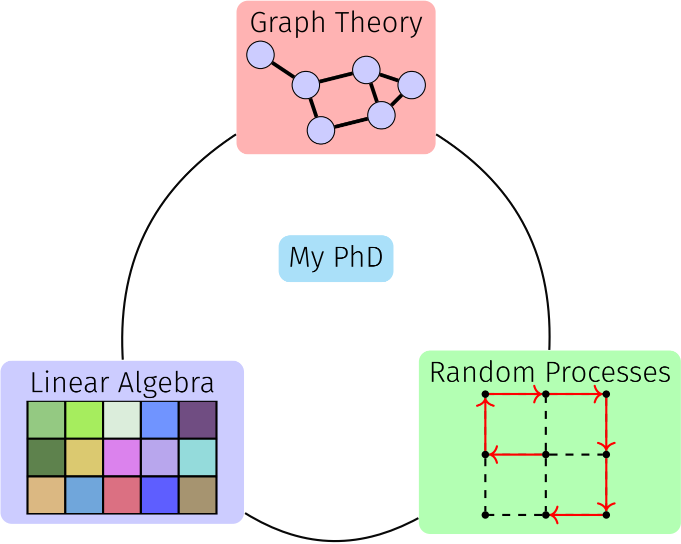
Wilson's Algorithm for Randomized Linear Algebra

Yusuf Yiğit Pilavcı

Advisors:
Pierre-Olivier Amblard
Simon Barthelmé
Nicolas Tremblay

15/11/2022

What's inside?



Graphs are *Ubiquitous*...

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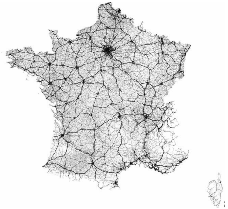

Road Networks

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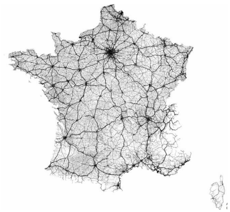

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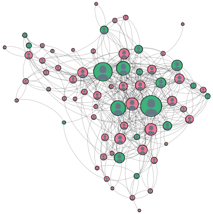

Social Networks

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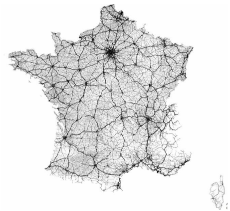

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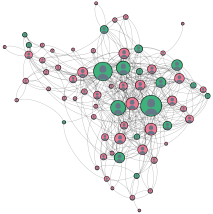

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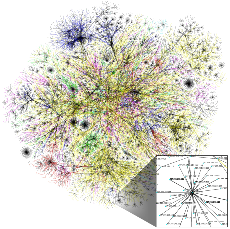

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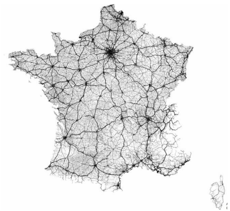

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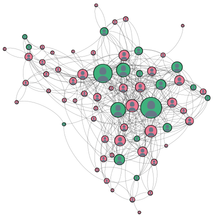

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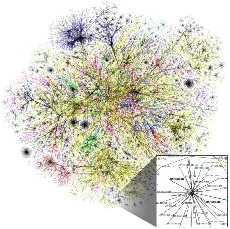

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Brain Networks

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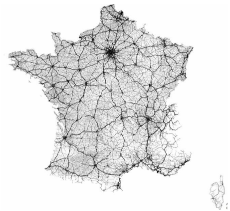

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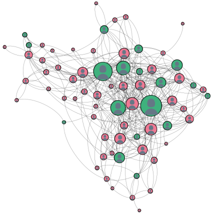

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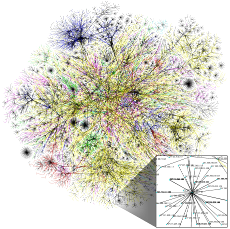

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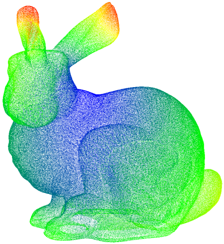

Point Clouds Networks

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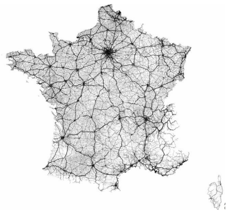

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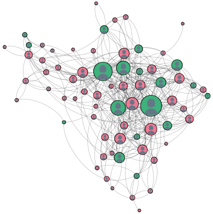

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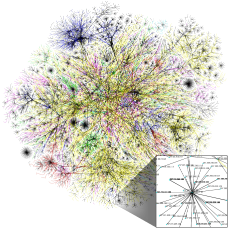

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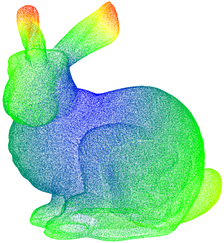

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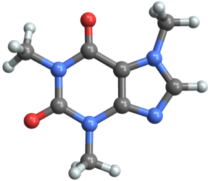

Molecule Networks

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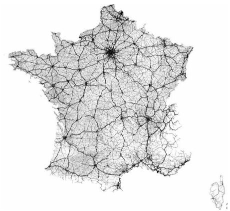

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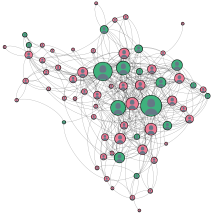

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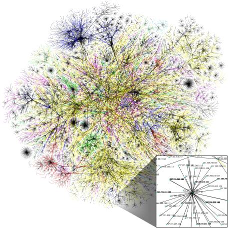

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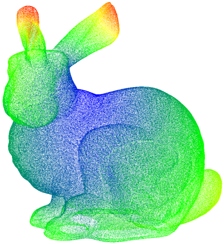

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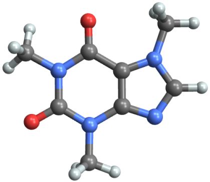

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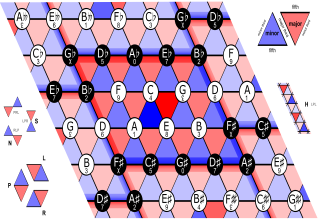

Tonnetz

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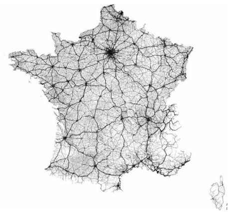

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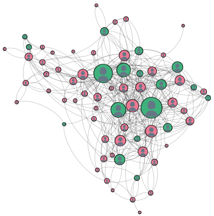

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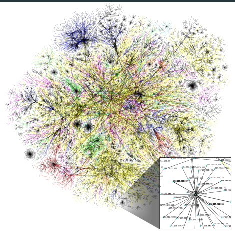

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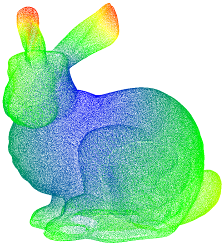

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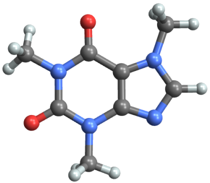

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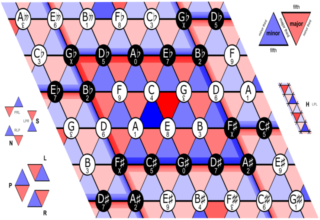

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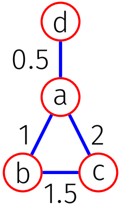
Graph related Linear Algebra



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

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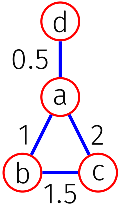
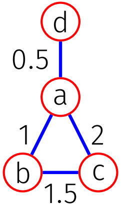


$\mathcal{G} = ({\color{red}\mathcal{V}}, {\color{blue}\mathcal{E}}, \mathrm{w})$

$$\begin{array}{cc} & \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{array}{c} a \\ b \\ c \\ d \end{array} & \begin{bmatrix} 0 & 1 & 2 & 0.5 \\ 1 & 0 & 1.5 & 0 \\ 2 & 1.5 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

Adjacency matrix W

Graph related Linear Algebra



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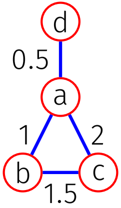
Degree matrix D

Graph related Linear Algebra



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Laplacian matrix

$L = D - W$

The Graph Laplacian is *Ubiquitous*...

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Theory

- Connectivity Analysis
- Graph Partitioning
- Spanning Trees
- Random Walks (Loop-Erased)...

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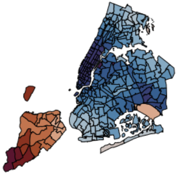
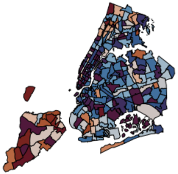
⚠ However, some computations do not scale with large graphs.

Original Signal:



$\mathbf{y}$:



Original Signal: $\quad y$: $\quad \hat{x}$:

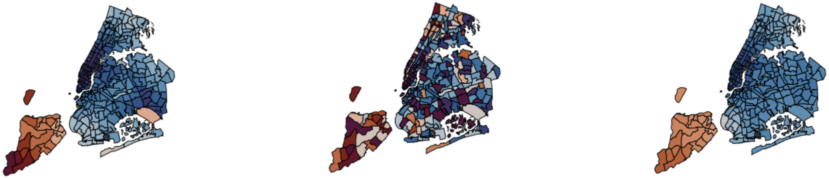


Figure 3: Median taxi fees paid in drop-off locations in NYC

Graph Signal Smoothing

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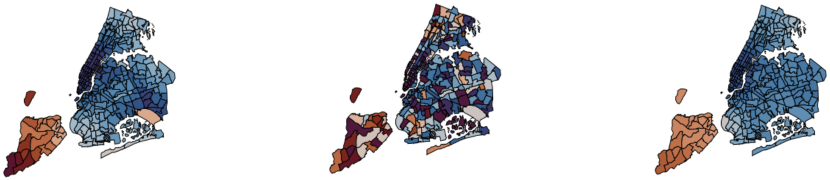

Figure 3: Median taxi fees paid in drop-off locations in NYC

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

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} q \underbrace{||\mathbf{y}-\mathbf{x}||_2^2}_{\text{Fidelity}} + \underbrace{\mathbf{x}^T L \mathbf{x}}_{\text{Regularization}}, \quad q > 0$$

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

- The explicit solution to this problem is:

$$\hat{\mathbf{x}} = \mathrm{K}\mathbf{y} \text{ with } \mathrm{K} = q(\mathrm{L} + q\mathrm{I})^{-1}$$

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- Direct computation of 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.
- For SDD linear systems, there is a growing body of works starting from (Spielman and Teng 2004).

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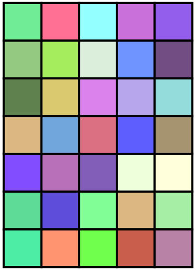
- How to choose a good value for the hyperparameter q?
- There are several methods such as Akaike's or Bayesian information criterion, generalized cross validation or Stein's unbiased risk estimator.
- Each uses a quantity called the effective degree of freedom which is equal to $\mathrm{tr}(K)$.

- RLA is a branch of numerical linear algebra developing Monte Carlo methods.



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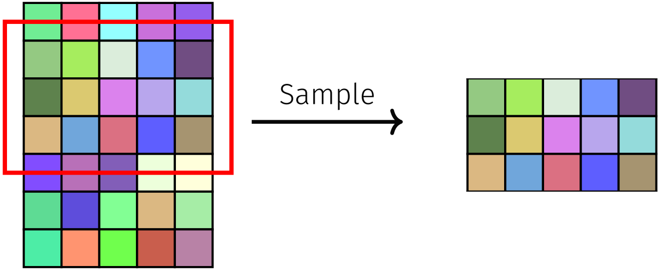

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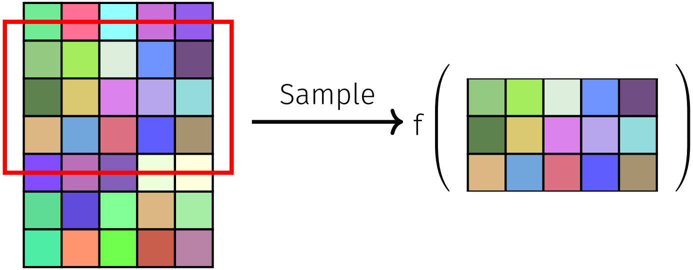
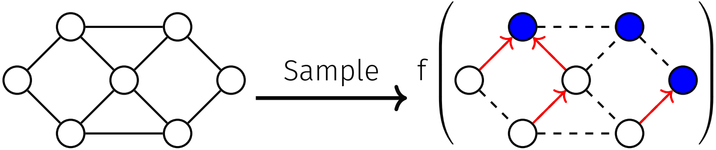


- RLA algorithms for Laplacian-based numerical algebra by using Random Spanning Forests.



Outline

Random Spanning Forests (RSF)

RSF-based Algorithms

Conclusion

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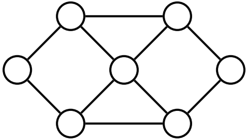
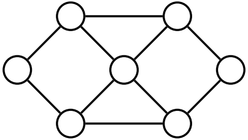
Spanning Forests



Graph

Spanning Forests



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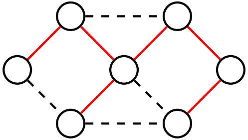
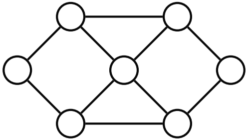


Spanning Tree

Spanning Forests



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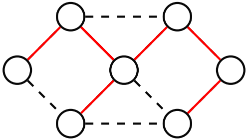

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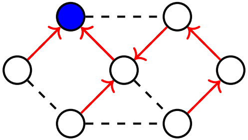
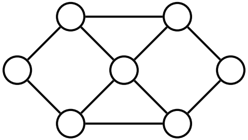


Rooted
Spanning Tree

Spanning Forests



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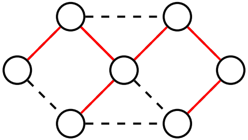

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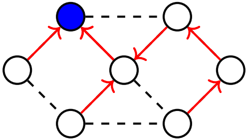

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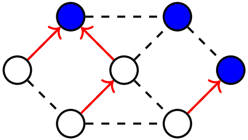
Spanning Tree



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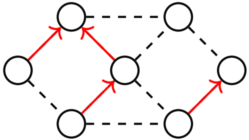
Forest Notations

- Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathrm{w})$, we denote:



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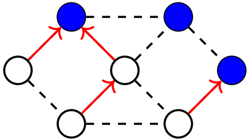

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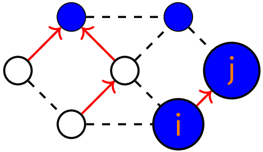

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A random spanning forest Φ_q on a graph $\mathcal{G}$ is spanning forest selected over all spanning forests of $\mathcal{G}$ according to the following distribution:

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

- The random roots $\rho(\Phi_q)$ is a determinantal point process with a marginal kernel $K = q(L + qI)^{-1}$ (Avena et al. 2018):

$$\forall S \subseteq \mathcal{V}, \quad \mathbb{P}(S \subseteq \rho(\Phi_q)) = \det K_S.$$

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- There is an efficient algorithm to sample RSFs, called Wilson's algorithm (Wilson 1996).

- Consider an simple random walk on $\mathcal{G}$ with the transition rule:
    - take a step from i to j with probability $\frac{w(i,j)}{q+d_i}$,
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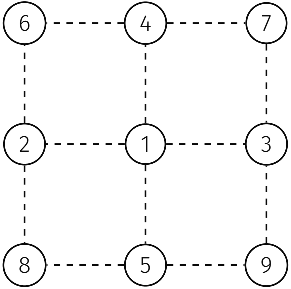

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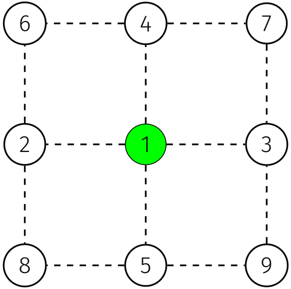

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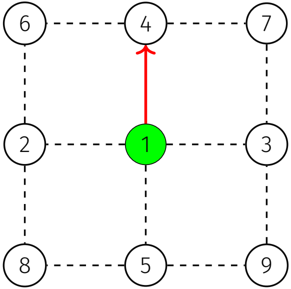

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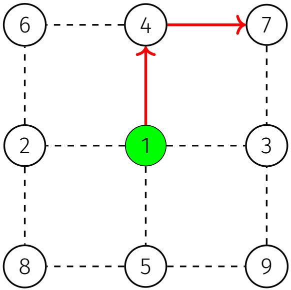

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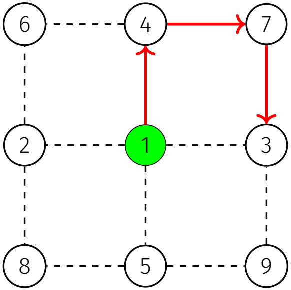

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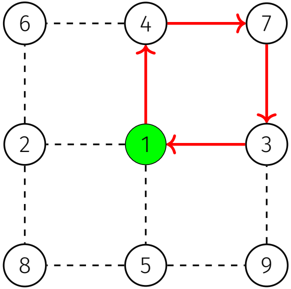

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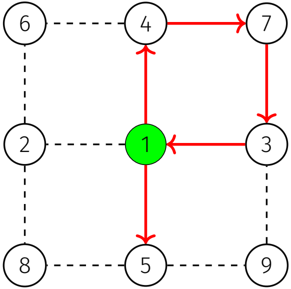

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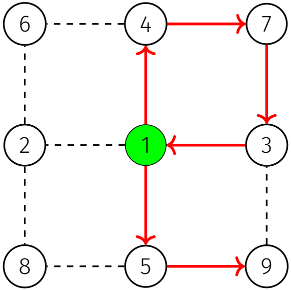

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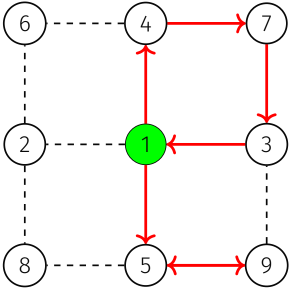

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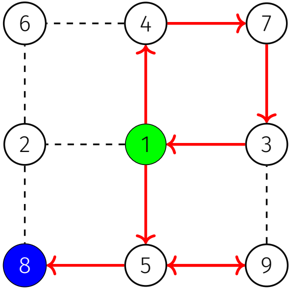

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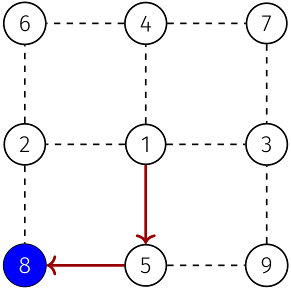

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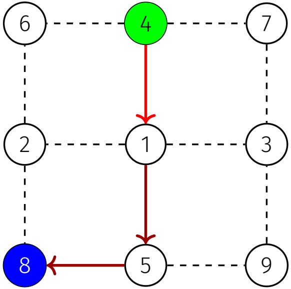

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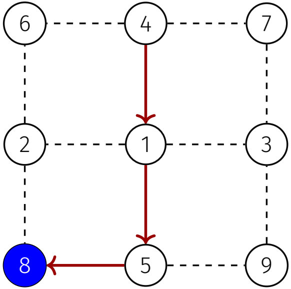

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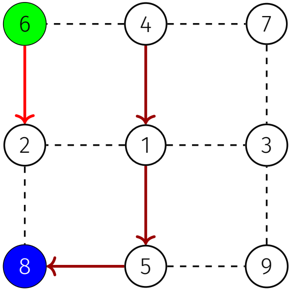

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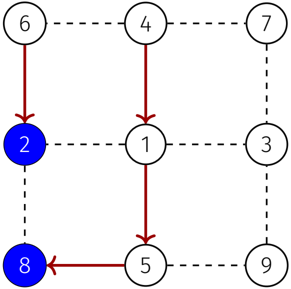

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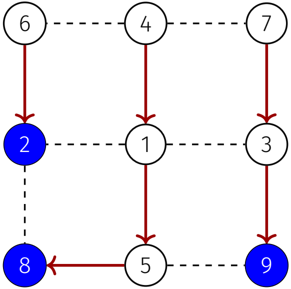

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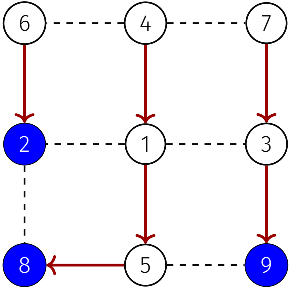


- The expected number of steps is known:

$$\mathrm{tr}\left[(\mathsf{L}+q\mathsf{I})^{-1}(\mathsf{D}+q\mathsf{I})\right] \leq \frac{2|\mathcal{E}|}{q} + |\mathcal{V}|.$$

Outline

Random Spanning Forests (RSF)

RSF-based Algorithms

Conclusion

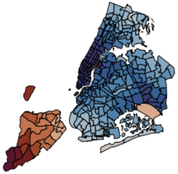
Main Contributions

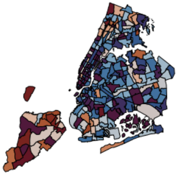
Challenges

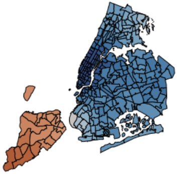
- Graph Signal Smoothing
- Trace Estimation
- Estimating Effective Resistances

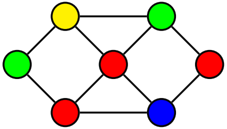
Challenges

- **Graph Signal Smoothing**

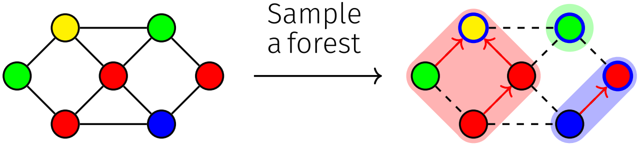
  Original Signal: 

  $\mathbf{y}$: 

  $\hat{\mathbf{x}} = \mathbf{K}\mathbf{y}$: 



Smoothing Via Forests



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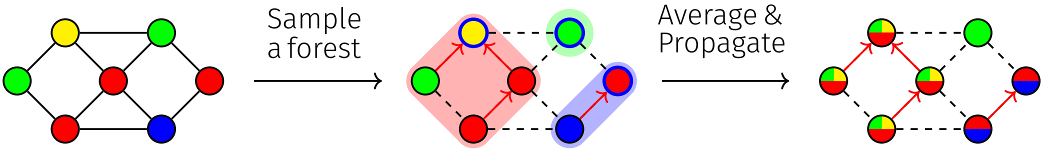

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- This yields an unbiased estimator $\bar{x}$.

Comparison with State of the art

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

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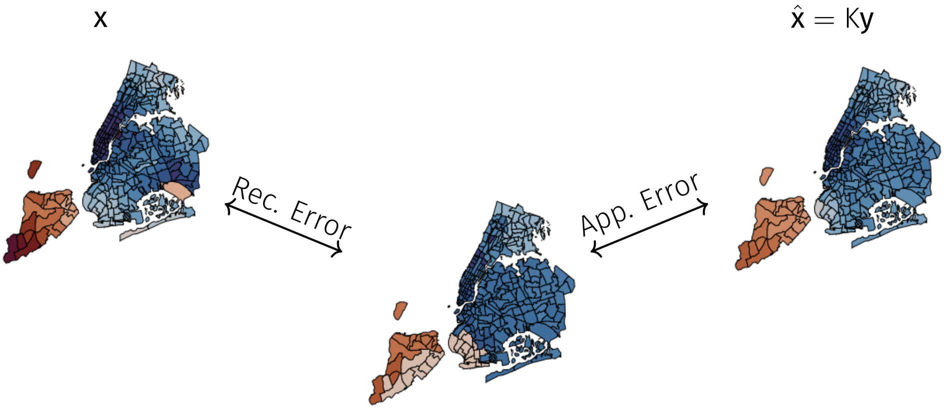

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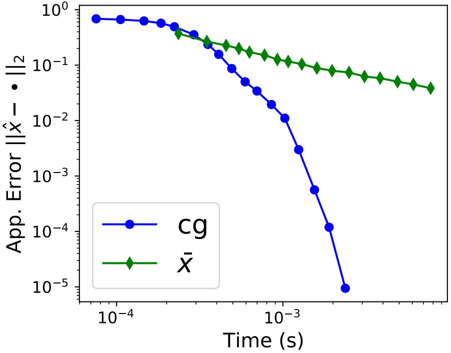

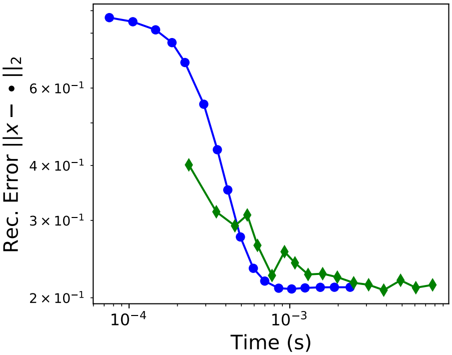

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  where $\alpha \in \mathbb{R}$ and $\nabla F(\mathbf{x}_k) = K^{-1}\mathbf{x}_k - \mathbf{y}$.
- We propose to apply the gradient descent update on the previous estimator $\bar{\mathbf{x}}$:

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

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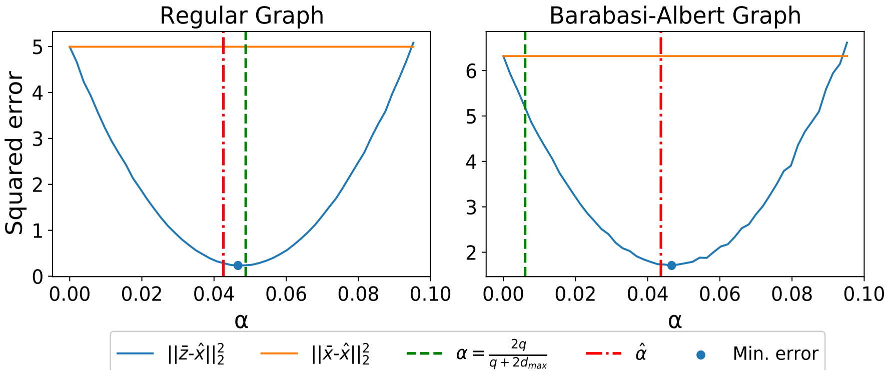
- One can either choose a value for α from the safe range (e.g. $\alpha = \frac{2q}{q+2d_{max}}$) or estimate from the samples:

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

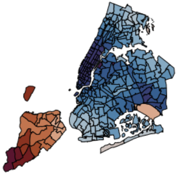
Range of α

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



An Illustration

x:



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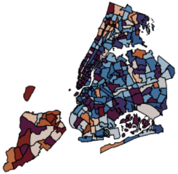

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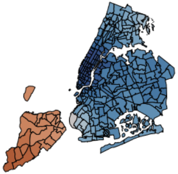

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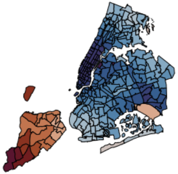

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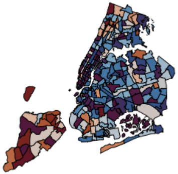

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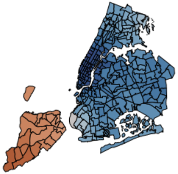

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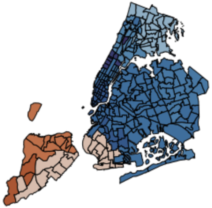

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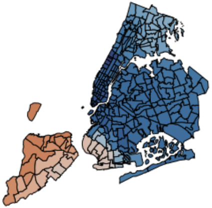

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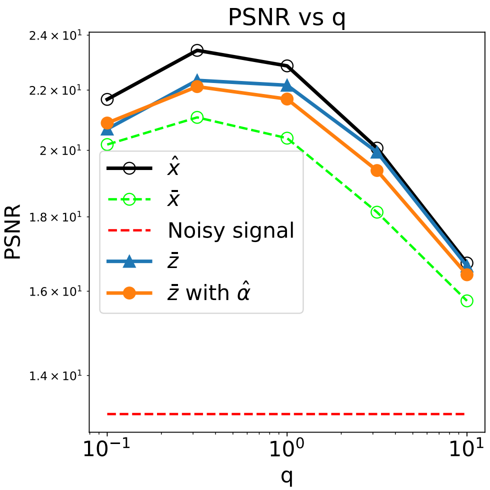

Figure 7: PSNR vs q, N=2

Challenges

- Graph Signal Smoothing
- **Trace Estimation**
- Estimating Effective Resistances

Inverse Trace Estimation: Hutchinson's Estimator

- A famous algorithm for estimating $\mathrm{tr}(K)$ is Hutchinson's estimator:

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

where $\mathbf{a}^{(i)} \in \{-1, 1\}^n$ is a random vector with $\mathbb{P}(\mathbf{a}_j^{(i)} = \pm 1) = 1/2$.

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- A famous algorithm for estimating $\mathrm{tr}(K)$ is Hutchinson's estimator:

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

  where $\mathbf{a}^{(i)} \in \{-1, 1\}^n$ is a random vector with $\mathbb{P}(\mathbf{a}_j^{(i)} = \pm 1) = 1/2$.
- It is an unbiased estimator of $\mathrm{tr}(K)$.
- The cumbersome computation here is $K\mathbf{a}^{(i)}$ for N vectors.
- It can be done via:
    - Direct computation via Cholesky decomposition
    - (Preconditioned) Iterative solvers
    - Algebraic Multigrid solvers
    - …

Forest based Trace Estimator

- Another unbiased estimator is by RSFs (Barthelme et al. 2019):

$$\mathsf{s} \coloneqq |\rho(\Phi_{\mathsf{q}})| \text{ with } \mathbb{E}[\mathsf{s}] = \mathrm{tr}(\mathsf{K})$$

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- This estimator gives an comparable performance with the existing algorithms.
- One can use this estimator in case of symmetric diagonally dominant matrices instead of the graph Laplacians.

- One can rewrite $\bar{\mathbf{x}} = \bar{\mathrm{S}}\mathbf{y}$.

Variance Reduction via Control Variates

- One can rewrite $\bar{\mathbf{x}} = \bar{\mathsf{S}}\mathbf{y}$.
- The control variate estimator for K:

$$\bar{\mathsf{Z}} = \bar{\mathsf{S}} - \alpha(\mathsf{K}^{-1}\bar{\mathsf{S}} - \mathsf{I}).$$

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

Variance Reduction via Stratification

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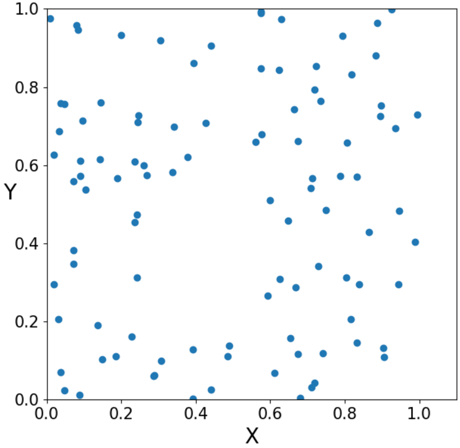

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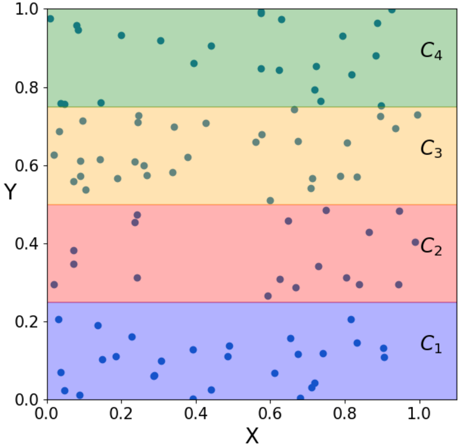

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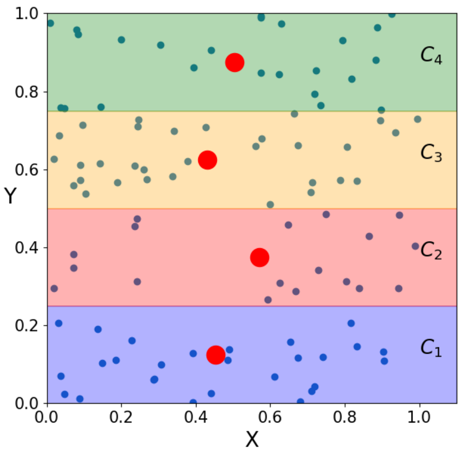

- The stratified estimator is:

$$X_{st} := \underbrace{\sum_{k=1}^{K} \underbrace{\frac{1}{N_k}\left(\sum_{\substack{j=1\\ Y\in C_k}}^{N_k} X^{(j)}\right)}_{\text{Conditional Expectation}} \mathbb{P}(Y \in C_i)}_{\text{Marginalization over Y}} .$$

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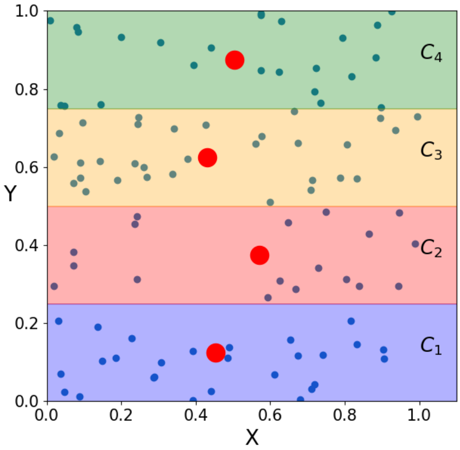

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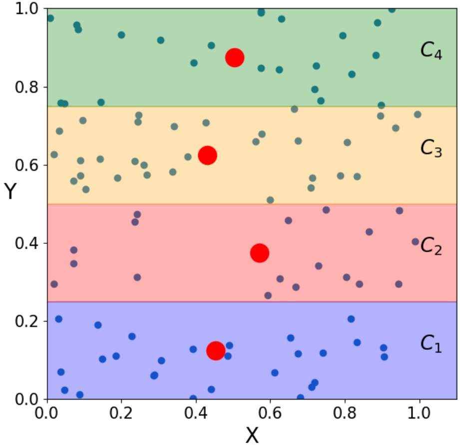

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- For certain allocations of N_k's, one has reduced variance
- We need to have a random variable Y such that:
    - $X|Y$ is easy to sample,
    - $\mathbb{P}(Y \in C_i)$ is accessible.

Variance Reduction via Stratification

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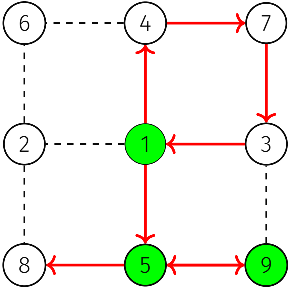

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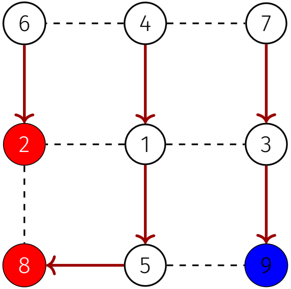
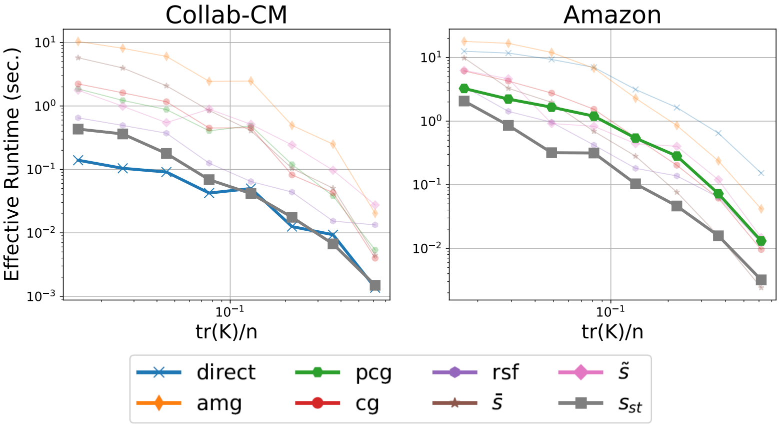


Comparison with Hutchinson's Estimator

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



Challenges

- Graph Signal Smoothing
- Trace Estimation
- Estimating Effective Resistances

Definition (Electrical Representation)
In the electrical representation of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathrm{w})$, each edge is a resistor with a resistance $\frac{1}{\mathrm{w(i,j)}}$.

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$$R_{i,j} := L^{\dagger}_{i,i} + L^{\dagger}_{j,j} - L^{\dagger}_{i,j} - L^{\dagger}_{j,i}$$

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- The effective conductance:

$$I_{i,j} := \frac{1}{R_{i,j}}$$

- $R_{i,j}$ is a distance metric between i and j.

Effective Resistances: What, **Why** and How ?

- $R_{i,j}$ is a distance metric between i and j.
- They are of central importance in many graph related applications:
    - Clustering (Alev et al. 2017),
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- In large scale, they are expensive to compute.

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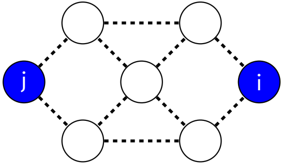
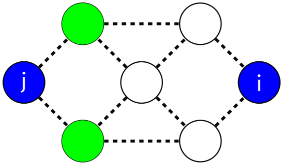
ESTIMATING $R_{i,j}$ VIA LOCAL FORESTS (LF)



Estimating $R_{i,j}$ via Local Forests (LF)



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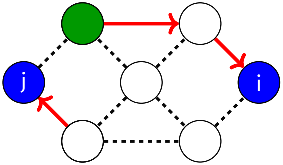

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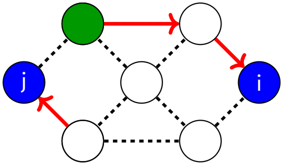

$\hat{l}_{i,j}^{(1)} = 1$

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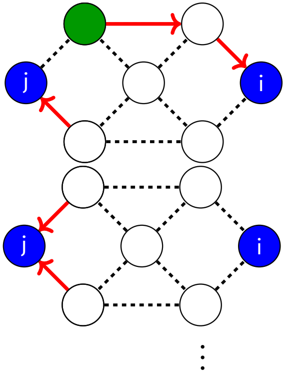

$\hat{I}^{(1)}_{i,j} = 1$

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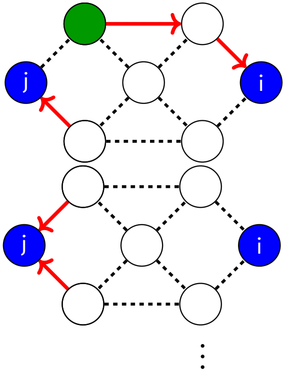

$\hat{\mathbb{I}}_{i,j}^{(1)} = 1$

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$$R_{i,j}^{LF} := \frac{N}{\sum_{k=1}^{N} \hat{\mathbb{I}}_{i,j}^{(k)}}$$

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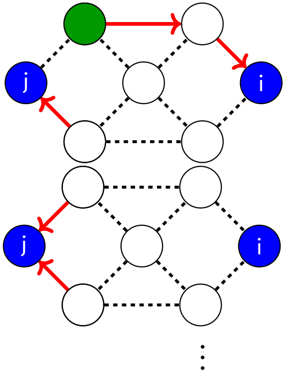

$\hat{I}^{(1)}_{i,j} = 1$

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$$R^{LF}_{i,j} := \frac{N}{\sum_{k=1}^{N} \hat{I}^{(k)}_{i,j}}$$

- R^{LF} is biased but the bias diminishes faster than the variance.

Experiments

- We report the run-time of the local algorithms for approximately the same relative error.

Dataset \ Algorithm	TP	MC2	LF(ours)
Cora	116	11	**2**
Citeseer	362	6	**1**
Pubmed	333	91	**12**
Collab-CM	82	156	**20**

Table 1: Runtime (ms) of the local algorithms over benchmark datasets

Outline

Random Spanning Forests (RSF)

RSF-based Algorithms

Conclusion

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$$\mathbb{P}(S \subseteq \rho_1(\Phi_q)) = \det K_1 \text{ with } K_1 = q(qI + D)^{-1}.$$

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- What happens between $\rho_1(\Phi_q)$ and $\rho(\Phi_q)$?

Publications

Journal

- Yusuf Yiğit Pilavcı, Pierre-Olivier Amblard, Simon Barthelme, and Nicolas Tremblay (2021). “Graph tikhonov regularization and interpolation via random spanning forests”. In: IEEE transactions on Signal and Information Processing over Networks 7, pp. 359–374

Conference

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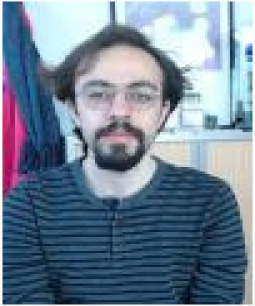
Thanks!



Just a PhD..

Random Spanning Forests

- For fixed subsets $V \subseteq \mathcal{V}$ and $S \subseteq \mathcal{E}$ with $|V| = |S|$, one has:

$$\det B_{S|V} = \begin{cases} \left(\prod_{(i,j)\in S} w(i,j)\right)^{1/2}, & \text{if S forms a spanning forest rooted in V} \\ 0, & \text{otherwise.} \end{cases}$$

- We can count the spanning forests rooted in $R \subseteq \mathcal{V}$:

$$\forall R \subseteq \mathcal{V}, \quad \det L_{-R} = \sum_{\phi \in \mathcal{F}_R} \prod_{(i,j)\in \mathcal{E}_\phi} w(i,j).$$

- The root probability can be seen as a ratio of counts:

$$\mathbb{P}(r_{\Phi_q}(i) = j) = K_{i,j} = q \frac{(-1)^{i+j} \det(L + qI)_{-i|-j}}{\det(L + qI)} = \frac{|\mathcal{F}^{i \to j}|}{|\mathcal{F}|}$$

Loop-Erased Random Walks

Theorem (Law of LERWs (Marchal 2000))
A loop-erased random walk LE(W) on $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathrm{w})$ that is stopped at the boundary $\Delta \subset \mathcal{V}$ has the following probability distribution:

$$\mathbb{P}(\mathrm{LE(W)} = \gamma) = \frac{\det \mathrm{L}_{-\Delta \cup \mathrm{s}(\gamma)}}{\det \mathrm{L}_{-\Delta}} \prod_{(\mathrm{i},\mathrm{j}) \in \gamma} \mathrm{w}(\mathrm{i}, \mathrm{j})$$

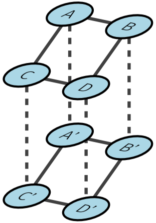
where γ is a fixed path and $\mathrm{s}(\gamma)$ denotes the nodes visited in γ.

Graph Filtering via Duplicated Graph

- The product K$\mathbf{y}$ corresponds to a graph filtering with the transfer function:

$$g_q(\lambda) = \frac{q}{q + \lambda}$$

- We duplicate the graph and the input $\mathbf{y}_d = \begin{bmatrix} \alpha \mathbf{y} \\ \beta \mathbf{y} \end{bmatrix}$



- The transfer function is paramerized by $\theta = (q_1, q_2, \alpha, \beta)$:

$$f_\theta(\lambda) = \frac{\alpha q_1(\lambda + h(0) + q_2) + \beta q_2(h(\lambda))}{(\lambda + h(0) + q_1)(\lambda + h(0) + q_2) - h(\lambda)^2},$$

L_1 Graph Regularization

- Another type of regularization is L_1 regularization:

$$x^\star = \operatorname*{argmin}_{x \in \mathbb{R}^n} \frac{q}{2}||x - y||_2^2 + ||Bx||_1$$

- Alternating direction of multipliers (ADMM) approximates $x^\star$ by:

$$x_{k+1} = \operatorname*{argmin}_{x \in \mathbb{R}^n} \left(\frac{q}{2}||x - y||_2^2 + \frac{\rho}{2}||Bx - z_k + u_k||_2^2 \right)$$
$$z_{k+1} = \operatorname*{argmin}_{z \in \mathbb{R}^m} \left(||z||_1 + \frac{\rho}{2}||Bx_{k+1} - z + u_k||_2^2 \right)$$
$$u_{k+1} = u_k + (Bx^{k+1} - z^{k+1}).$$

Extension to SDDs

- Let $G = U^\top \Lambda U = A^{(p)} + A^{(n)} + D^{(1)} + D^{(2)}$ be an symmetric diagonally dominant matrix where $D^{(1)}_{i,i} = \sum_{i \neq j} G_{i,j}$ and $D^{(2)}_{i,i} = G_{i,i} - D^{(1)}_{i,i}$.
- Construct the graph Laplacians:

$$L_1 = D^{(1)} + A^{(n)} - A^{(p)}/2 = U_1^\top \Lambda_1 U_1$$

$$L_2 = \begin{bmatrix} D^{(1)} + A^{(n)} + D^{(2)}/2 & -D^{(2)}/2 - A^{(p)} \\ -D^{(2)}/2 - A^{(p)} & D^{(1)} + A^{(n)} + D^{(2)}/2 \end{bmatrix}$$

- The eigenvectors of L_2 are $U_2 = \begin{bmatrix} U & U_1 \\ -U & U_1 \end{bmatrix}$
- The eigenvalues of L_2 are $\lambda_2 = \lambda_1 \cup \lambda$

Cross-Validation for GTR

- The leave-one-out cross-validation for graph Tikhonov regularization boils down to:

$$\mathrm{LOOCV}(q) = \frac{1}{n}\left(\sum_{i=1}^{n} \frac{y_i - \hat{x}_i}{1 - K_{i,i}}\right)^2 .$$

- The generalized CV approximation is:

$$\mathrm{GCV}(q) = \frac{1}{N}\left(\sum_{i=1}^{n} \frac{y_i - \hat{x}_i}{1 - \left(\mathrm{tr}(K)/n\right)}\right)^2 .$$

References I

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