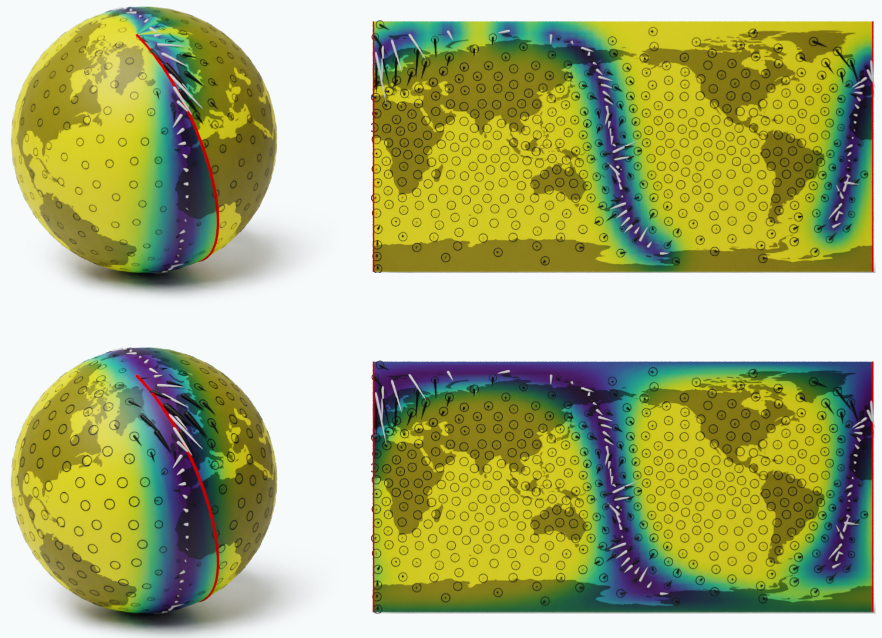


Figure 2: Modelling wind fields over the Earth involves placing kernels over the manifold $\mathcal{S}^2$. Taking into account the correct geometry prevents warping of inference at the poles and discontinuities at the seam where we unwrap the sphere.

References

[1] V. Borovitskiy, A. Terenin, P. Mostowsky, and M. P. Deisenroth. Matern gaussian processes on riemannian manifolds. In *Advances in Neural Information Processing Systems*, 2020.