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Variance Reduction for Inverse Trace Estimation via Random Spanning Forests

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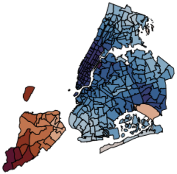
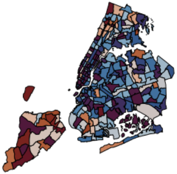
- However, it is not always easy to compute...
- In this work, we focus on

$$f(\mathsf{L}) = q(\mathsf{L} + q\mathsf{I})^{-1},$$

where $q > 0$ and L is symmetric and diagonally dominant *i.e.* $\forall i \in \mathcal{V}$, $\sum_{j=1}^{n} |\mathsf{L}_{i,j}| \leq |\mathsf{L}_{i,i}|$.

Hyperparameter Selection for Graph Signal Smoothing

Original Signal: 

y: 

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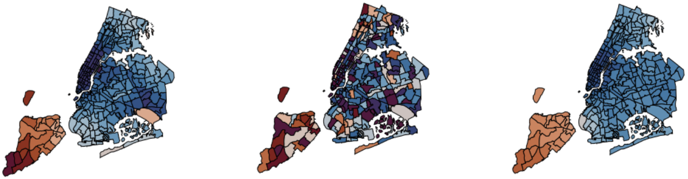

Figure: Median taxi fees paid in drop-off locations in NYC

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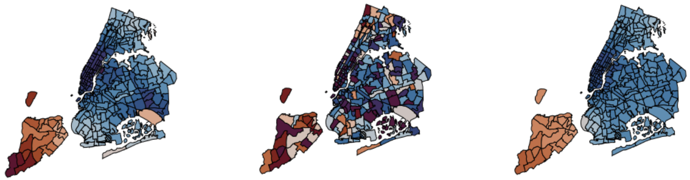

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Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, w)$,

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} q \underbrace{||\mathbf{y} - \mathbf{x}||^2}_{\text{Fidelity}} + \underbrace{\mathbf{x}^T \mathrm{L}\mathbf{x}}_{\text{Regularization}} \quad , \quad q > 0$$

where L is the graph Laplacian and $\mathbf{x}^T \mathrm{L}\mathbf{x} = \sum_{(i,j)\in\mathcal{E}} w(i,j)(x_i - x_j)^2$.

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- The denoising error $||\mathbf{x} - \hat{\mathbf{x}}||_2^2$ highly depends on q.
- Many methods of finding good value of q needs to compute $\mathrm{tr}(\mathsf{K})$.
- However, computing the inverse takes $\mathcal{O}(n^3)$ operations.

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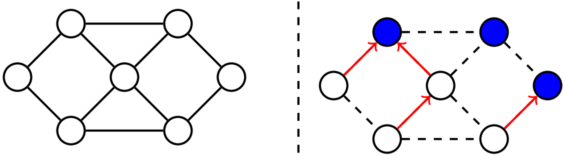

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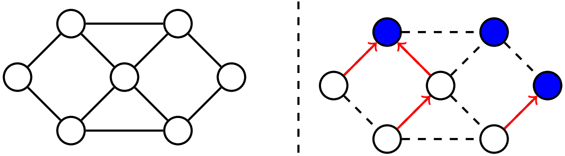

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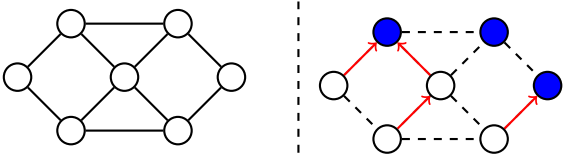

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- For a particular distribution [AG13], we have useful links with graph-related algebra.

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- Empirical results shows that is comparable with Girard's estimator.
- In this work, we give two ways of improving this estimator.

Gradient Descent Update as Control Variate

- Estimation of K can be considered as minimizing the loss following function:

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$$\mathsf{S}_{k+1} = \mathsf{S}_k - \alpha(\mathsf{K}^{-1}\mathsf{S}_k - \mathsf{I}).$$

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- Then, we improve them as follows [Pil+21a]:

$$\tilde{\mathsf{Z}} := \tilde{\mathsf{S}} - \alpha(\mathsf{K}^{-1}\tilde{\mathsf{S}} - \mathsf{I})$$
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- Focusing on the trace, we define $\tilde{s} := \mathrm{tr}(\tilde{\mathsf{Z}})$ and $\bar{s} := \mathrm{tr}(\bar{\mathsf{Z}})$.

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- For example, the optimal value of α for $\bar{s}$ is:

$$\alpha^\star = \frac{\mathsf{Cov}(s, \mathsf{tr}(\mathsf{K}^{-1}\bar{\mathsf{S}} - \mathsf{I}))}{\mathsf{Var}(\mathsf{tr}(\mathsf{K}^{-1}\bar{\mathsf{S}} - \mathsf{I}))}.$$

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- One can either choose a value for α from the safe range ($e.g.$ $\alpha = \frac{2q}{q+2d_{max}}$) or estimate from the samples:

$$\hat{\alpha} = \frac{\widehat{\mathsf{Cov}}(s, \mathsf{tr}(\mathsf{K}^{-1}\bar{\mathsf{S}} - \mathsf{I}))}{\widehat{\mathsf{Var}}(\mathsf{tr}(\mathsf{K}^{-1}\bar{\mathsf{S}} - \mathsf{I}))}.$$

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- For certain allocations N_k's, s_{st} has a reduced variance.
- We find a such random variable Y in RSFs!

Comparison with SOTA

- We compare the proposed algorithms with Hutchinson's estimator combined with several linear solvers.

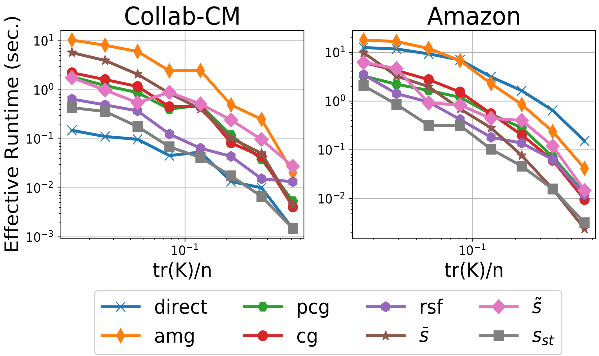

Figure: Effective Runtime vs $\mathrm{tr}(K)/n$.

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- We validate these methods over real-life datasets.
- We hope to extend these results for estimating other Laplacian-based quantities, such as effective resistances.

References

Luca Avena and Alexandre Gaudillière. “Random spanning forests, Markov matrix spectra and well distributed points”. In: *arXiv preprint arXiv:1310.1723* (2013).

Simon Barthelmé et al. “Estimating the inverse trace using random forests on graphs”. In: *arXiv preprint arXiv:1905.02086* (2019).

Yusuf Pilavcı et al. “Variance reduction in stochastic methods for large-scale regularised least-squares problems”. In: *arXiv preprint arXiv:2110.07894* (2021).

Yusuf Yiğit Pilavcı et al. “Graph tikhonov regularization and interpolation via random spanning forests”. In: *IEEE transactions on Signal and Information Processing over Networks* 7 (2021), pp. 359–374.

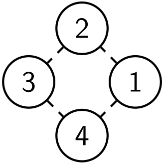
Questions

If you are hiring post-docs, scan me!

Thanks! Questions?

Estimating K with Forests

- We previously proposed two estimators for K [Pil+21b]:



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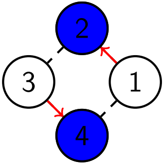

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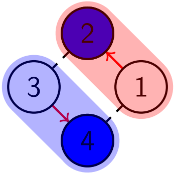

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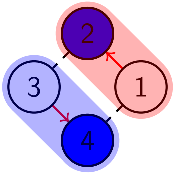

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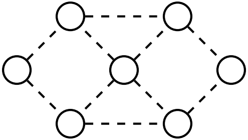

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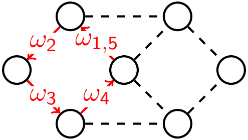

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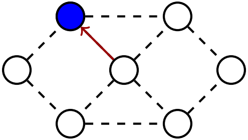

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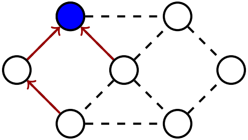

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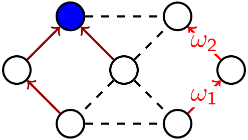

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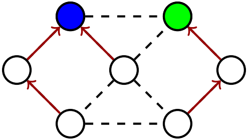

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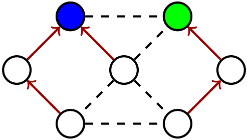

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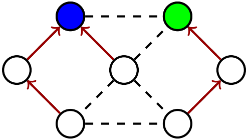

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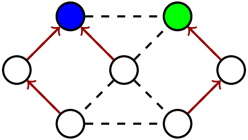

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  - $s' \sim \sum_{i=1}^{n} \text{Ber}\left(\frac{q}{q+d_i}\right)$
  - Sampling RSFs given $s' \in C_k$ is easy.

Inverse Trace Estimation: Hutchinson's Estimator

- SOTA for estimating tr(K) is Hutchinson's estimator []:

$$h := \frac{1}{N}\sum_{i=1}^{N} \mathbf{a}^{(i)\top} \mathsf{K} \mathbf{a}^{(i)}$$

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- It can be done via:
  - Direct computation via Cholesky decomposition
  - (Preconditioned) Iterative solvers
  - Algebraic Multigrid solvers
  - ...