Matérn Gaussian Processes on Graphs

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Abstract

Gaussian processes are a versatile framework for learning unknown functions in a manner that permits one to utilize prior information about their properties. Although many different Gaussian process models are readily available when the input space is Euclidean, the choice is much more limited for Gaussian processes whose input space is an undirected graph. In this work, we leverage the stochastic partial differential equation characterization of Matérn Gaussian processes—a widely-used model class in the Euclidean setting—to study their analog for undirected graphs. We show that the resulting Gaussian processes inherit various attractive properties of their Euclidean and Riemannian analogs and provide techniques that allow them to be trained using standard methods, such as inducing points. This enables graph Matérn Gaussian processes to be employed in mini-batch and non-conjugate settings, making them more accessible to practitioners and easier to deploy within larger learning frameworks.

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 $\quad\kappa$: length scale $\quad\nu$: smoothness

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

Defines a Gaussian process $f : \mathbb{R}^d \to \mathbb{R}$

This work: given a graph $G = (V, E)$ define GPs $f : V \to \mathbb{R}$

Matérn GPs: solutions of stochastic partial differential equations

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

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

This work: replace Δ with graph Laplacian and $\mathcal{W}$ with $\mathrm{N}(\mathbf{0}, \mathbf{I})$

Matérn kernels for graphs

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

$\mathbf{\Delta}$: graph Laplacian $\qquad \boldsymbol{\mathcal{W}}$: standard Gaussian

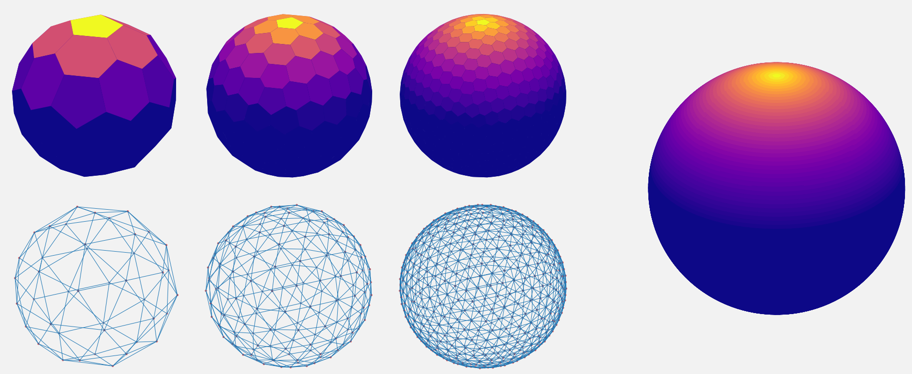
Matérn: $\quad k_\nu(x,x') = \frac{\sigma^2}{C_\nu} \sum_{n=1}^{|G|} \left(\frac{2\nu}{\kappa^2} + \lambda_n\right)^{-\nu} \boldsymbol{f}_n(x)\boldsymbol{f}_n(x')$

Sq. exp.: $\quad k_\infty(x,x') = \frac{\sigma^2}{C_\infty} \sum_{n=1}^{|G|} e^{-\frac{\kappa^2}{2}\lambda_n} \boldsymbol{f}_n(x)\boldsymbol{f}_n(x')$

$\lambda_n, \boldsymbol{f}_n$: eigenvalues, eigenvectors of graph Laplacian

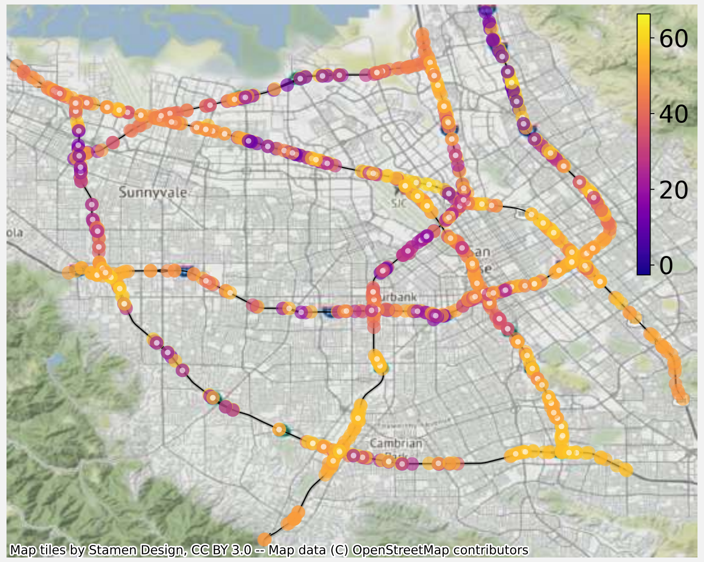
Large graphs: approximate with top N eigenpairs and truncate sum

Connection with Riemannian Matérn GPs

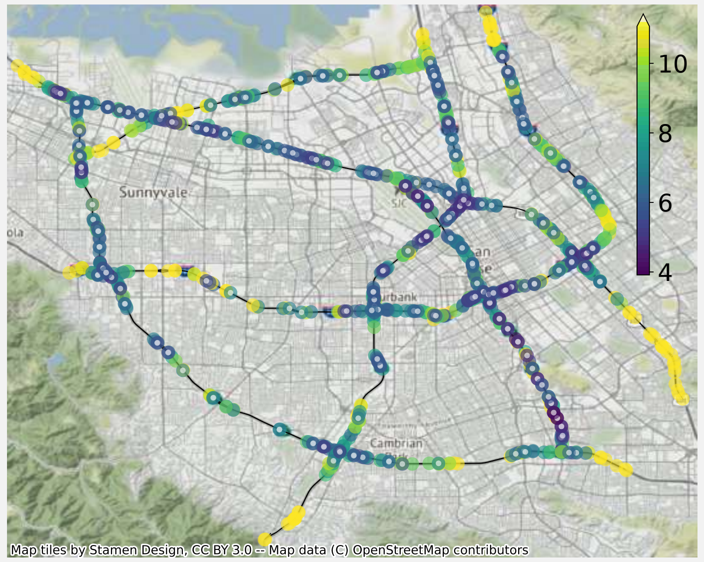


Riemannian Matérn GPs: limits of graph Matérn GPs

Example: graph interpolation with traffic data



(a) Mean



(a) Standard deviation:

(a) Mean

(b) Standard Deviation

References

[1] V. Borovitskiy, A. Terenin, P. Mostowsky, and M. P. Deisenroth. Matérn Gaussian Processes on Riemannian Manifolds. NeurIPS, 2020.
[2] H. Rue and L. Held. Markov Random Fields: Theory and Applications. CRC Press, 2005.