Matérn Gaussian Processes on Riemannian Manifolds

Viacheslav Borovitskiy*[1,4] · Alexander Terenin*[2] · Peter Mostowsky*[1] · Marc Peter Deisenroth[3]

*Equal contribution · [1]St. Petersburg State University · [2]Imperial College London · [3]University College London
[4]St. Petersburg Department of Steklov Mathematical Institute of Russian Academy of Sciences

Abstract

Gaussian processes are an effective model class for learning unknown functions, particularly in settings where accurately representing predictive uncertainty is of key importance. Motivated by applications in the physical sciences, the widely-used Matérn class of Gaussian processes has recently been generalized to model functions whose domains are Riemannian manifolds, by re-expressing said processes as solutions of stochastic partial differential equations. In this work, we propose techniques for computing the kernels of these processes on compact Riemannian manifolds via spectral theory of the Laplace–Beltrami operator, allowing them to be trained via standard scalable techniques such as inducing points. This enables Riemannian Matérn GPs to be used in mini-batch, online, and non-conjugate settings, and makes them more accessible to machine learning practitioners.

The Euclidean Matérn kernel

$$k(x,x') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{\|x-x'\|}{\kappa}\right)^{\nu} K_\nu\left(\sqrt{2\nu}\frac{\|x-x'\|}{\kappa}\right)$$

σ^2: variance κ: length scale ν: smoothness

$\nu \to \infty$: recovers squared exponential kernel

The Matérn kernel defines a Gaussian process $f : \mathbb{R}^d \to \mathbb{R}$.

A no-go theorem for kernels on manifolds

We'd like to define analogs of Matérn and squared exponential GPs $f : M \to \mathbb{R}$, where (M, g) is a Riemannian manifold.

Candidate generalization for $\nu \to \infty$ via geodesics

$$k_{\text{naïve}}(x,x') = \sigma^2 \exp\left(-\frac{d_g(x,x')^2}{2\kappa^2}\right)$$

Theorem. (Feragen et al. [2]) Let M be a complete Riemannian manifold without boundary. If $k_{\text{naïve}}$ is a positive semi-definite kernel for all κ, then M is isometric to a Euclidean space.

$\Longrightarrow$ need a different candidate generalization

Stochastic partial differential equations

GPs with Matérn kernels can be regarded as solutions of SPDEs [3].

$$\underbrace{\left(\frac{2\nu}{\kappa^2} - \Delta\right)^{\frac{\nu}{2}+\frac{d}{4}} f = \mathcal{W}}_{\text{Matérn}} \qquad \underbrace{e^{-\frac{\kappa^2}{4}\Delta} f = \mathcal{W}}_{\text{squared exponential}}$$

Δ : Laplacian $\mathcal{W}$: (rescaled) white noise

✓ Generalizes well to the Riemannian setting
☒ Not very constructive, requires solving SPDEs

This work: compute the Matérn kernel on compact Riemannian manifolds

Computing the kernels of SPDE Riemannian Matérn GPs

Matérn: $$k_\nu(x,x') = \frac{\sigma^2}{C_\nu} \sum_{n=0}^{\infty} \left(\frac{2\nu}{\kappa^2} - \lambda_n\right)^{\nu - \frac{d}{2}} f_n(x) f_n(x')$$

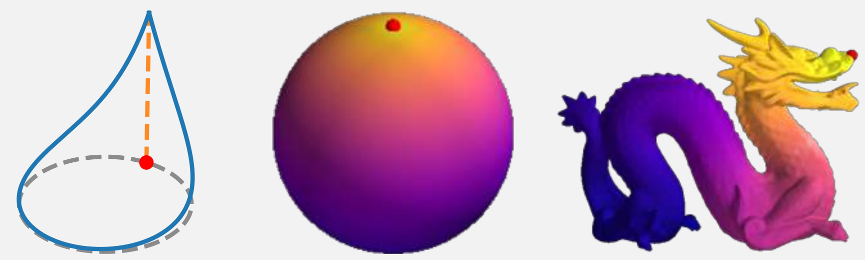
Sq. exp.: $$k_\infty(x,x') = \frac{\sigma^2}{C_\infty} \sum_{n=0}^{\infty} e^{-\frac{\kappa^2}{2}\lambda_n} f_n(x) f_n(x')$$

λ_n, f_n : Laplace–Beltrami eigenpairs

For many spaces, λ_n and f_n are known analytically, and in others they can be obtained numerically by solving a differential equation.

This gives a Karhunen—Loéve-type expansion, with $f_n(\cdot)$ analogous to Fourier features.

Riemannian Matérn kernel



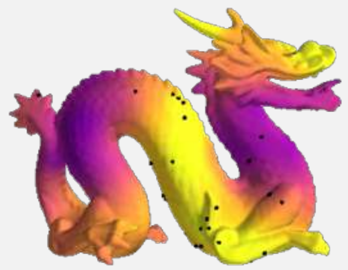
Matérn-1/2 kernel: $k_{1/2}(\boldsymbol{x}, \cdot)$

Posterior samples

(a) Ground truth

(b) Posterior mean

(c) Standard deviation



(d) One posterior sample

References

[1] V. Borovitskiy, A. Terenin, P. Mostowski, and M. P. Deisenroth. Matérn gaussian processes on Riemannian manifolds. NeurIPS, 2020.
[2] A. Feragen, F. Lauze, and S. Hauberg. Geodesic exponential kernels: When curvature and linearity conflict. CVPR, 2015.
[3] F. Lindgren, H. Rue, and J. Lindström. An explicit link between Gaussian fields and Gaussian–Markov random fields: the stochastic partial differential equation approach. JRSSB 73(4), 2011.