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

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

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

Matérn Edge GPs

Derived from SDEs on the edge set

- $\mathbf{f}_1 \sim \mathrm{GP}(\mathbf{0}, \mathbf{K}_1)$
- Matérn kernels on the edge space

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

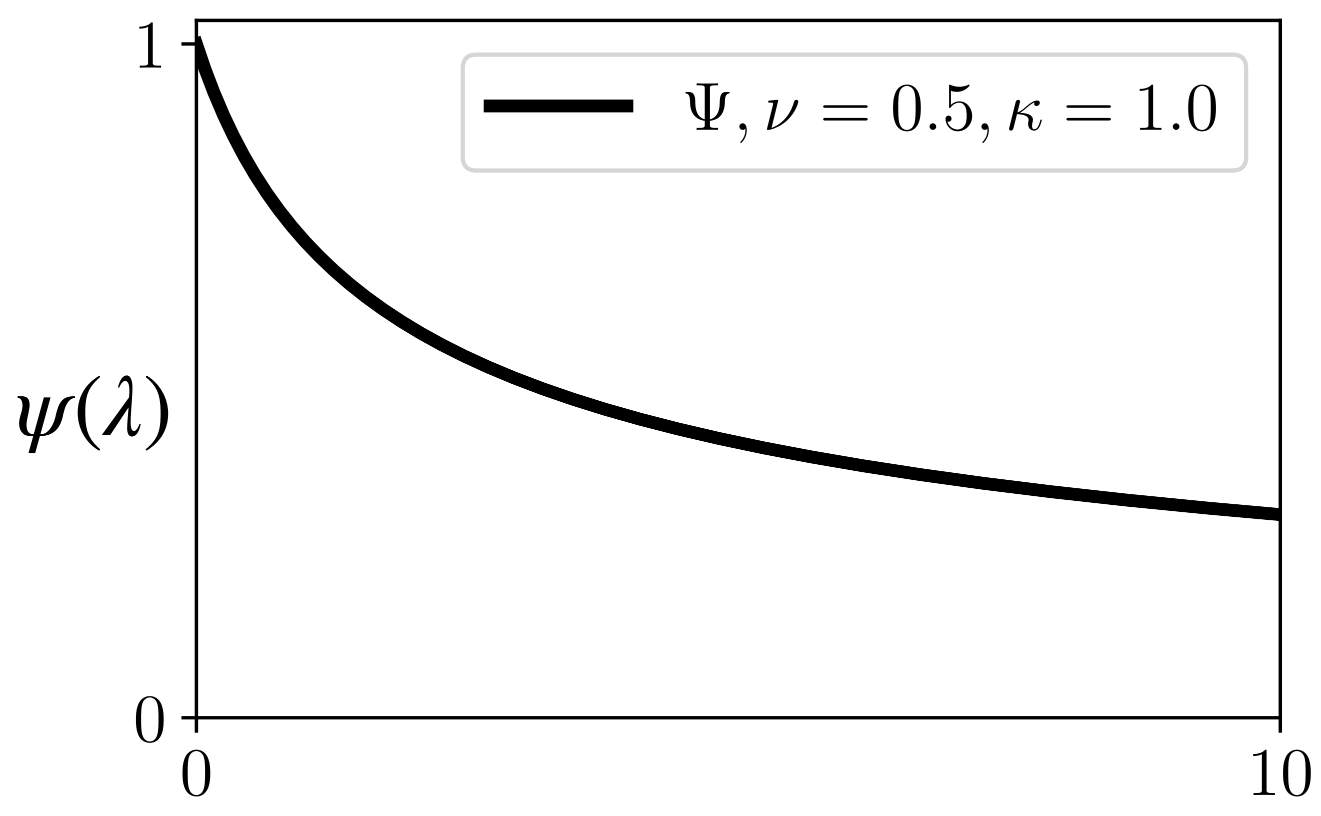
$\Phi(\mathbf{L}_1)\mathbf{f}_1 = \mathbf{w}_1$, with

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

- The solution gives edge GPs

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

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



- Low-pass in the eigen-spectrum

Smoothness

Node function — 0-form (scalar field)

Edge function — 1-form (vector field)

Divergence

Curl