GPs on graphs
Modeling node functions

GPs from Euclidean to non-Euclidean

GP in Euclidean settings

Function on a set $f : X \to \mathbb{R}$

$$f \sim \mathrm{GP}(\mu, k)$$

- Predictive distribution $f_{|\mathbf{y}}$
- Matérn GP family, e.g., diffusion

$$k(x, x') = \sigma^2 \exp\left(-\frac{d(x, x')^2}{2\kappa^2} \right)$$

- Distance-based: geometry-aware, but not well-defined for manifolds, graphs …
- Instead, as solutions of SDEs (Whittle (1963); Lindgren et al. (2011))

$$\left(\frac{2\nu}{\kappa^2} - \Delta \right)^{\frac{\nu}{2}+\frac{d}{4}} f = w$$

- Δ: Laplacian, w: white noise
- implicit, generalizable, domain-aware
- explicit for some domains

GPs on graphs

Modeling node functions

- $\mathbf{f}_0 \sim \mathrm{GP}(\mathbf{0}, \mathbf{K}_0)$ (Borovitskiy et al. 2021)
- Matérn graph kernel

$$\Phi(\mathbf{L}_0)\mathbf{f}_0 = \mathbf{w}_0, \text{ with}$$

$$\Phi(\mathbf{L}_0) = \left(\frac{2\nu}{\kappa^2}\mathbf{I} + \mathbf{L}_0\right)^{\frac{\nu}{2}} \text{ and } \mathbf{w}_0 \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

- The solution has kernel

$$\mathbf{K}_0 = \sigma^2 \sum_{n=0}^{N_0-1} \psi(\lambda_n)\mathbf{u}_n\mathbf{u}_n^\top = \sigma^2\left(\frac{2\nu}{\kappa^2}\mathbf{I} + \mathbf{L}_0\right)^{-\nu}$$

$$\psi(\lambda) = \begin{cases} (\frac{2\nu}{\kappa^2} + \lambda)^{-\nu} & \nu < \infty, \text{Matern} \\ e^{-\frac{\kappa^2}{2}\lambda} & \nu = \infty, \text{Diffusion} \end{cases}$$