

Wilson's Algorithm for Randomized Linear Algebra

Yusuf Yiğit Pilavcı

09/06/2022



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- ▶ In large scale, faster algorithms might be necessary
- ▶ Randomized numerical linear algebra (RNLA) aims to facilitate them via Monte Carlo methods [Martinsson and Tropp 2020].
- ▶ The algorithms in this branch run under a scheme called sample-and-solve.



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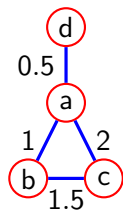


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 - ▶ Machine learning (semi-supervised learning, GNNs, ...) [Zhu; Wu et al.]
 - ▶ Graph visualization, clustering, sparsification ...
- ▶ We leverage the rich theoretical links between the graph Laplacians and a special random process over graphs, called Random Spanning Forests.

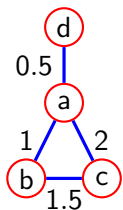


Graphs and Matrices



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

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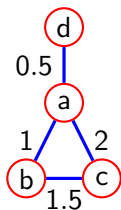


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Adjacency matrix W

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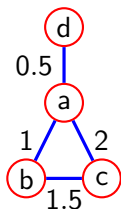
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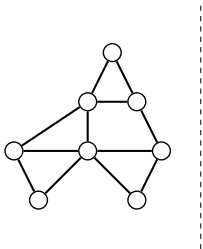
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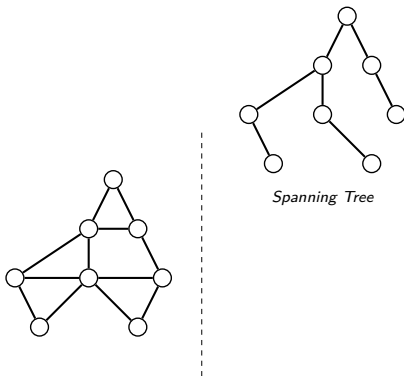
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Laplacian matrix $L = D - W$

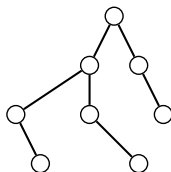
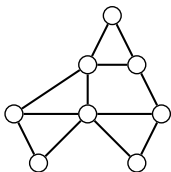
Spanning Forests, Roots and Partitions



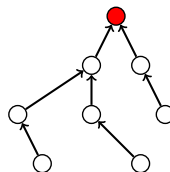
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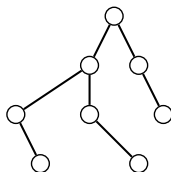
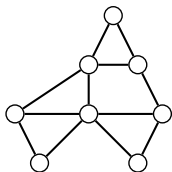


Spanning Tree

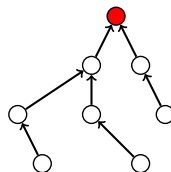


Rooted Spanning Tree

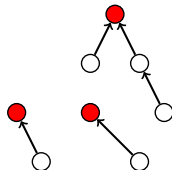
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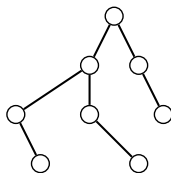
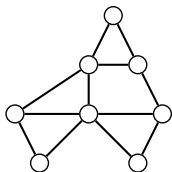


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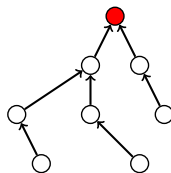


Rooted Spanning Forest

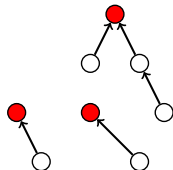
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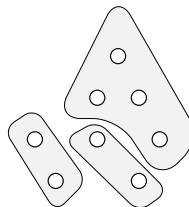
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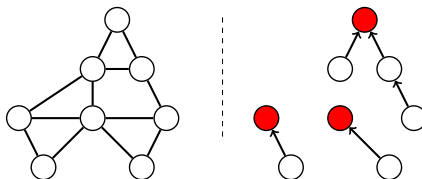
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Partition

A few more notation

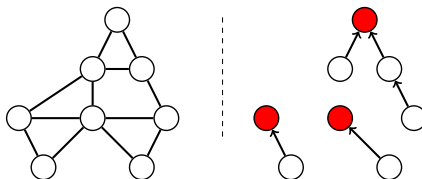
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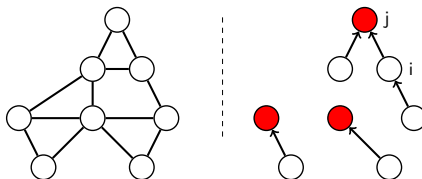
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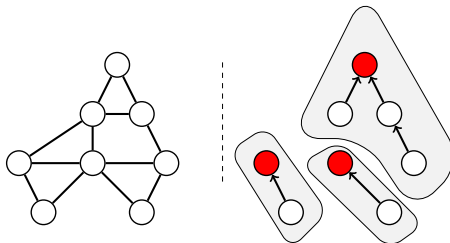
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Random Spanning Forests: **What**, Why and How?

Definition (RSF)

A random spanning forest Φ_q on a graph \mathcal{G} is spanning forest selected over all spanning forests of \mathcal{G} according to the following distribution:

$$P(\Phi_q = \phi) \propto q^{|\rho(\phi)|} \prod_{(i,j) \in \mathcal{E}_\phi} w(i,j)$$



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- $q > 0$ changes the expected number of roots.



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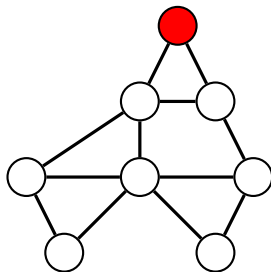
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- ▶ Moreover, we have the following identity:

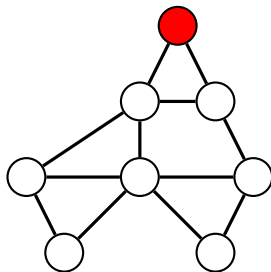
$$\forall i, j \in \mathcal{V}, \quad \mathbb{P}(r_{\Phi_q}(i) = j) = K_{i,j}, \text{ with } K = q(L + qI)^{-1}.$$



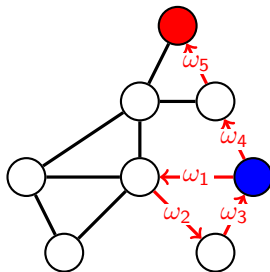
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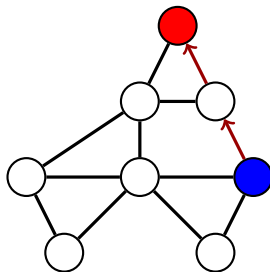
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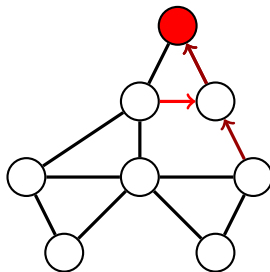
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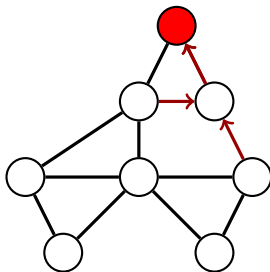
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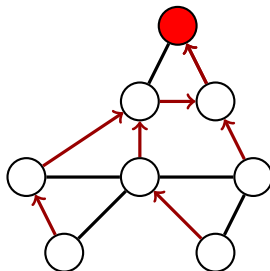
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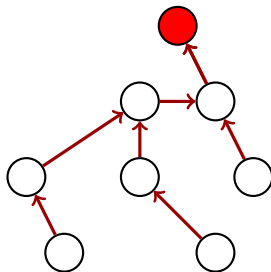
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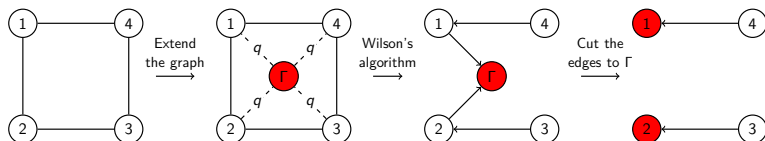


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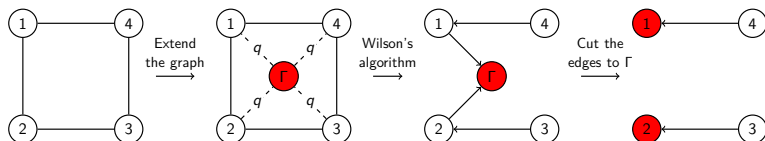


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- ▶ The time complexity is $\mathcal{O}(\frac{|\mathcal{E}|}{q})$.

Problems

- ▶ Graph signal smoothing.
- ▶ Trace estimation.



Graph Signal Smoothing

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

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

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



Graph Signal Smoothing

- ▶ The explicit solution to this problem is:

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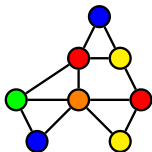
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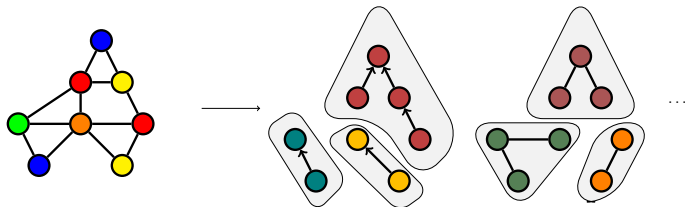
- ▶ Direct computation of \mathbf{K} requires $\mathcal{O}(n^3)$ elementary operations due to the inverse.
- ▶ For large n , iterative methods and polynomial approximations are state-of-the-art. Both compute $\hat{\mathbf{x}}$ in linear time in the number of edges $|\mathcal{E}|$.



Forest Estimator

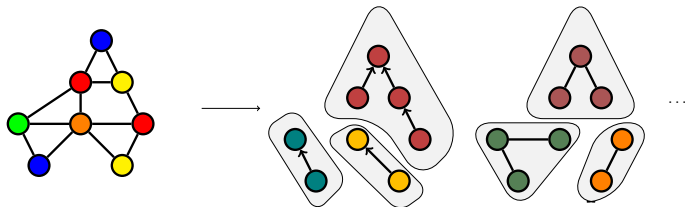


Forest Estimator



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- ▶ Random partitions are sampled via random spanning forests.
- ▶ This yields an unbiased estimator $\bar{\mathbf{x}}$.

Comparison with State of the art (SOTA)

- ▶ We compare $\bar{\mathbf{x}}$ with:
 - ▶ Direct computation via Cholesky decomposition,
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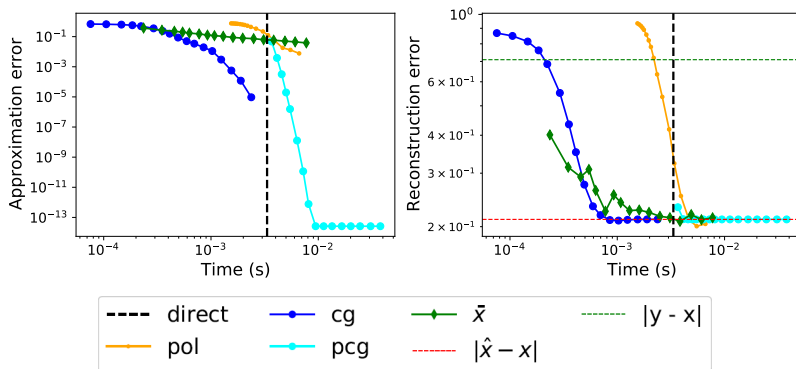
- ▶ We compare $\bar{\mathbf{x}}$ with:
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 - ▶ (Preconditioned) Conjugate gradient descent,
- ▶ We assume a smooth original signal \mathbf{x} and noisy measurements $\mathbf{y} = \mathbf{x} + \epsilon$ with $\epsilon \in \mathcal{N}(0, \sigma)$.



Comparison with State of the art (SOTA)

- We compare all algorithms in approximation error (error respect to $\hat{\mathbf{x}}$) and reconstruction error (error respect to \mathbf{x})

Cora Graph



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Gradient Descent Update as Control Variate

- ▶ The solution $\hat{\mathbf{x}}$ also minimizes:

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{K}^{-1}\mathbf{x} - \mathbf{x}^\top \mathbf{y}.$$



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$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla F(\mathbf{x}_k)$$

where $\alpha \in \mathbb{R}$ and $\nabla F(\mathbf{x}_k) = \mathbf{K}^{-1} \mathbf{x}_k - \mathbf{y}$.



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- ▶ We propose to apply the gradient descent update on the previous estimator $\bar{\mathbf{x}}$:

$$\bar{\mathbf{z}} := \bar{\mathbf{x}} - \alpha (\mathbf{K}^{-1} \bar{\mathbf{x}} - \mathbf{y})$$



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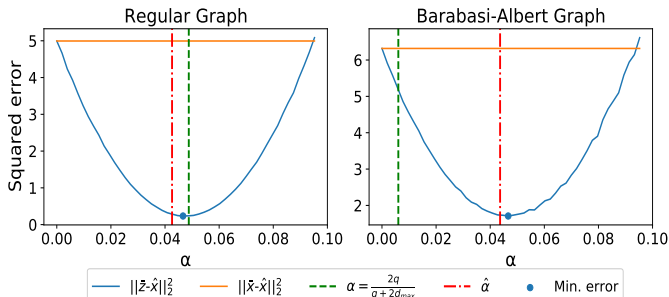
- ▶ One can either choose a value for α from the safe range (e.g. $\alpha = \frac{2q}{q+2d_{\max}}$) or estimate from the samples:

$$\hat{\alpha} = \frac{\text{tr}(\widehat{\text{Cov}}(\mathbf{K}^{-1}\bar{\mathbf{x}}, \bar{\mathbf{x}}))}{\text{tr}(\widehat{\text{Var}}(\mathbf{K}^{-1}\bar{\mathbf{x}}))}.$$



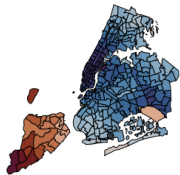
Range of α

- We empirically compare these options of α over a regular and irregular graph:

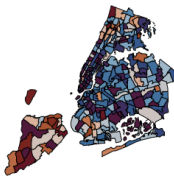


An Illustration

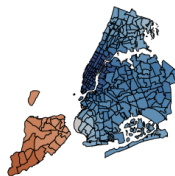
x:



y:

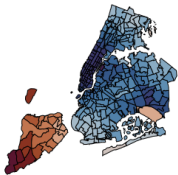


\hat{x} :

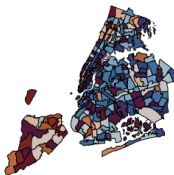


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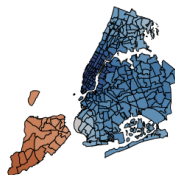
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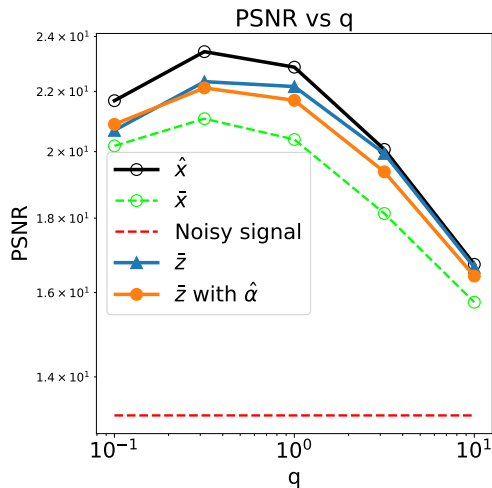


Figure: PSNR vs q , $N=2$

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Inverse Trace Estimation: SOTA

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- ▶ For some samples of a random vector \mathbf{a} , it needs to calculate $\mathbf{a}^T K \mathbf{a}$.
- ▶ Solving for $K \mathbf{a}$ can be done via:
 - ▶ Direct computation via Cholesky decomposition
 - ▶ (Preconditioned) Iterative solvers
 - ▶ Algebraic Multigrid solvers
 - ▶ ...



Forest based Trace Estimator

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- ▶ One can use this estimator in case of symmetric diagonally dominant matrices instead of the graph Laplacians.



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- ▶ A safe value of α is $\frac{2q}{q+d_{\max}}$. We also observe that $\frac{q}{q+d_{\text{avg}}}$ is usually a good estimate of α^* .



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- ▶ Stratified sampling can substantially decrease approximation error when applicable.
- ▶ Thanks to rich theory of RSFs, we can apply stratified sampling on s .



Comparison with SOTA

- We compare the time needed by the estimators for reaching a certain accuracy.

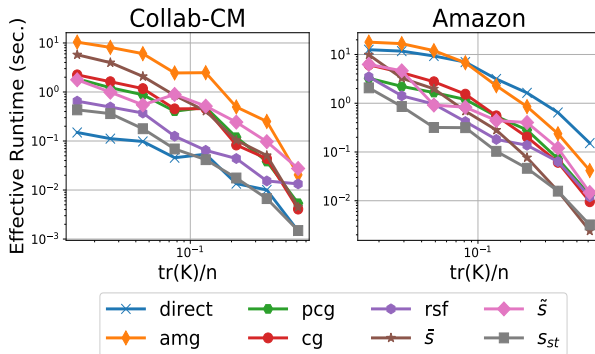


Figure: Effective Runtime vs $\text{tr}(\mathbf{K})/n$.

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- ▶ Estimating effective resistances.






$$R_{i,j} = L_{i,i}^{\dagger} + L_{j,j}^{\dagger} - L_{i,j}^{\dagger} - L_{j,i}^{\dagger}.$$



Questions

Thanks! Questions?



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