Scalable Deep Gaussian Markov Random Fields for General Graphs

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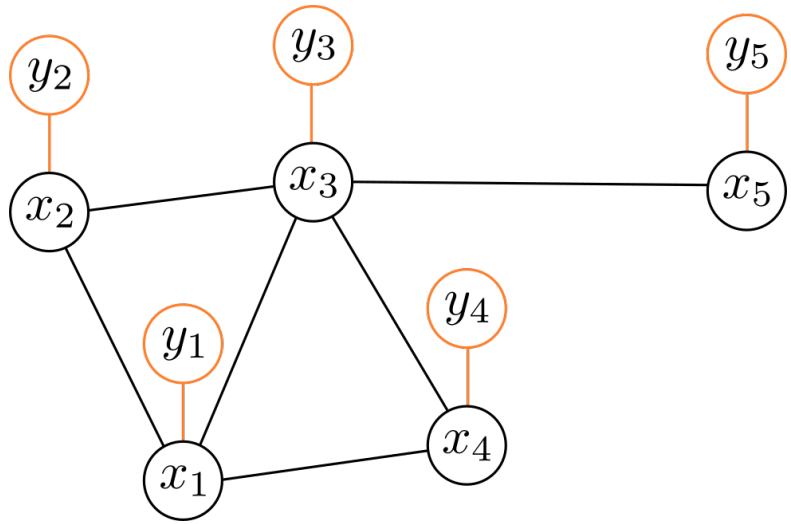
A Layered Gaussian Model on Graphs



- Latent nodes $\boldsymbol{x}$
  - Gaussian prior $\boldsymbol{x} \sim \mathcal{N}\left(\boldsymbol{\mu}, Q^{-1}\right)$
  - Gaussian Markov Random Field (GMRF)
- Noisy observations
  - $\boldsymbol{y} = \boldsymbol{x} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 I\right)$
- Predictions for unobserved nodes
- Conjugate setting

Deep GMRFs (DGMRFs)[1]

- Define GMRF using affine map g

$$\boldsymbol{z} = g(\boldsymbol{x}) = G\boldsymbol{x} + \boldsymbol{b}, \quad \boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, I) \tag{1}$$

[1] Per Sidén and Fredrik Lindsten. "Deep Gaussian Markov Random Fields". In: *Proceedings of the 37th International Conference on Machine Learning*. 2020

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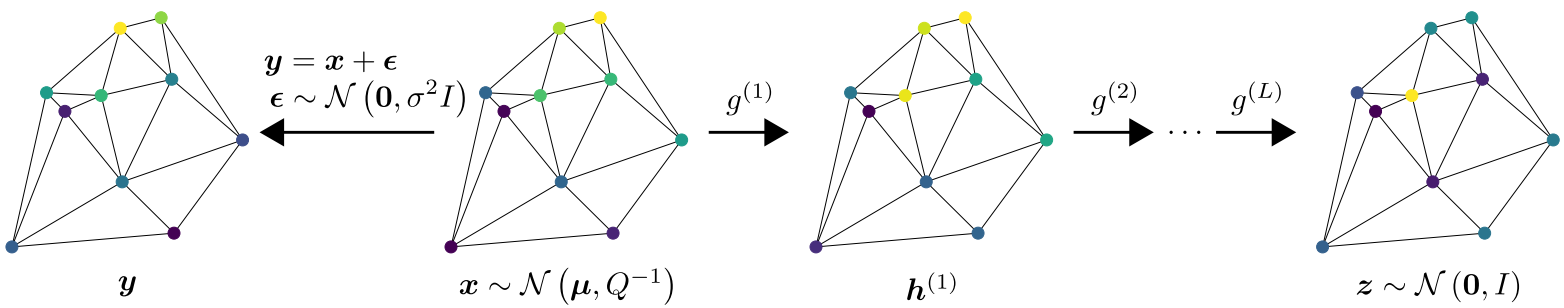
- Layer structure

$$g = g^{(L)} \circ g^{(L-1)} \circ \cdots \circ g^{(1)} \tag{2}$$



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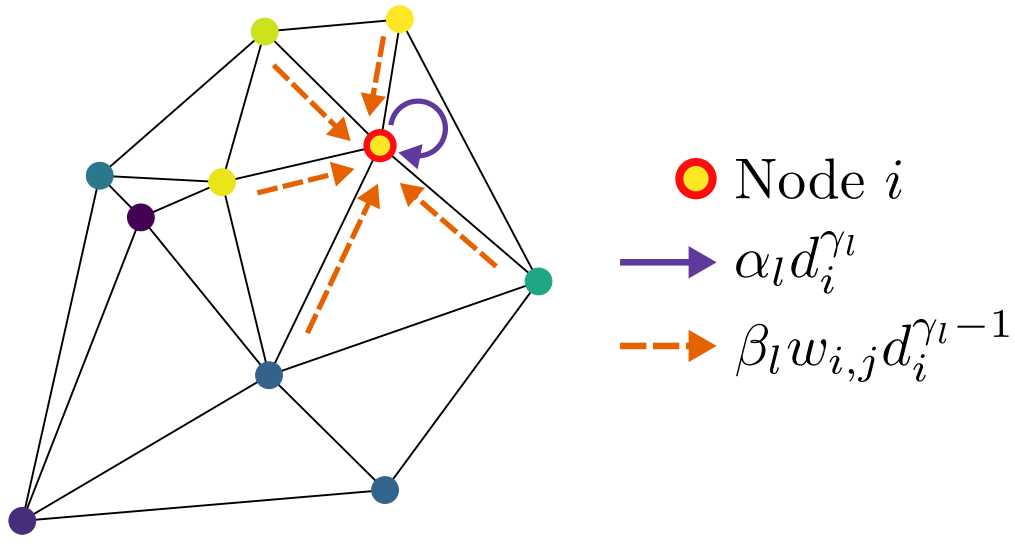
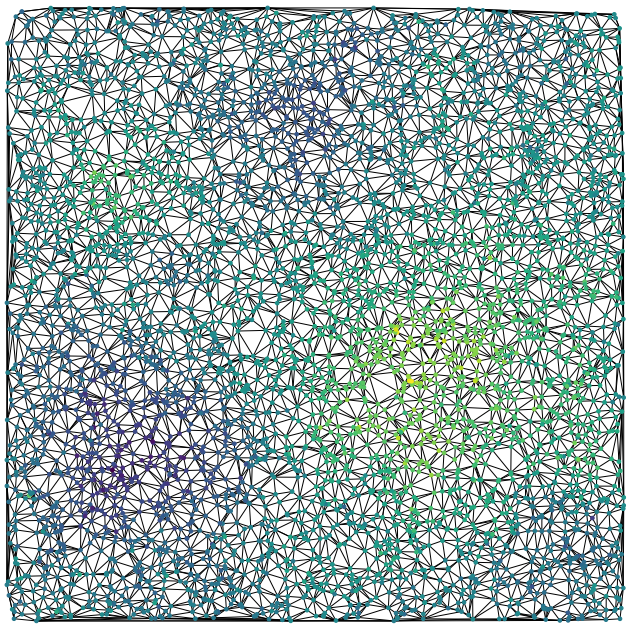
A Deep GMRF Layer for Graphs



$$h_i^{(l)} = b_l + \alpha_l d_i^{\gamma_l} h_i^{(l-1)} + \beta_l d_i^{\gamma_l - 1} \sum_{j \in n(i)} w_{i,j} h_j^{(l-1)} \tag{3}$$

Training and Inference



- Efficient training of layer parameters
  - Maximize ELBO
  - Scalable methods for $\log|\det(G)|$
  - Re-use layers to define variational distribution
- Exact posterior inference for latent field $\boldsymbol{x}$

Experiments

- Experiments on Synthetic, Wikipedia, and Spatial graphs
- Principled uncertainty estimates

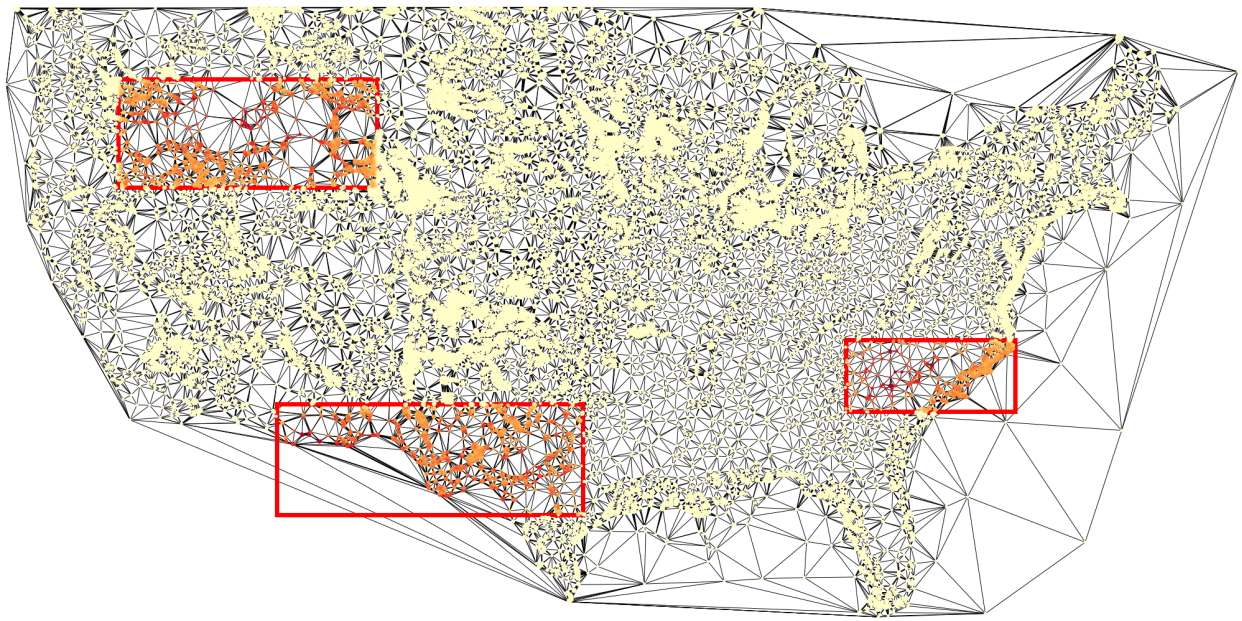


Figure: Posterior marginal std.-dev.

Links and Contact Information

Code available: `github.com/joeloskarsson/graph-dgmrf`

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