Kriging

in the age of ML

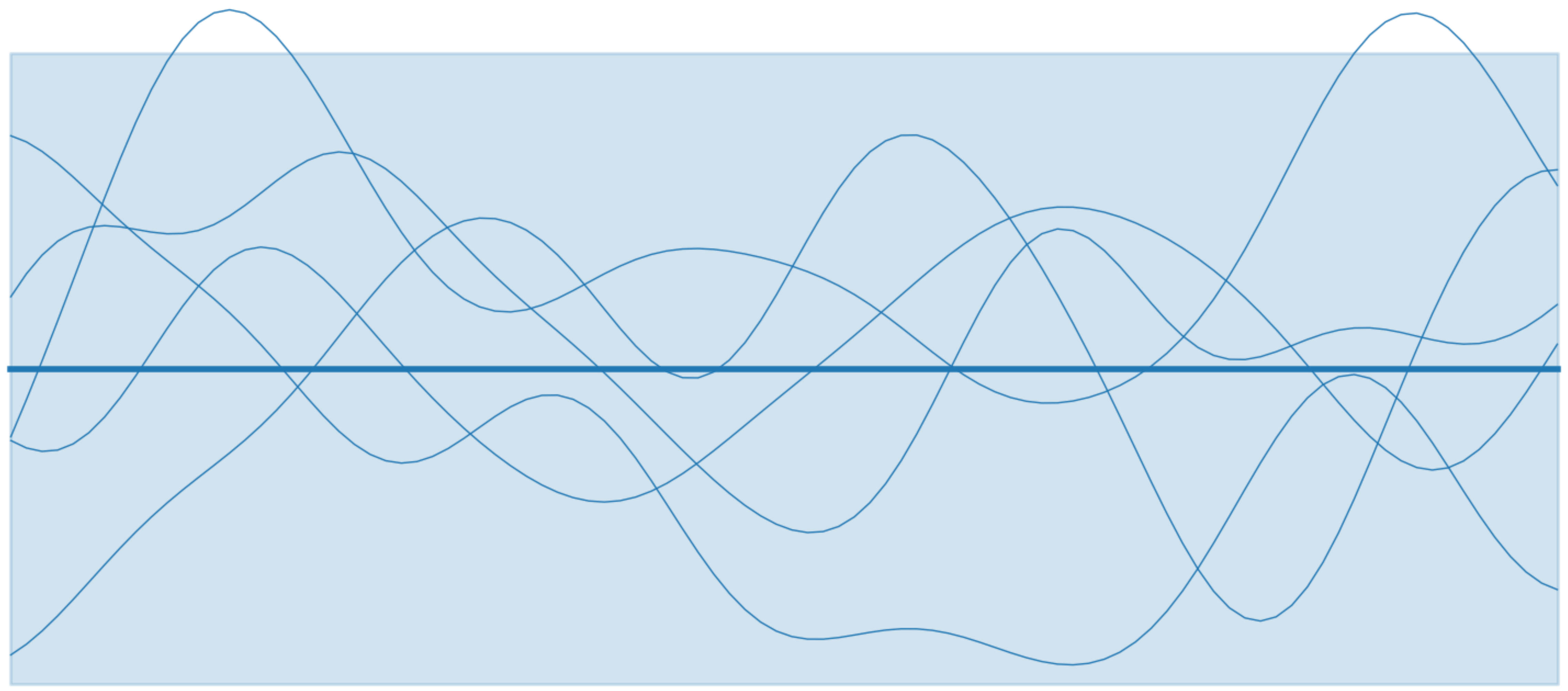
Link to accompanying tutorial: https://github.com/sotakao/moap-bml-workshop

So Takao **17/02/2022** **UCL-MOAP Workshop on Bayesian ML for Weather and Climate**

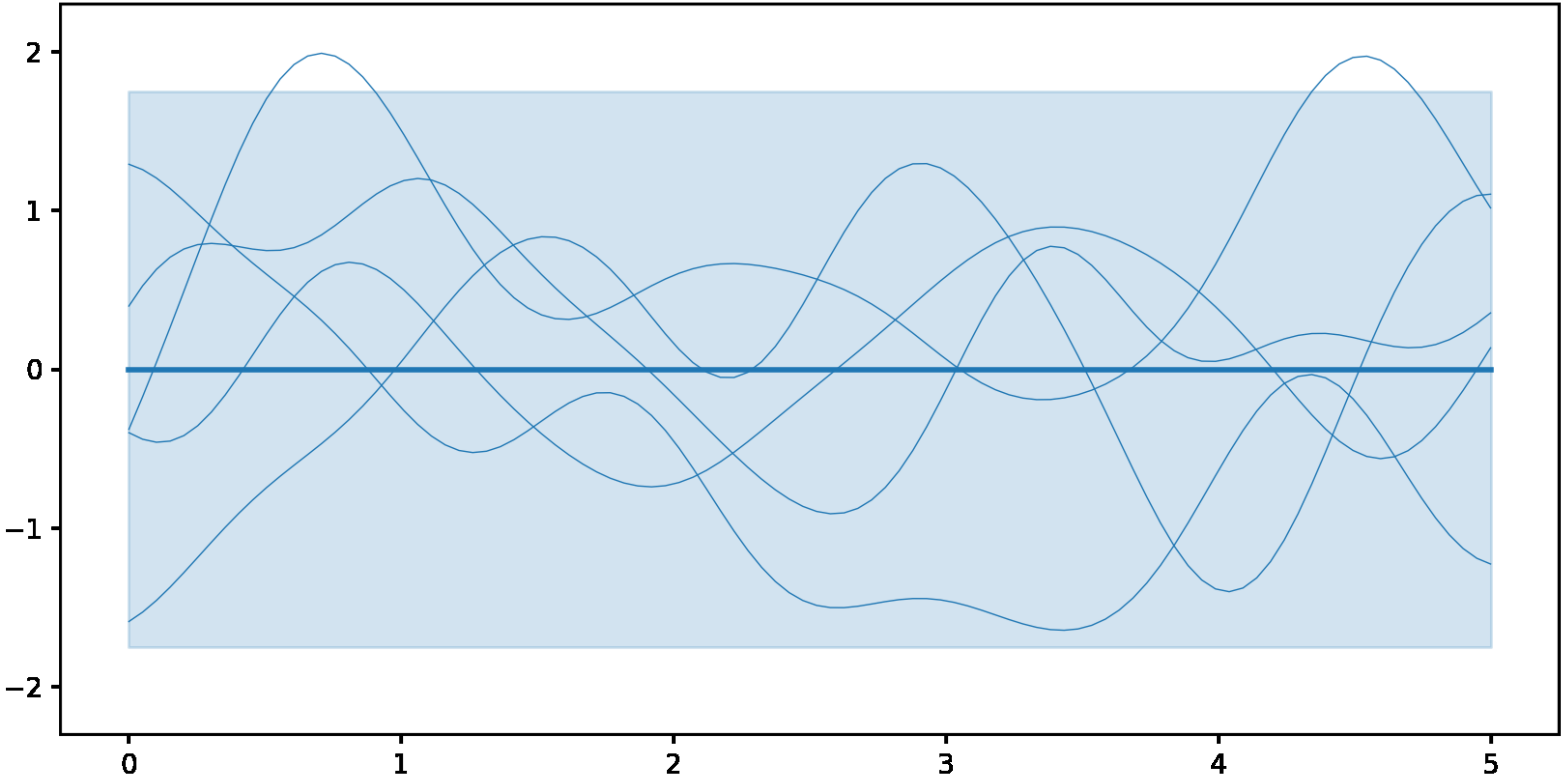
Gaussian Processes

GPs are Gaussian random variables on *the space of functions*

- Mean: $m(x) = \mathbb{E}[f(x)]$
- Kernel: $k(x, y) = \mathrm{Cov}[f(x), f(y)]$



$$p(f \mid y) = \frac{p(y \mid f)p(f)}{p(y)}$$



Limitations of GPs

- $\mathcal{O}(N^3)$ computational complexity

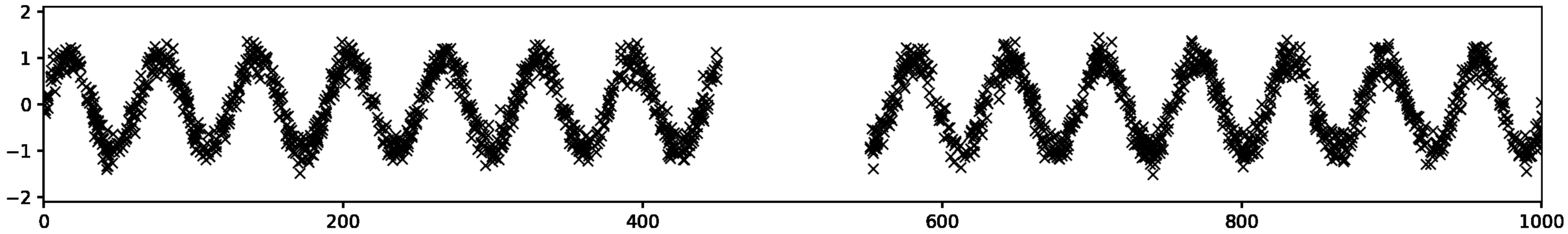
- Limited to basic kernel choices

Overcoming the limitations

Inducing point method

Idea: Can we *summarise* the training data using $M \ll N$ pseudo datapoints?

- Sparse Variational Gaussian Processes by **Titsias (2009)** can do this:



- Time complexity reduced from $\mathcal{O}(N^3)$ to $\mathcal{O}(NM^2)$

Temporal GPs

In the time dimension, the complexity can be reduced further down to $\mathcal{O}(N)$!

Idea: GPs can be reformulated as stochastic differential equations (SDEs)

Examples (see Hartikainen et al. (2010))

- Matérn-1/2

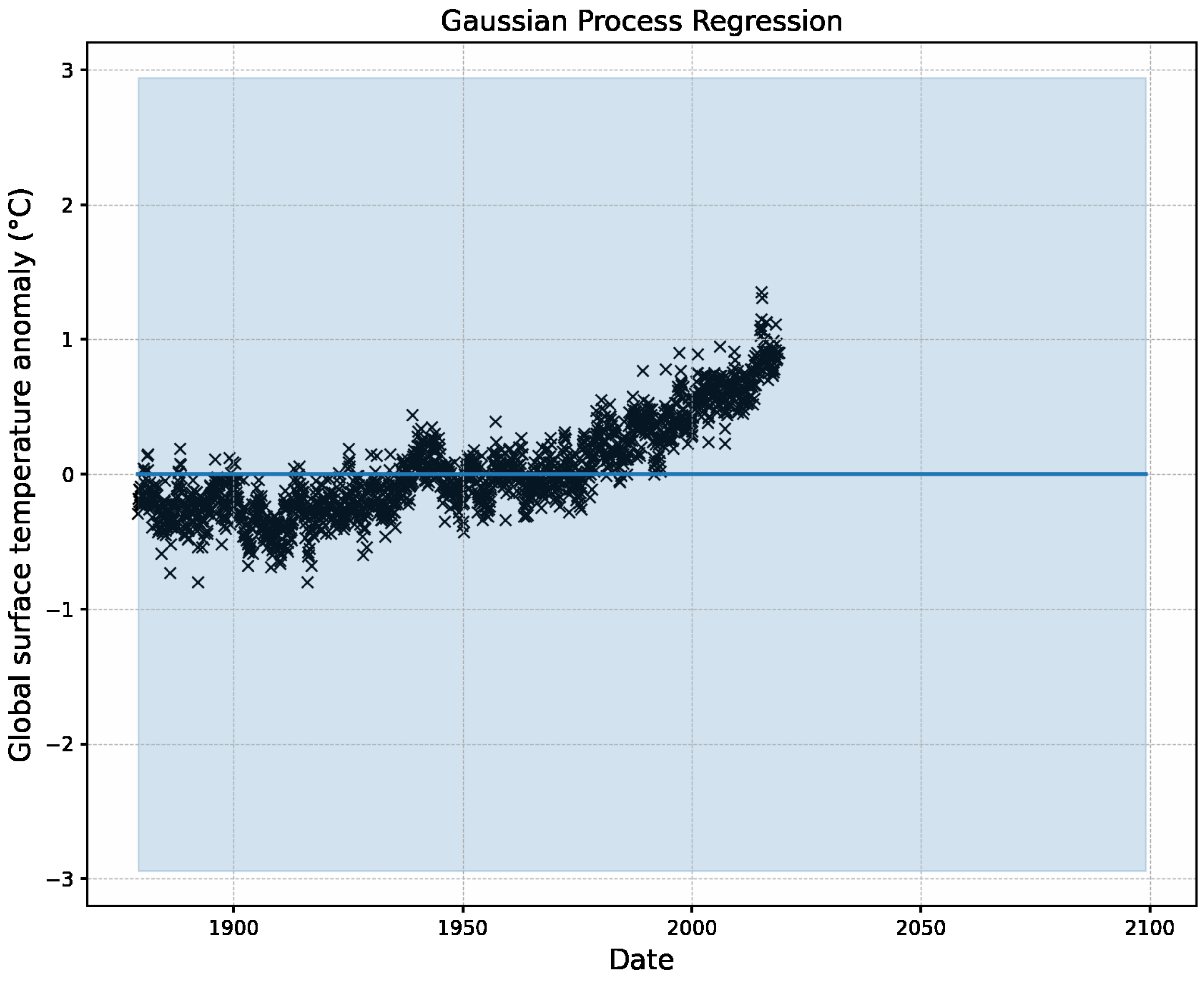
$$\mathrm{d}X_t = -\frac{\sqrt{2\nu}}{l} X_t \, \mathrm{d}t + q_c \, \mathrm{d}W_t$$

- Matérn-3/2

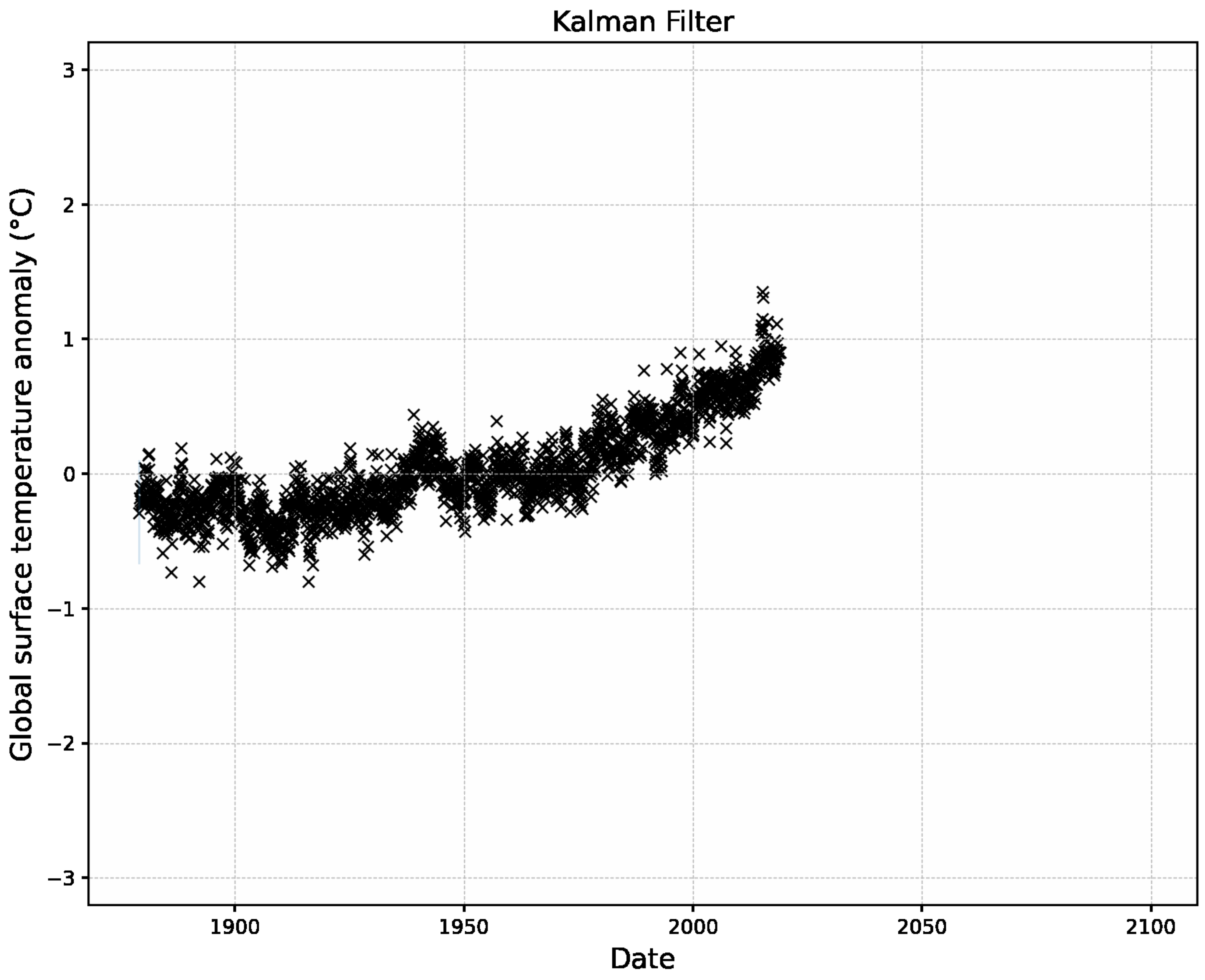
$$\begin{cases} \mathrm{d}X_t & = V_t \, \mathrm{d}t \\ \mathrm{d}V_t & = -\left(\frac{\sqrt{2\nu}}{l}\right)^2 X_t \, \mathrm{d}t - 2\frac{\sqrt{2\nu}}{l} V_t \, \mathrm{d}t + q_c \, \mathrm{d}W_t \end{cases}$$

Conditioning on data can now be achieved via Kalman filtering/smoothing

Temporal GPs

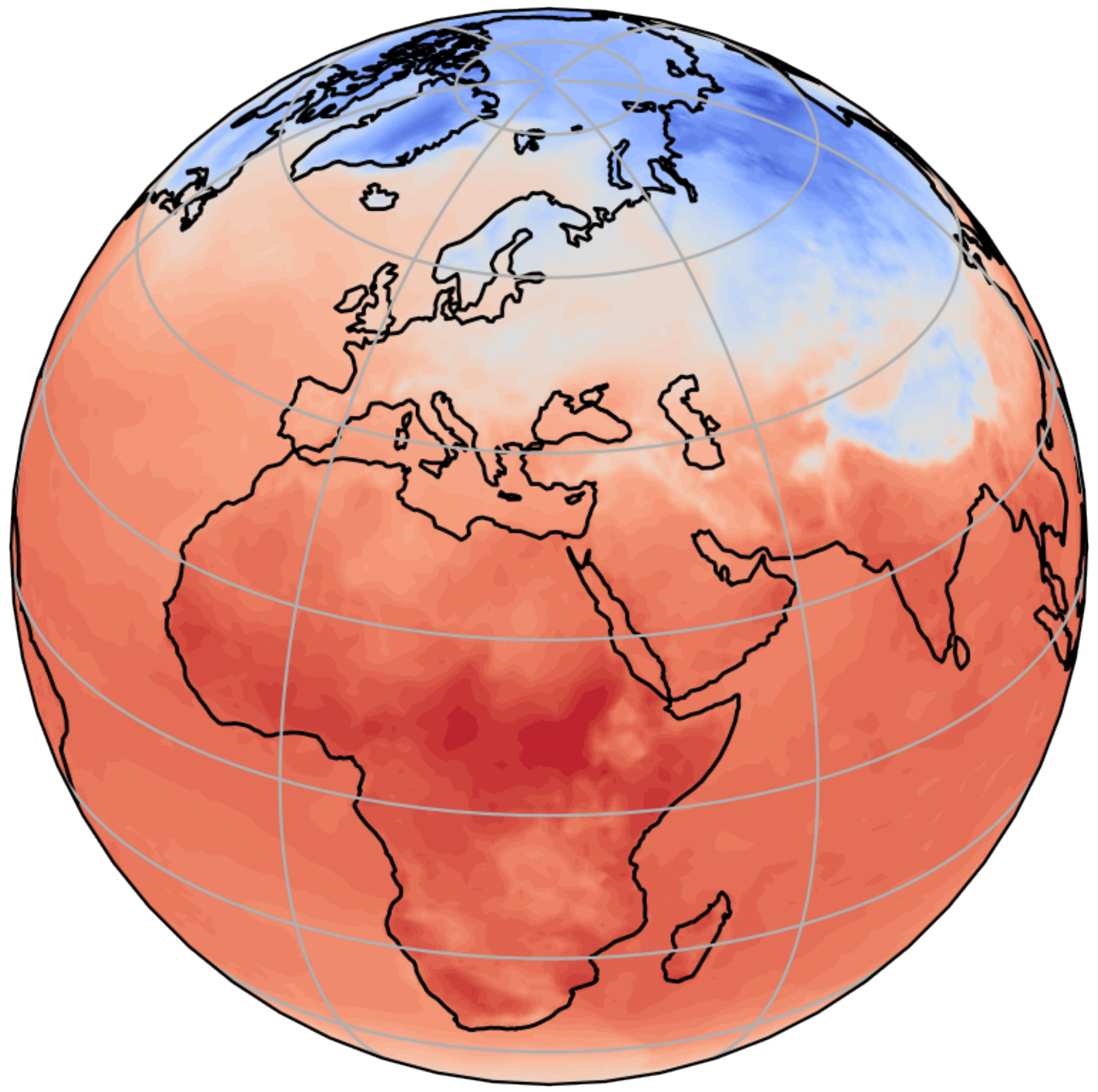


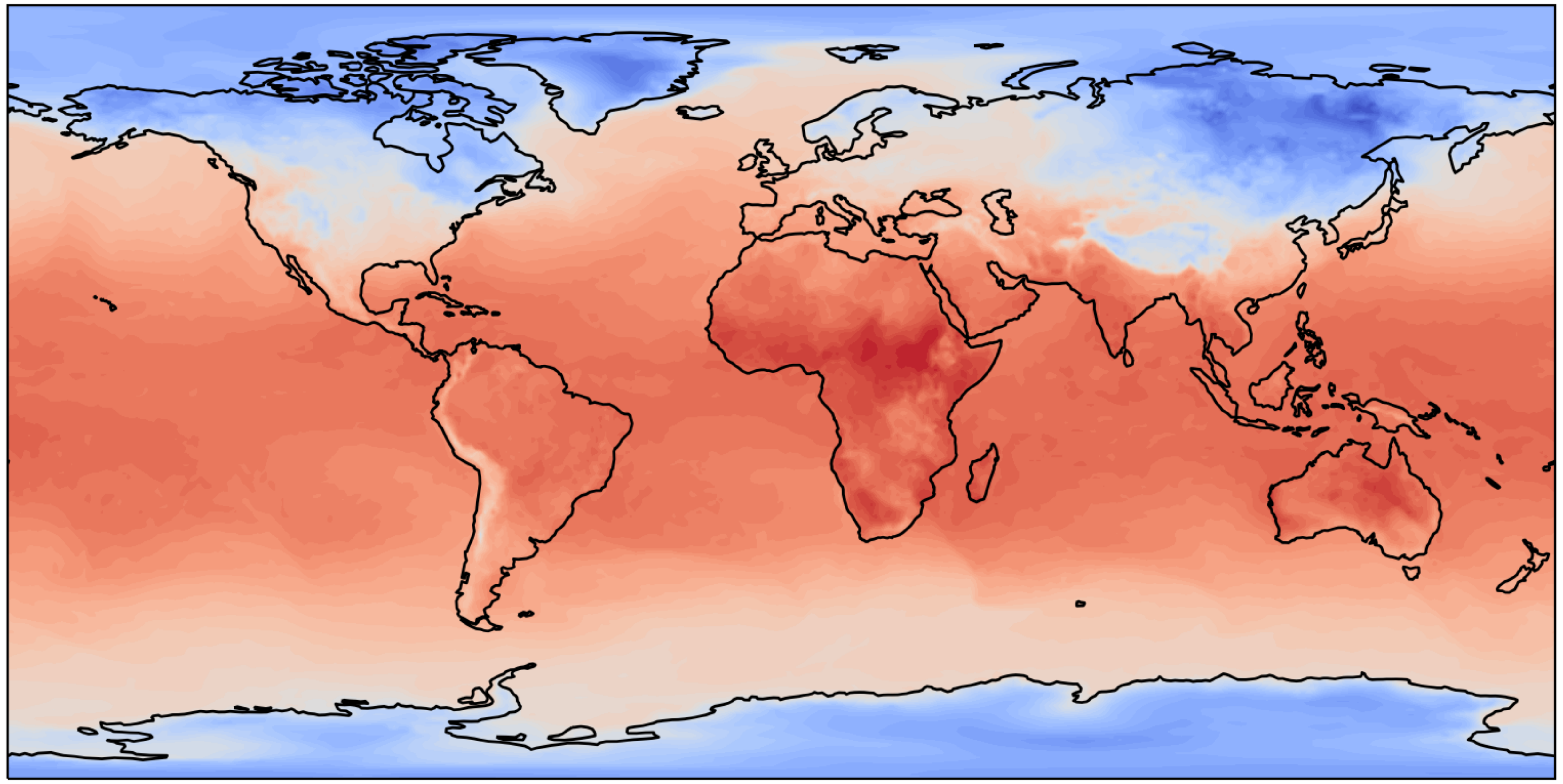
$\mathcal{O}(N^3)$



$\mathcal{O}(N)$

Kriging on manifolds





Matérn GPs can be reformulated as Stochastic PDEs:

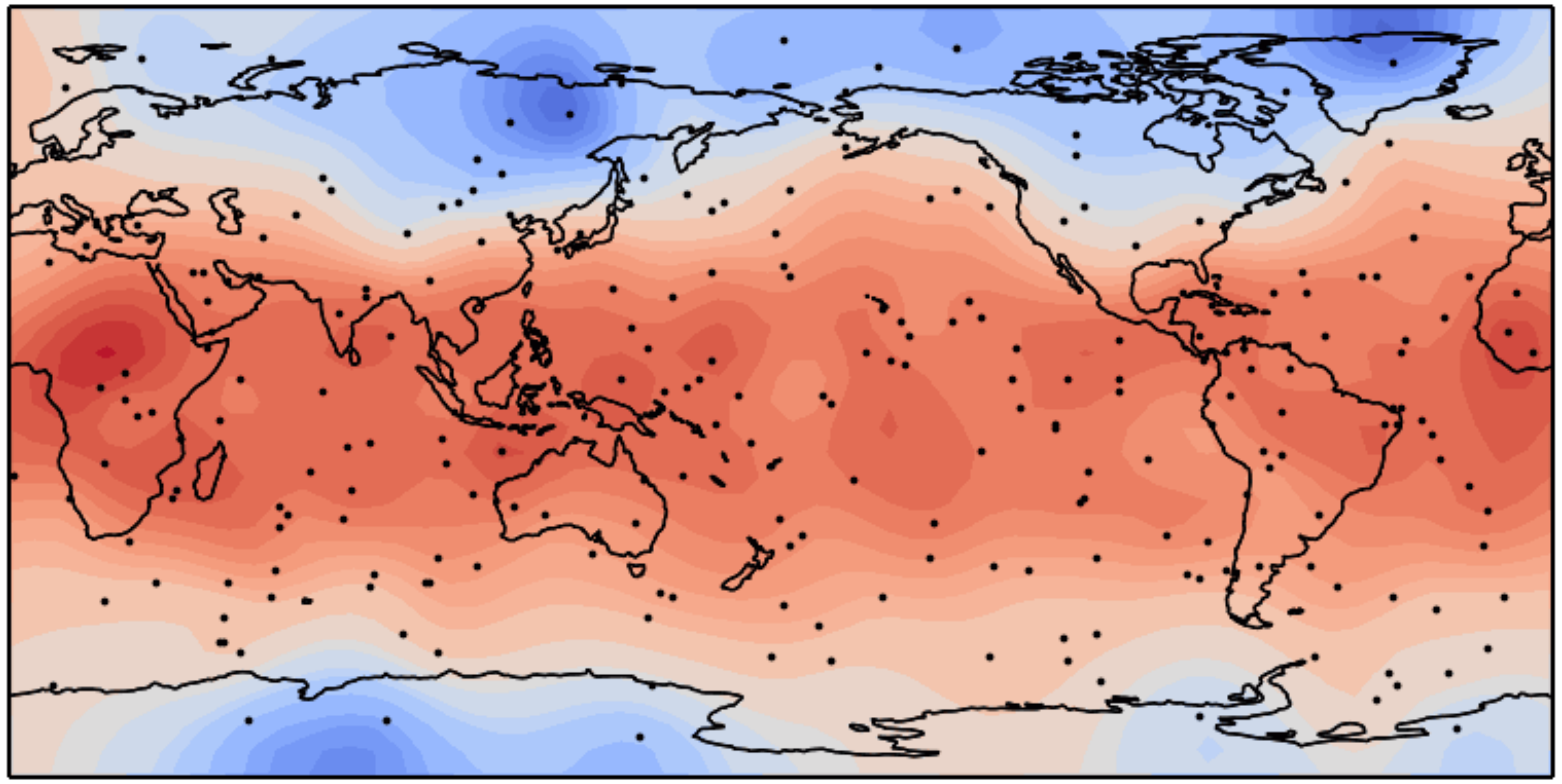
$$\left(\frac{2\nu}{\rho^2} - \Delta\right)^{\frac{\nu}{2}+\frac{d}{4}} f = \mathcal{W}$$

Kernel obtained by studying the spectral properties of the SPDE (Borovitskiy et al. 2021)

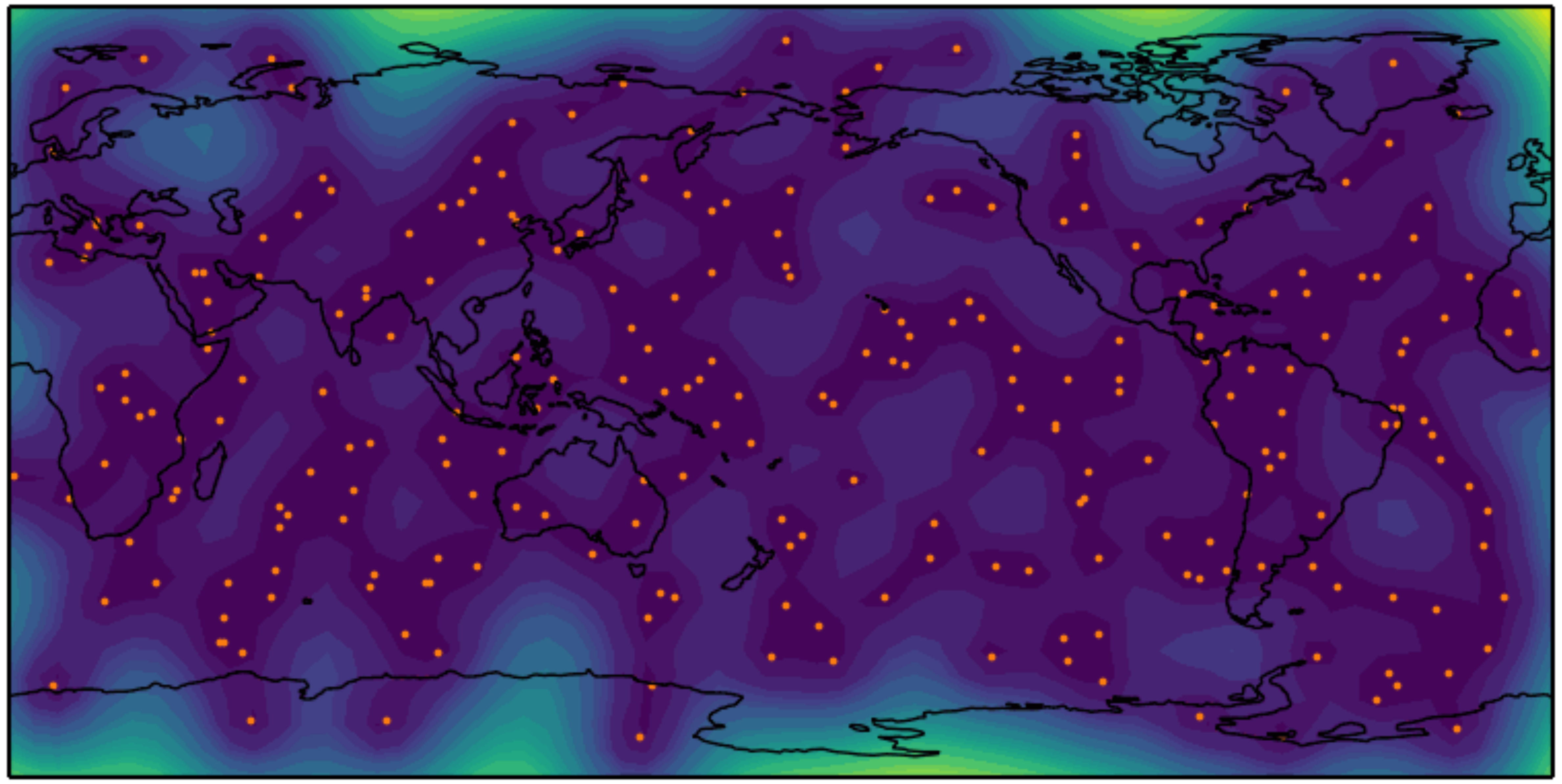
Comparison with Euclidean GPs

Euclidean GP

Prediction



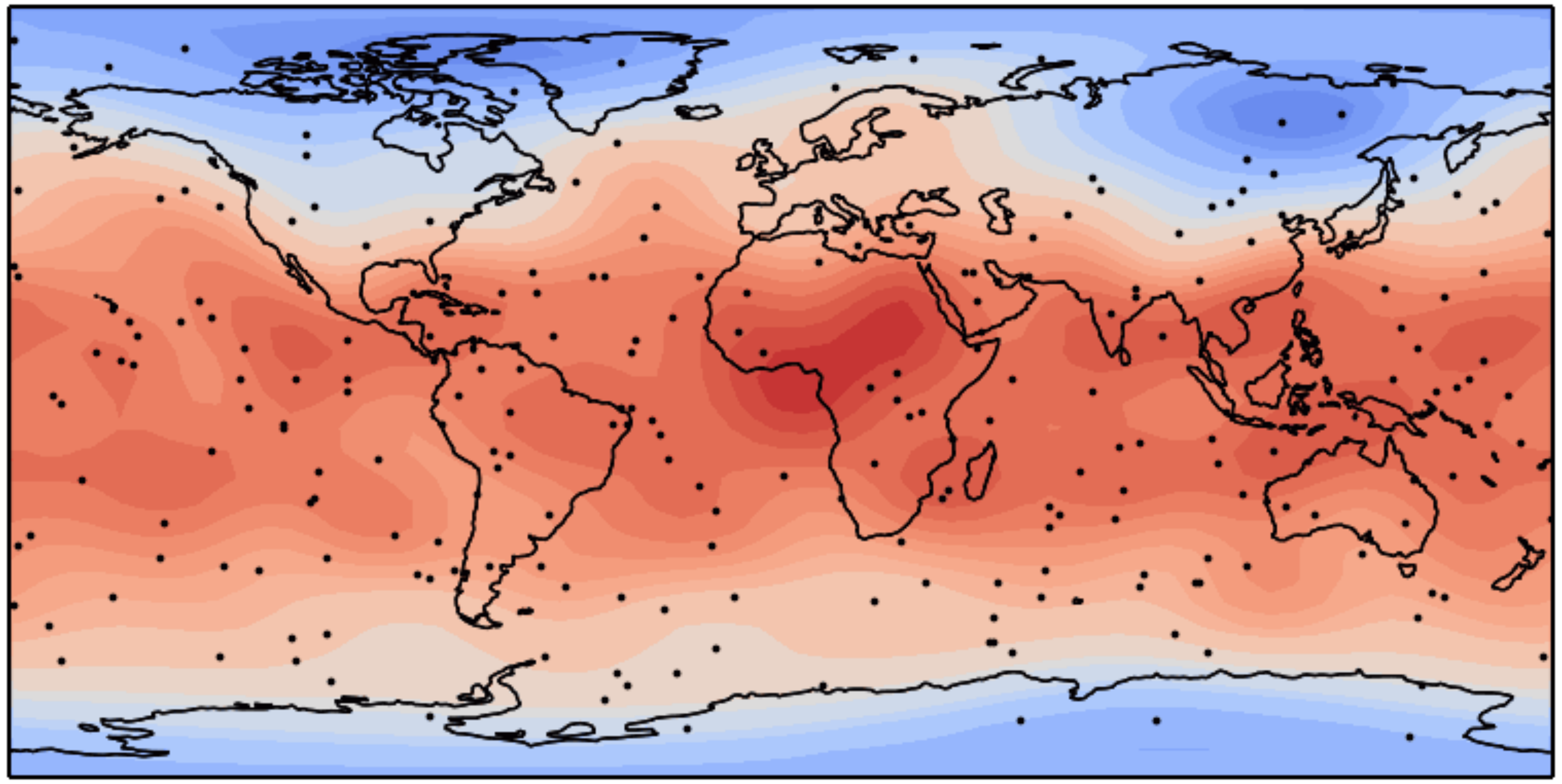
Variance



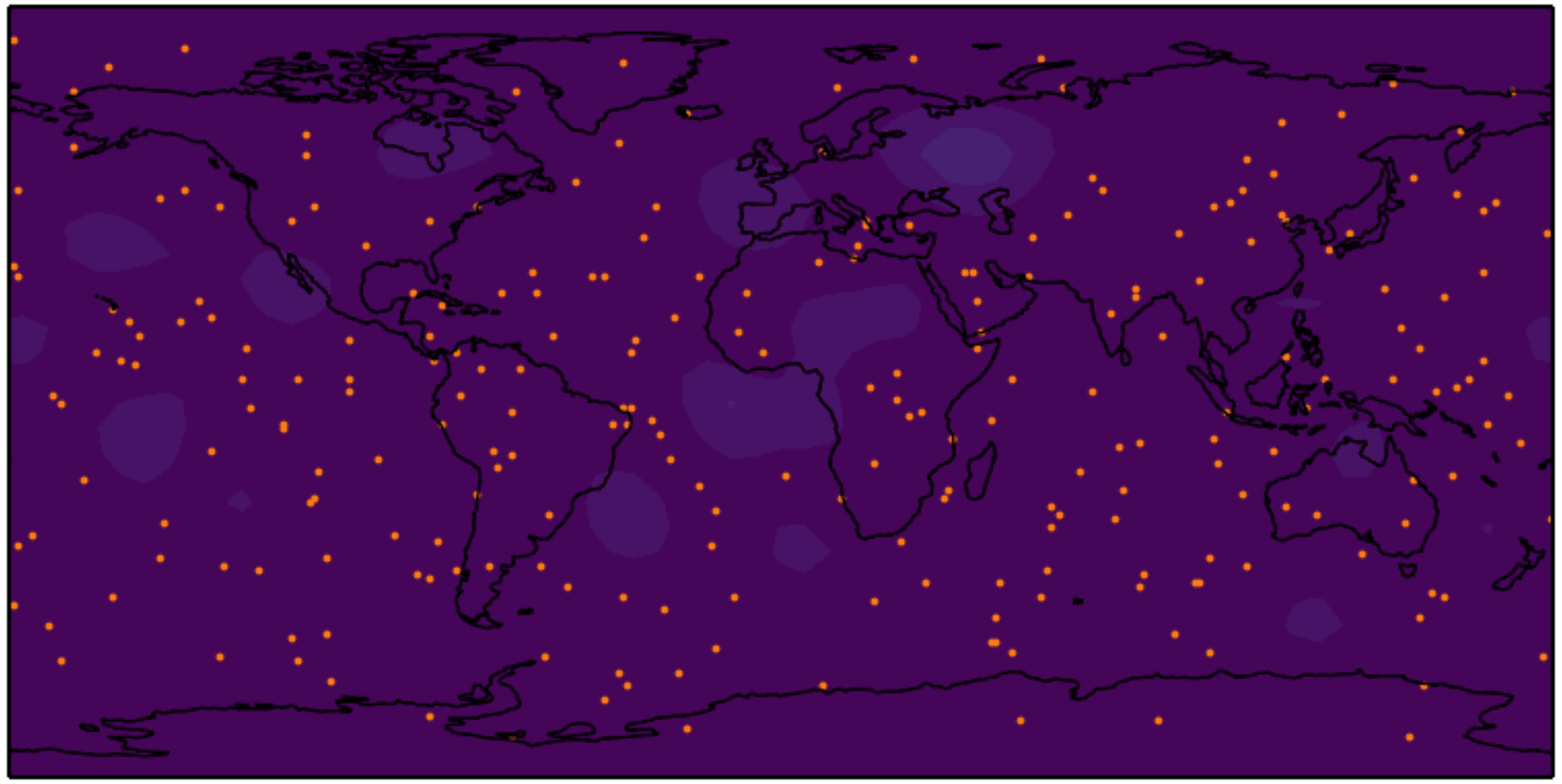
Comparison with Euclidean GPs

Spherical GP

Prediction

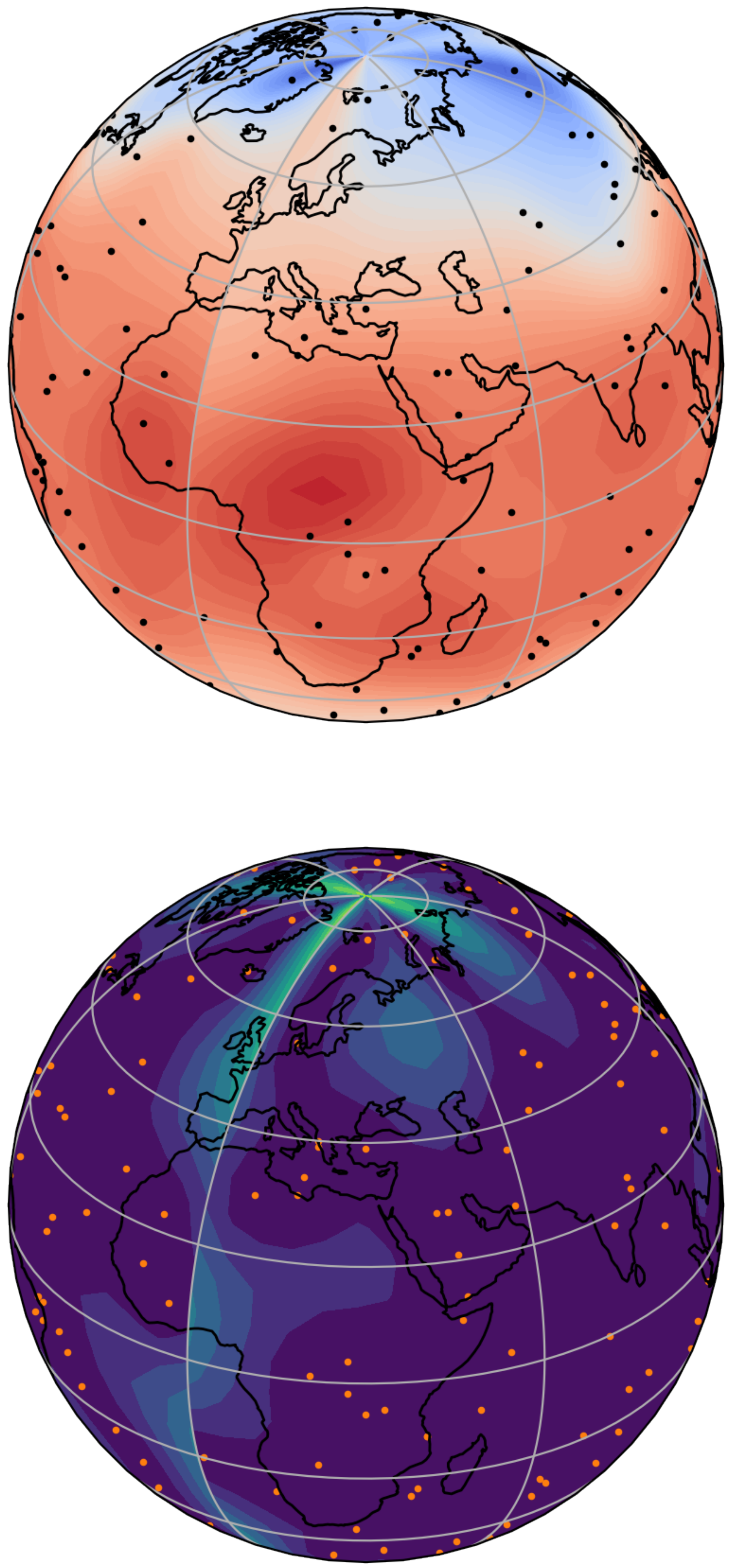


Variance

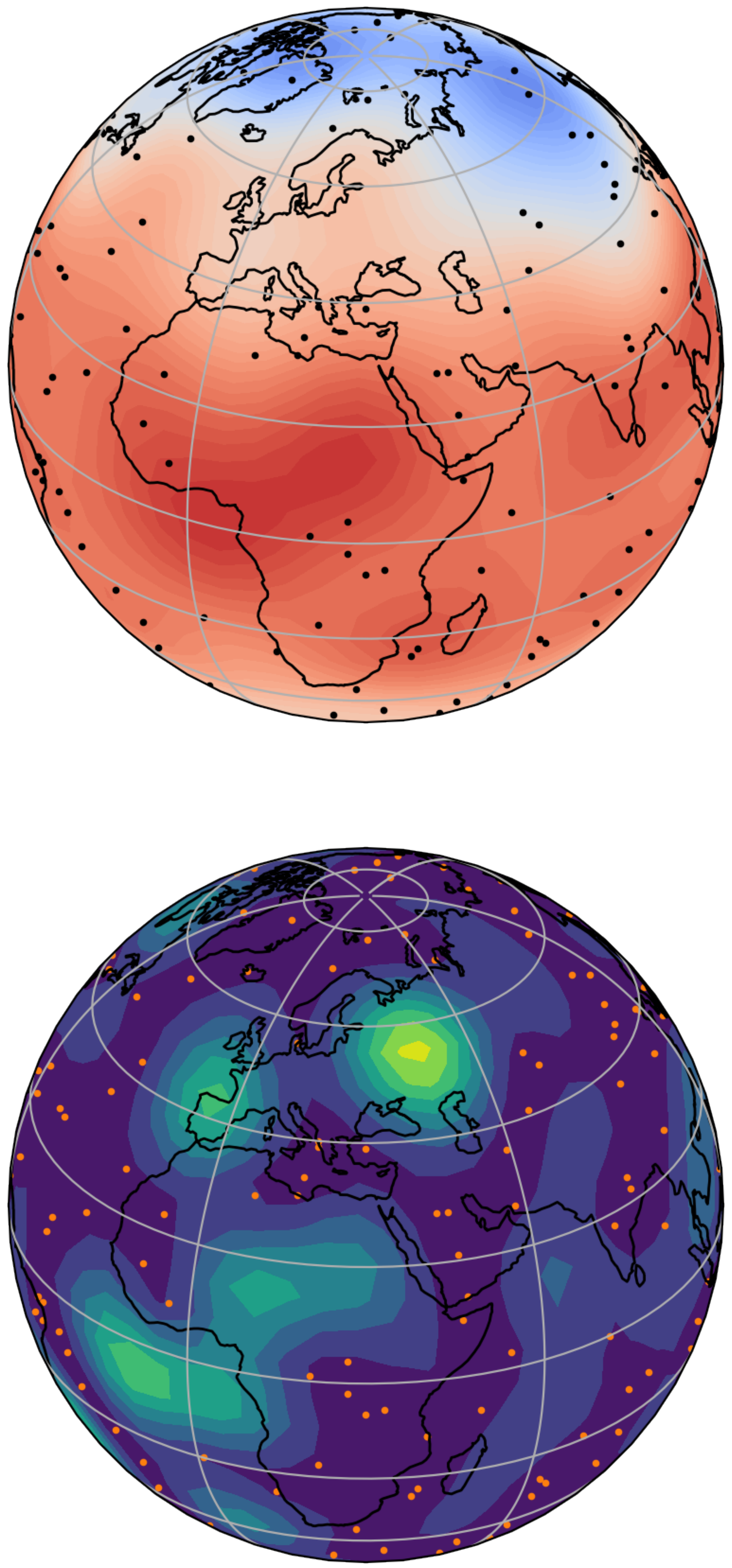


Comparison with Euclidean GPs

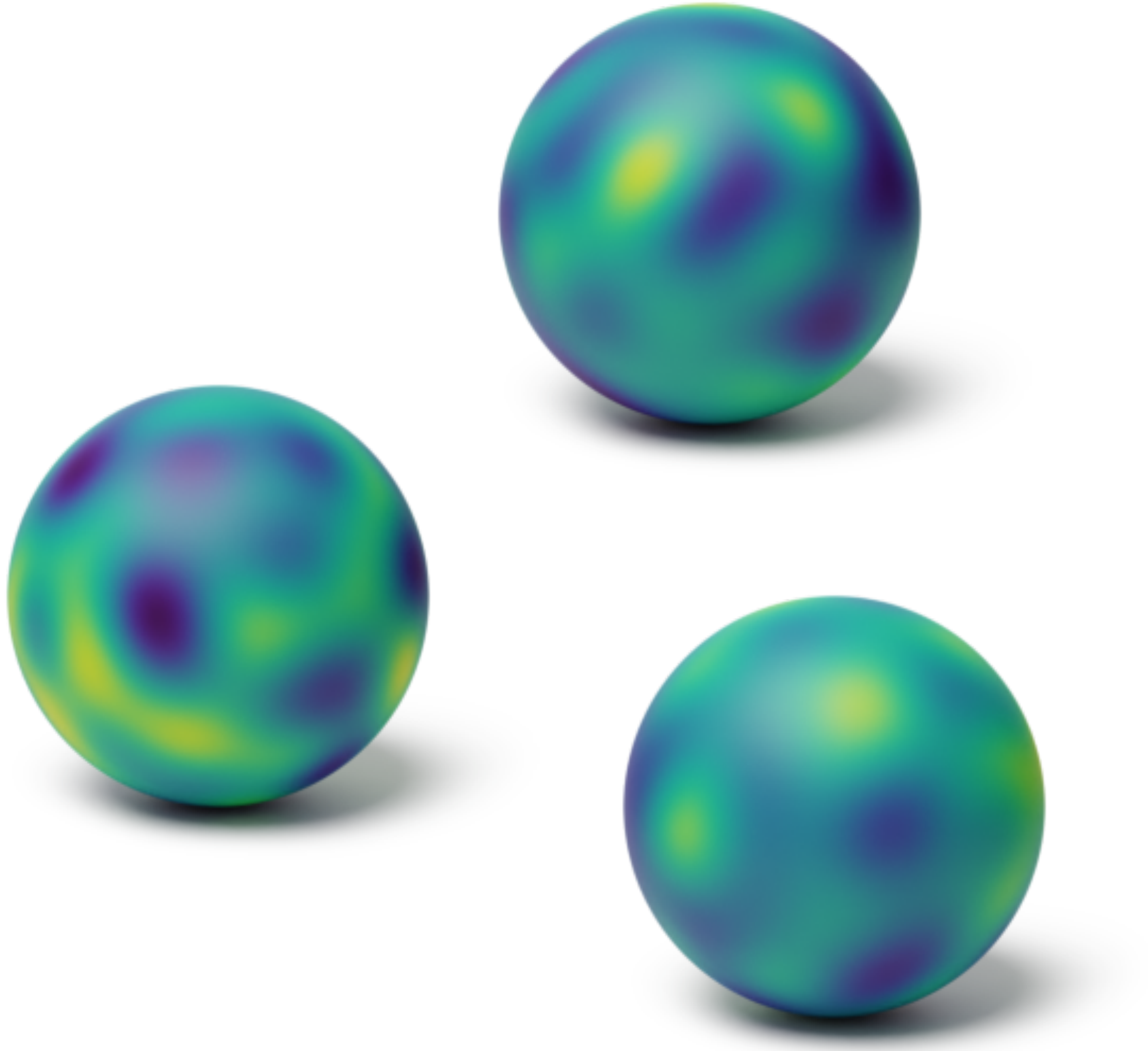
Euclidean



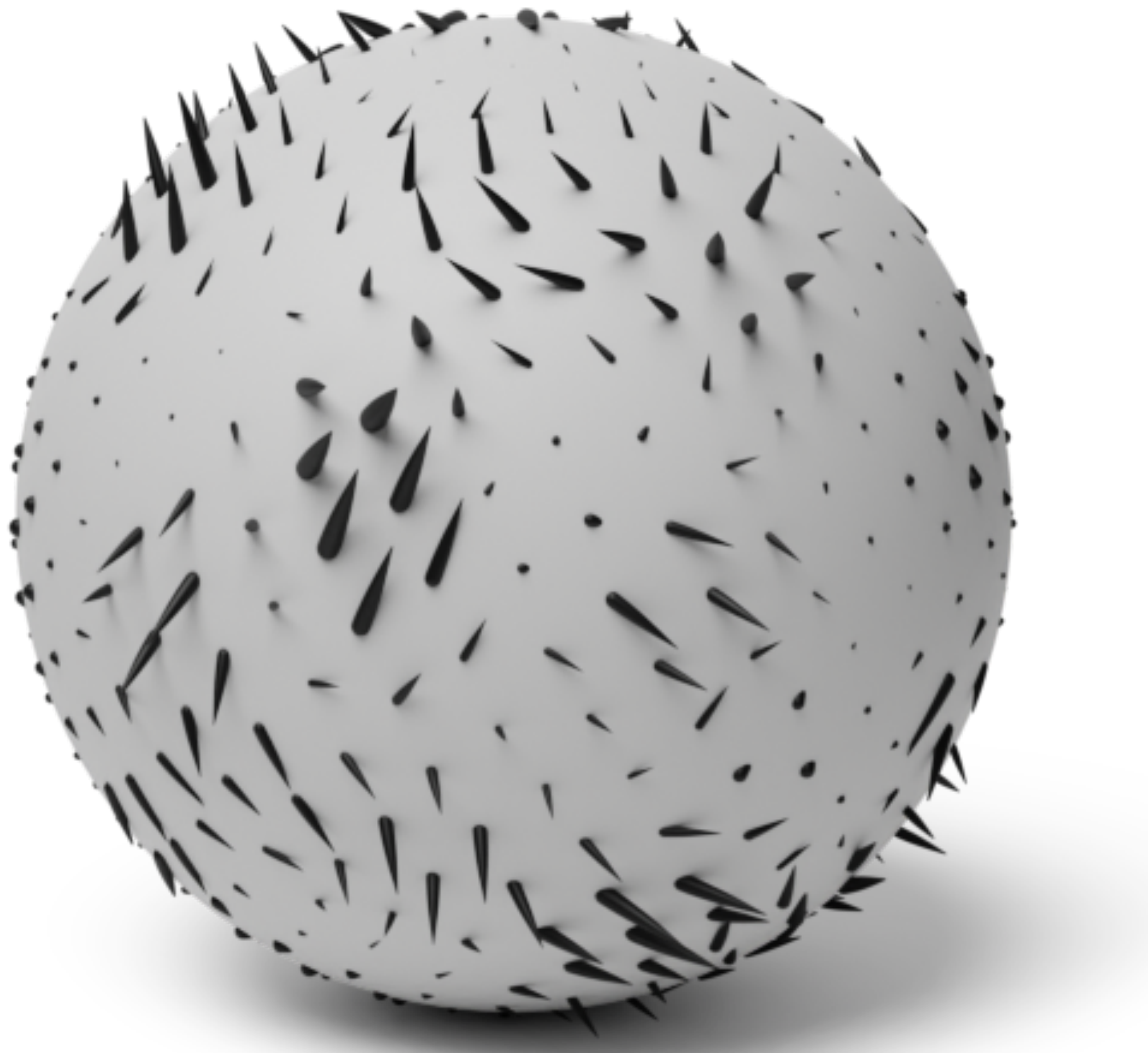
Spherical



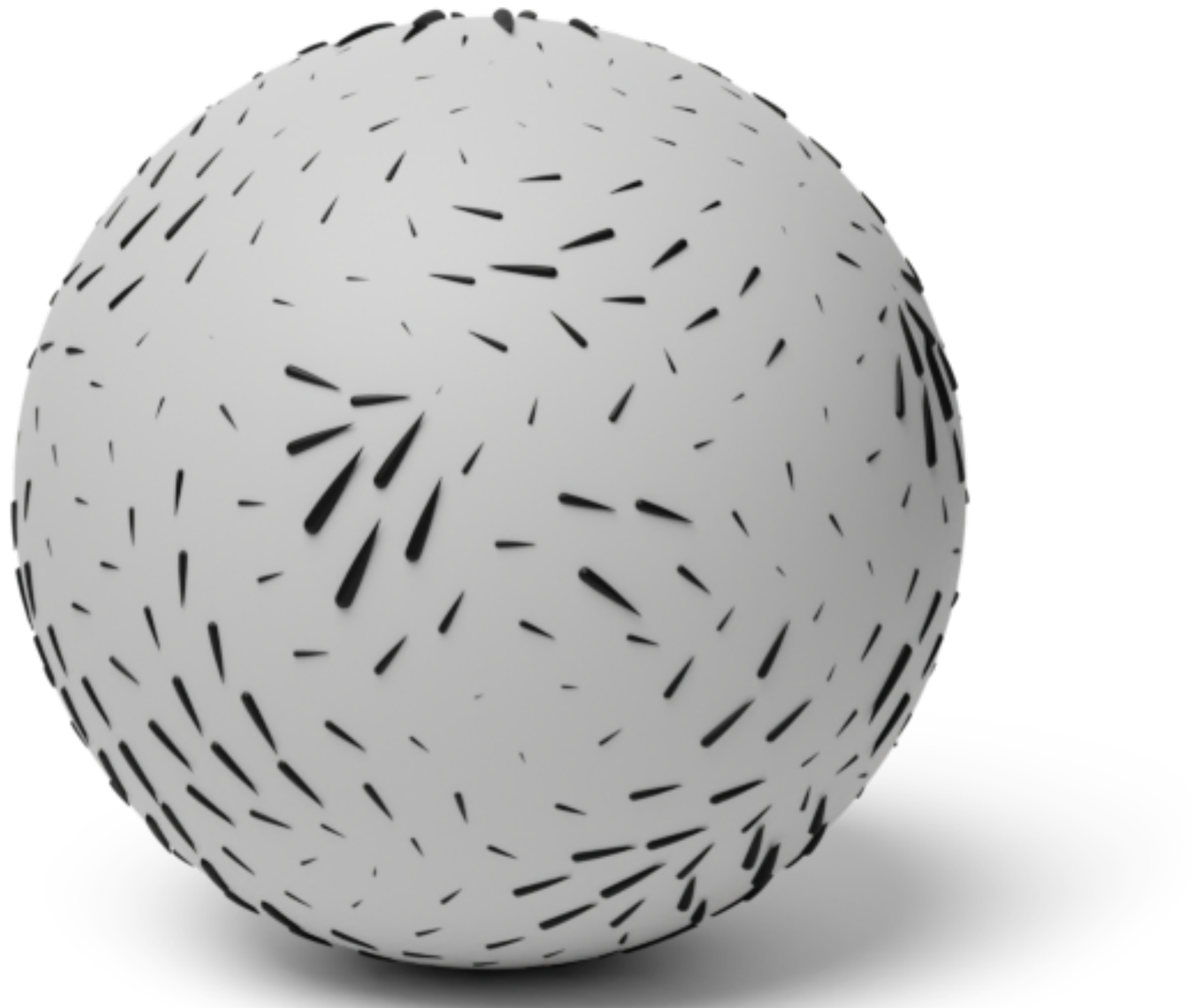
Modelling vector fields on manifolds with GPs



1. Spherical GPs x 3



2. Vector-valued GP $\mathbb{S}^2 \rightarrow \mathbb{R}^3$

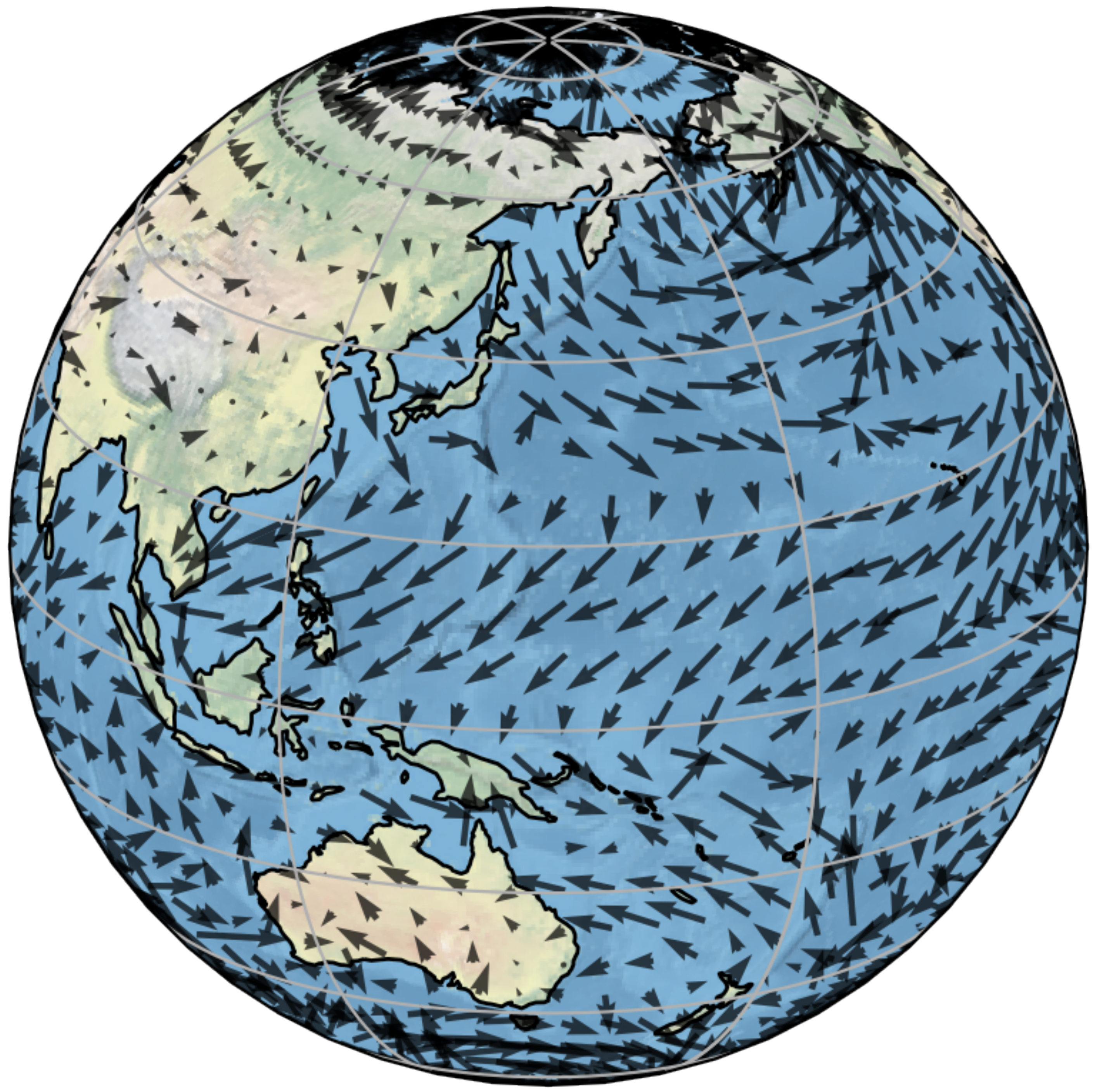


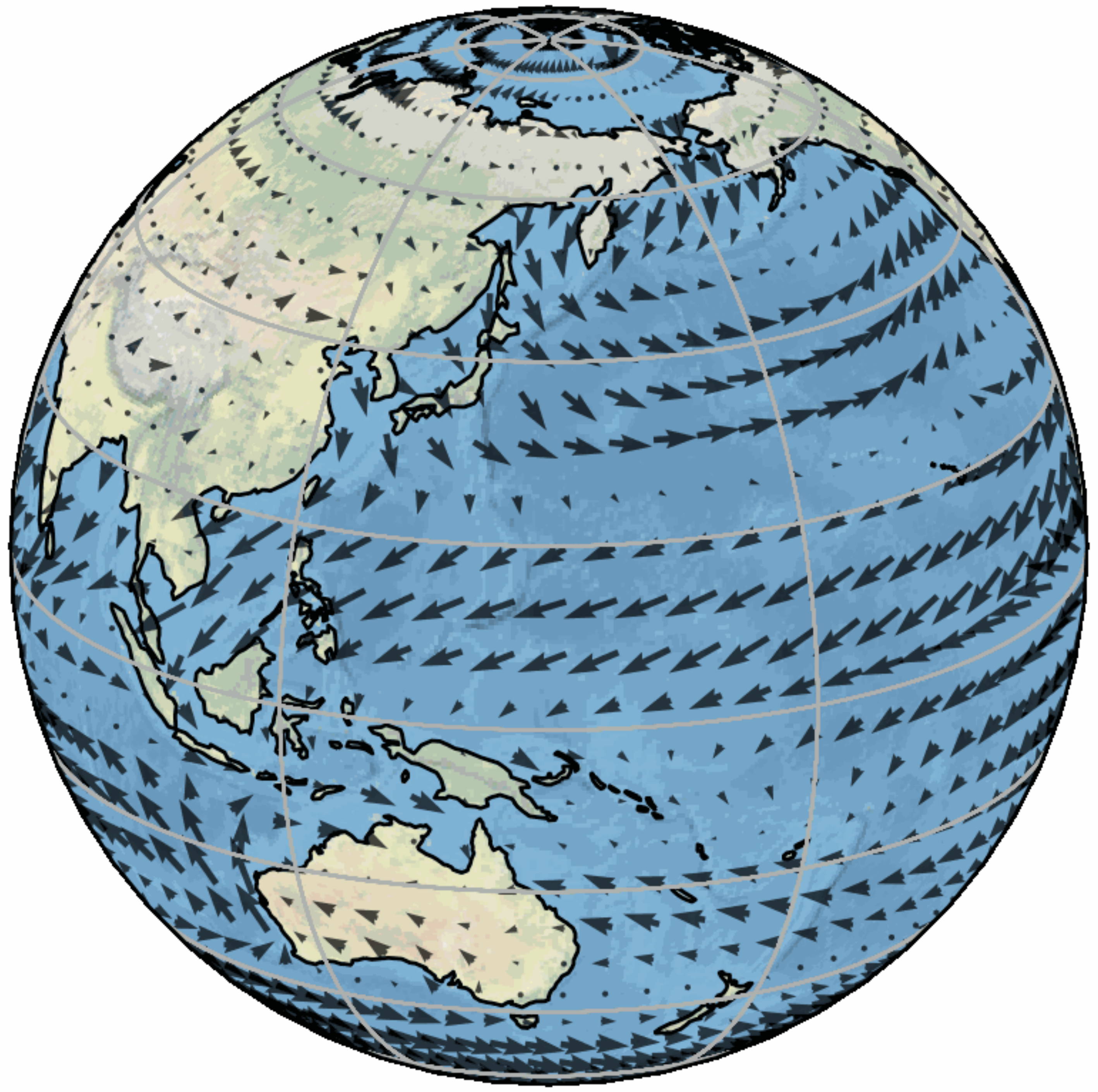
3. Projected GP $\mathbb{S}^2 \rightarrow T\mathbb{S}^2$

Our paper: https://arxiv.org/pdf/2110.14423.pdf

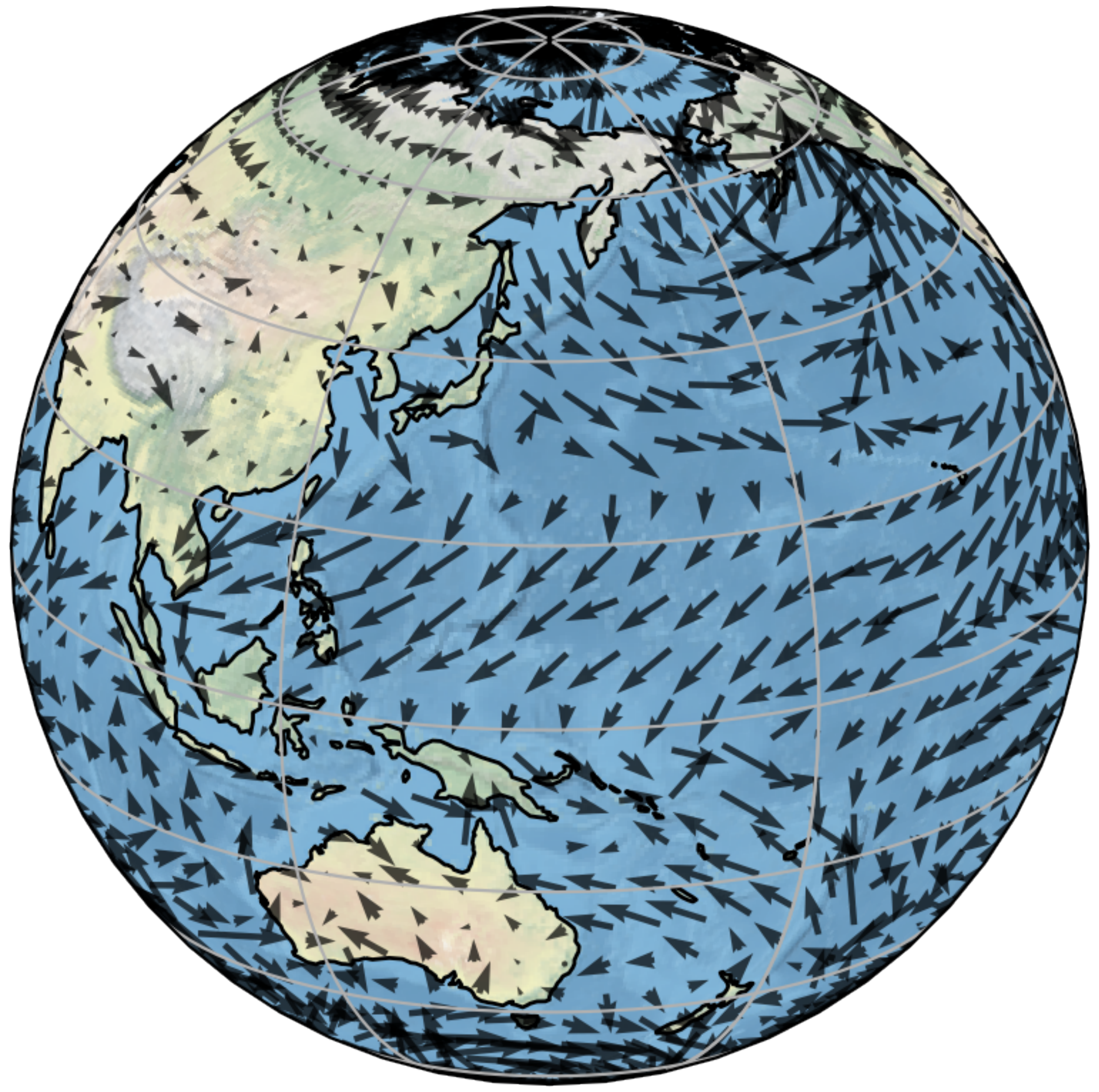
Wind modelling experiment

Ground Truth

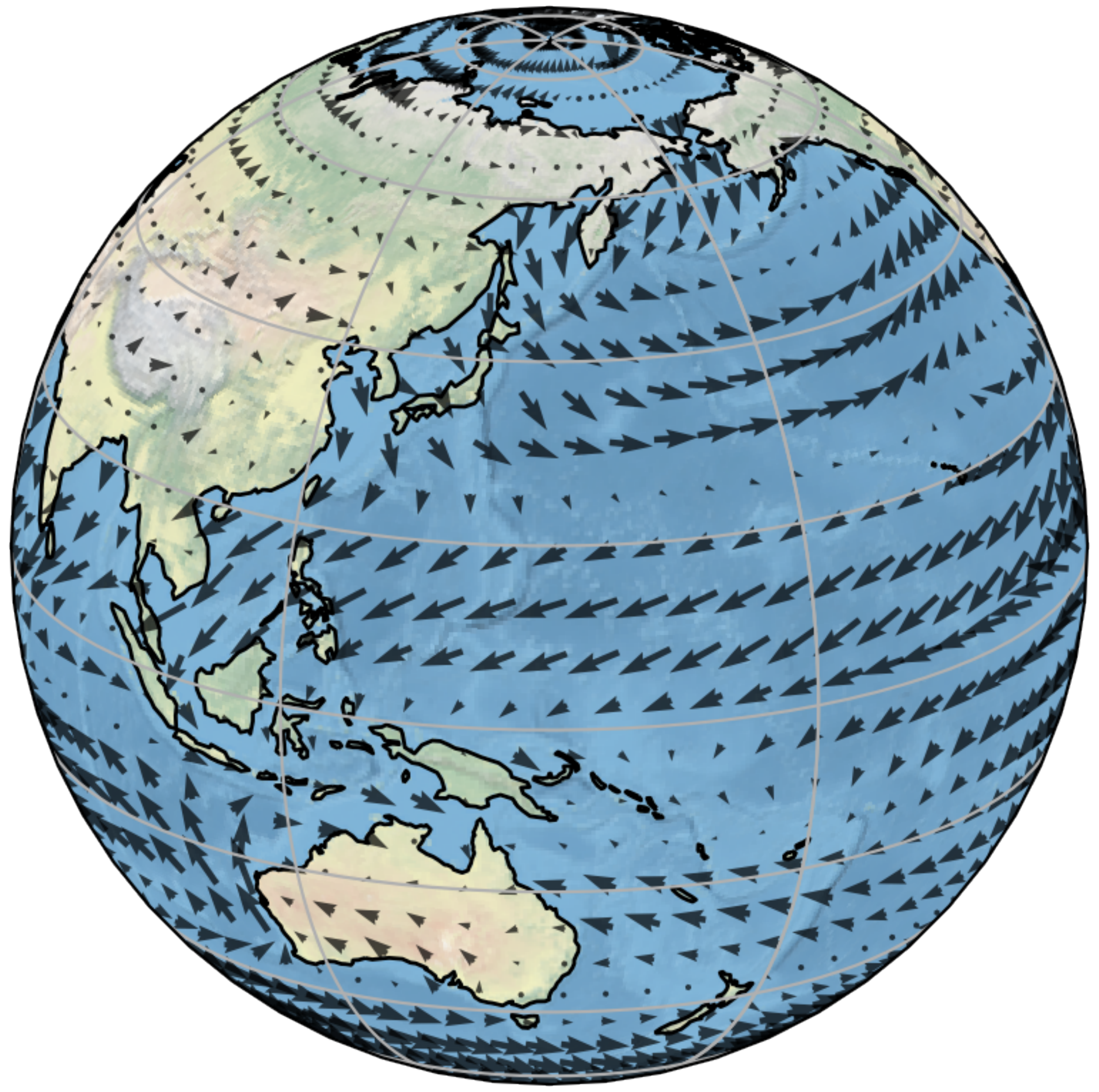




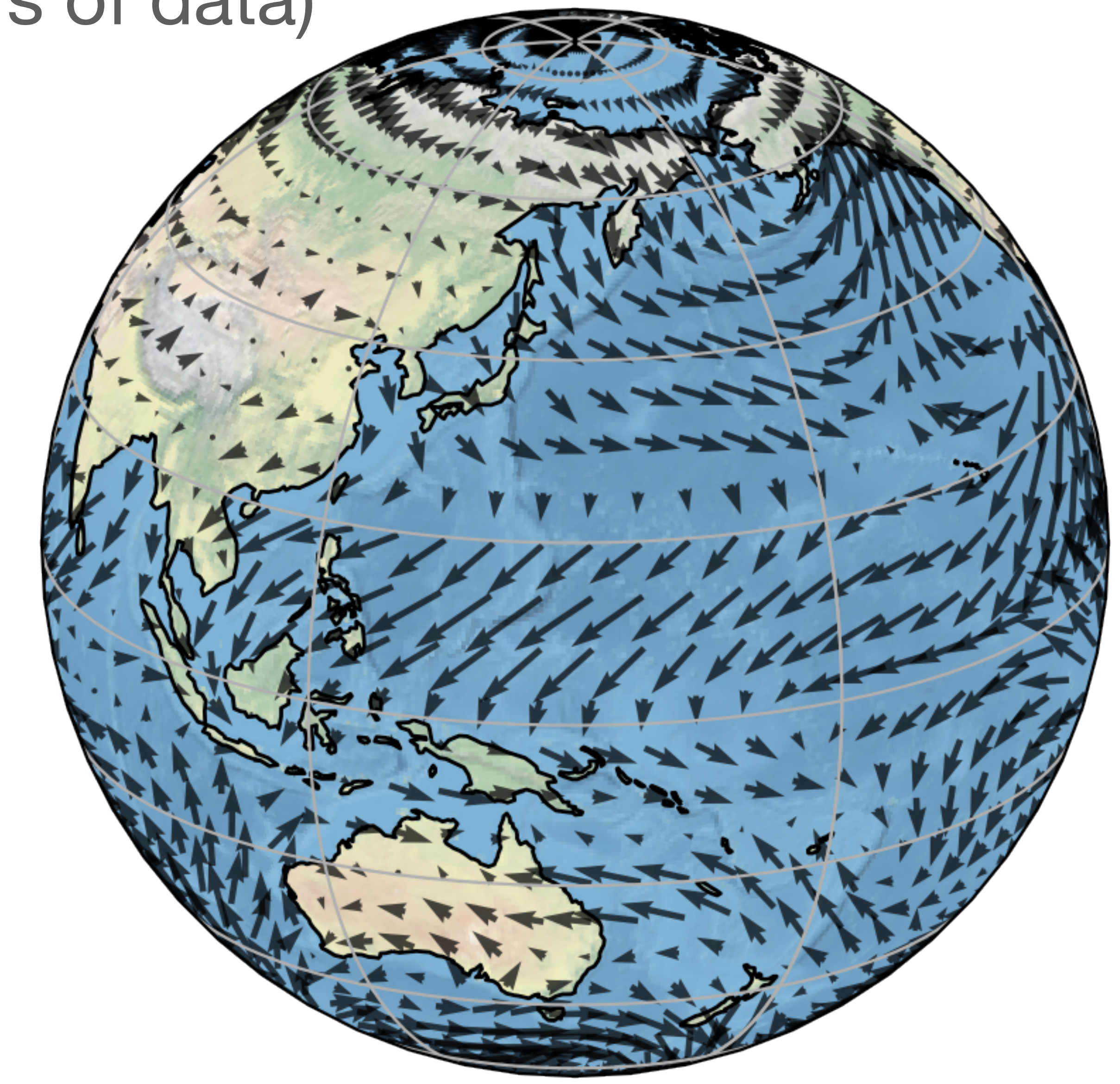
Ground Truth



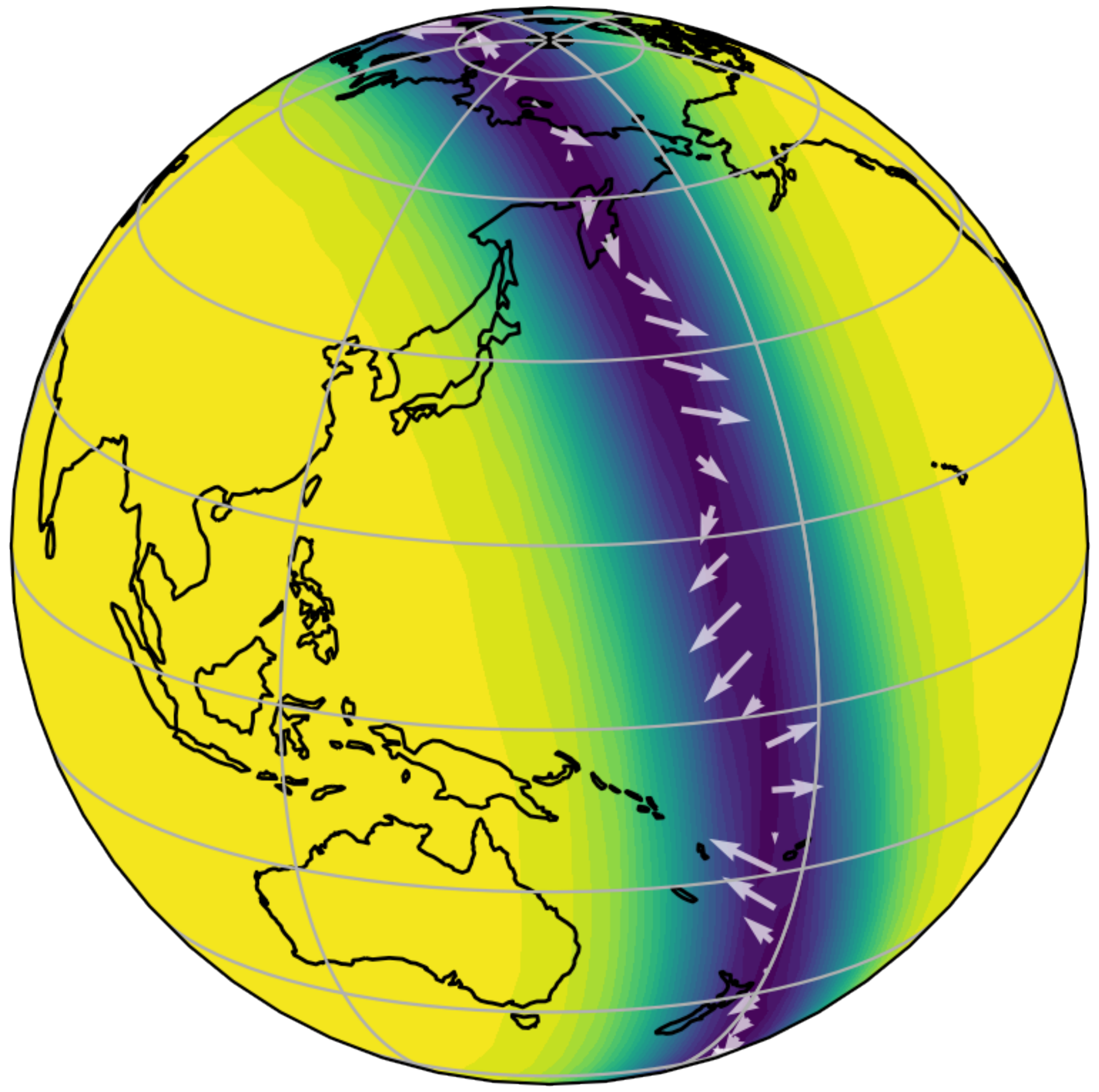
Prior mean



Posterior mean
(12 hrs of data)



Uncertainty
(one hour of data)



Github repo: https://github.com/MJHutchinson/ExtrinsicGaugeIndependentVectorGPs

Summary

- Research in GPs has come a long way to deal with modern requirements
  - Big data
  - Non-Euclidean domains (and vector fields!)
- Many applications to weather/climate science yet to be explored
  - Speeding up computations
  - Black-box data assimilation
  - Dealing with more complicated geometry (e.g. boundary conditions)
- Happy to discuss other applications!