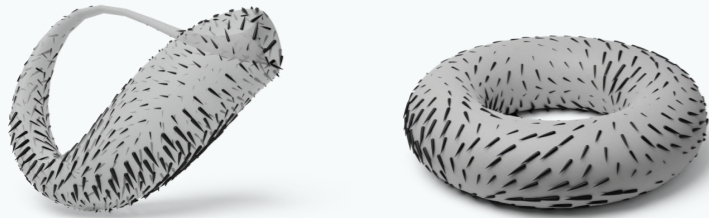


## Abstract

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**  $f$   $f : X \rightarrow TX$  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  $f : X \rightarrow TX$  between manifolds: range is *not* a vector space.  
 $\Rightarrow$  need an appropriate notion of Gaussianity for bundles

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

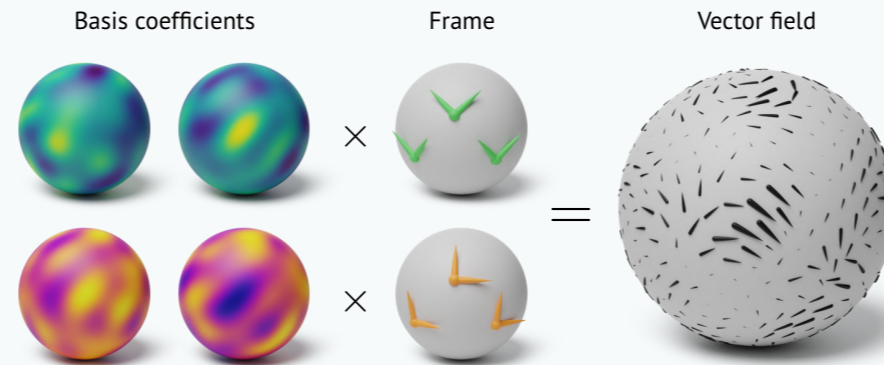
Provides an appropriate notion of finite-dimensional marginals

**Definition.** We say that a scalar-valued function  $k : T^*X \times T^*X \rightarrow \mathbb{R}$  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  $\alpha_1, \dots, \alpha_n \in T^*X$ , 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

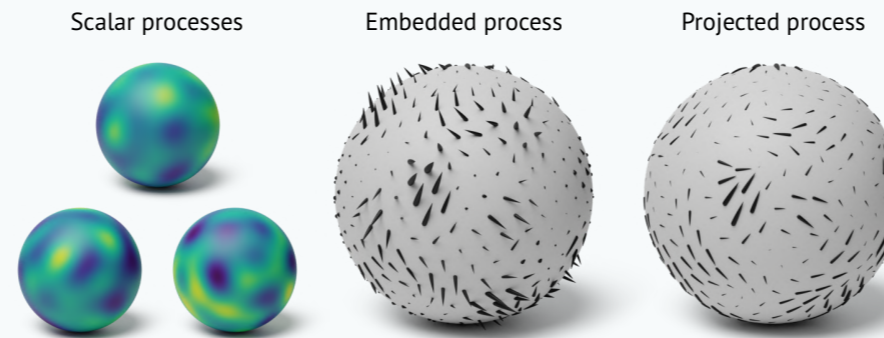


Frame: simultaneous systems of coordinates chosen in all tangent spaces

**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  $f : X \rightarrow \mathbb{R}^d$ ,
- (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*:

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

$\kappa$ : 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

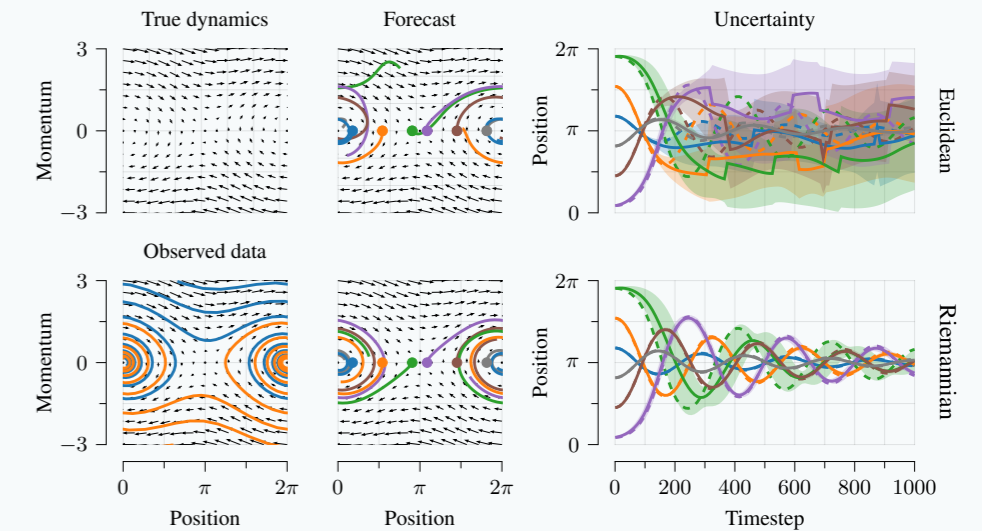


Figure 1: An ideal pendulum with pivot friction has a state space that is a cylinder,  $[0, 2\pi] \times \mathbb{R}$ . Taking into account the geometry ensures no discontinuity at  $2\pi$ , and facilitates stable long term predictions.

## Weather Modelling

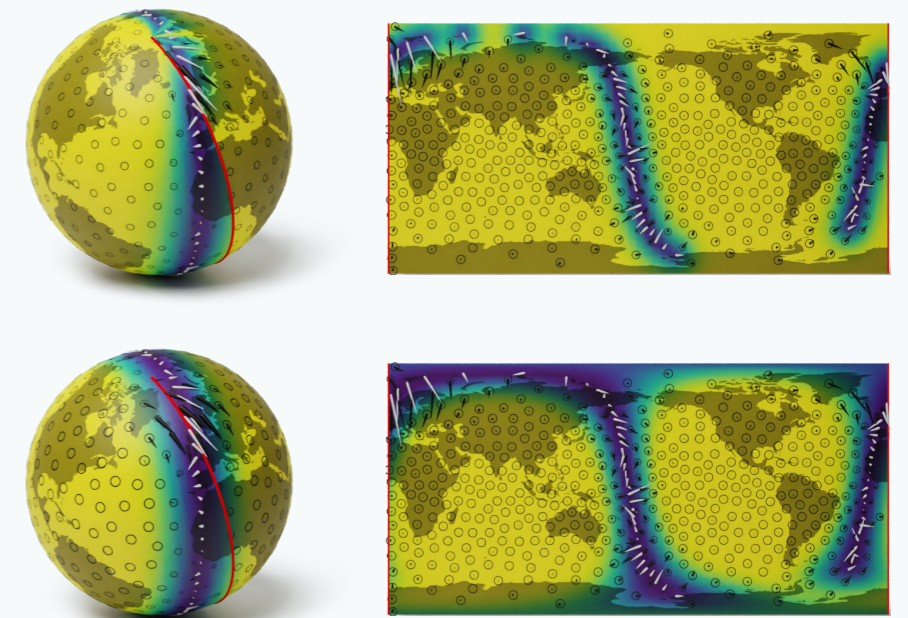


Figure 2: Modelling wind fields over the Earth involves placing kernels over the manifold  $S^2$ . Taking into account the correct geometry prevents warping of inference at the poles and discontinuities at the seam where we unwrap the sphere.

## 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.