

GPs on graphs

Modeling node functions

- $\mathbf{f}_0 \sim \text{GP}(\mathbf{0}, \mathbf{K}_0)$ (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

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

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

GPs from Euclidean to non-Euclidean

GP in Euclidean settings

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

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

- Predictive distribution $f_{|y}$

- 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

Matérn Edge GPs

Derived from SDEs on the edge set

- $\mathbf{f}_1 \sim \text{GP}(\mathbf{0}, \mathbf{K}_1)$
- Matérn graph kernel

$$\text{EVD: } \mathbf{L}_1 = \mathbf{U}_1 \mathbf{\Lambda}_1 \mathbf{U}_1^\top$$

$$\Phi(\mathbf{L}_1) \mathbf{f}_1 = \mathbf{w}_1, \text{ with}$$

$$\Phi(\mathbf{L}_1) = \left(\frac{2\nu}{\kappa^2} \mathbf{I} + \mathbf{L}_1 \right)^{\frac{\nu}{2}} \text{ and } \mathbf{w}_1 \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$$

- The solution gives edge GPs

$$\text{Matérn: } \mathbf{f}_1 \sim \text{GP}\left(0, \left(\frac{2\nu}{\kappa^2} \mathbf{I} + \mathbf{L}_1 \right)^{-\nu}\right)$$

$$\text{Diffusion: } \mathbf{f}_1 \sim \text{GP}\left(0, e^{-\frac{\kappa^2}{2} \mathbf{L}_1}\right)$$

Diffusion on nodes vs on edges

