Heat Kernels in Graphs:

A Journey from Random Walks to Geometry, and Back

He Sun

University of Bristol

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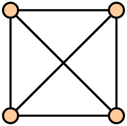

$$\mathcal{L}_G = \begin{pmatrix} 1 & -1/3 & -1/3 & -1/3 \\ -1/3 & 1 & -1/3 & -1/3 \\ -1/3 & -1/3 & 1 & -1/3 \\ -1/3 & -1/3 & -1/3 & 1 \end{pmatrix}$$

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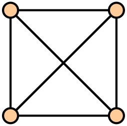

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Matrix $\mathcal{L}$ has eigenvalues $0 = \lambda_1 \leq \ldots \leq \lambda_n$ with corresponding eigenvectors

$$f_1, \ldots, f_n.$$

Heat Kernel: a Fundamental Solution of a PDE

Let $\mathcal{M}$ be a compact Riemannian manifold, and

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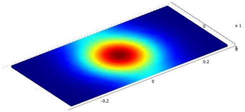

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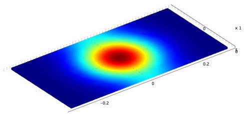

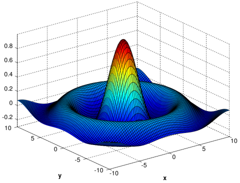

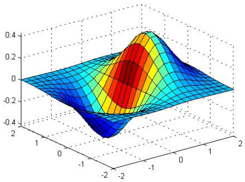

Heat Kernel Defines a Continuous-Time Random Walk

Heat Kernel in Graphs

When Δ is the Laplacian matrix $\mathcal{L}$ of graph G, for any $t \geq 0$ the heat kernel of G can be written as

$$\mathbf{H}_t = \mathrm{e}^{-t\mathcal{L}} = \sum_{k=0}^{\infty} \frac{t^k \mathrm{e}^{-t}}{k!} \mathbf{P}^k,$$

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The heat kernel defines a semi-group, i.e.,

$$\mathbf{H}_{t+s} = \mathbf{H}_t \cdot \mathbf{H}_s, \forall t, s \geq 0 \qquad \text{and} \qquad \lim_{t \to 0} \mathbf{H}_t = \mathbf{I}.$$

Heat Kernel in Graphs: Towards a Geometric Interpretation

For any time-step $t \geq 0$, define an embedding $\psi_t : V \mapsto \mathbb{R}^n$ by

$$\psi_t(v) = \left(\mathrm{e}^{-t\lambda_1} f_1(v), \mathrm{e}^{-t\lambda_2} f_2(v), \ldots, \mathrm{e}^{-t\lambda_n} f_n(v) \right).$$

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A simple calculation shows that $d_t(u,v) = \sum_{w \in V} \left(\mathbf{H}_t(w,u) - \mathbf{H}_t(w,v) \right)^2$.

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Meaning of the heat kernel distance, with a proper choice of t:

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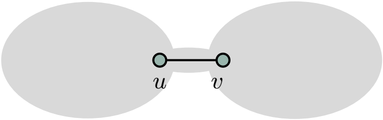

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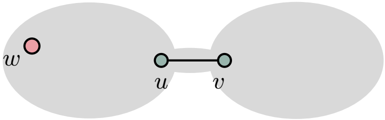

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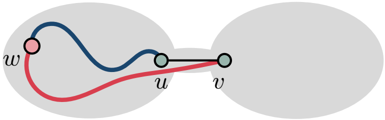

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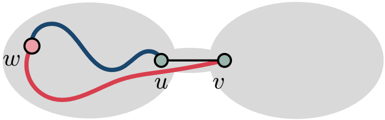

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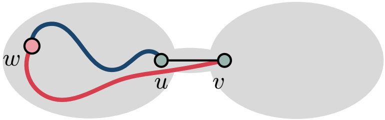

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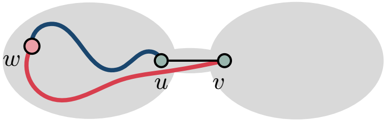

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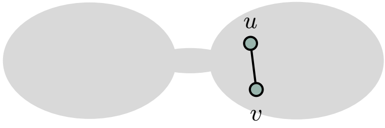

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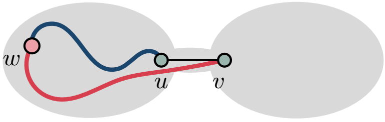

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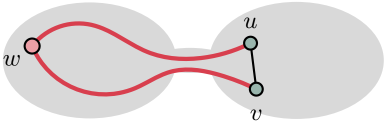

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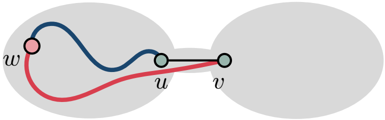

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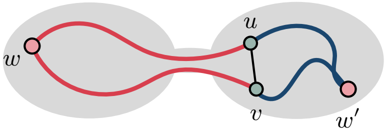

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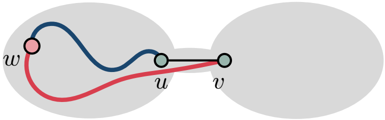

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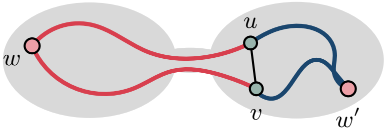

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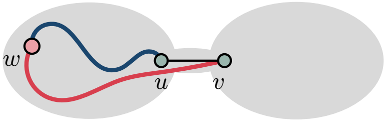

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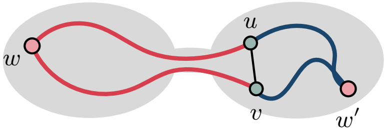

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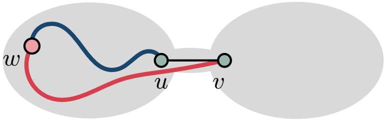

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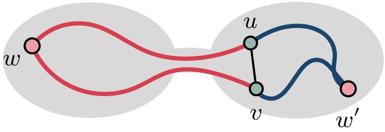

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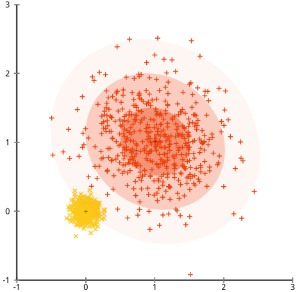
- Do PDEs lead to an entirely new technique to design algorithms for large datasets?

Graph Clustering

Applications in clustering:



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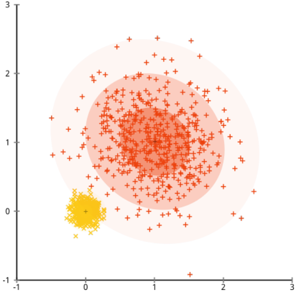

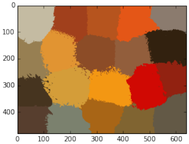

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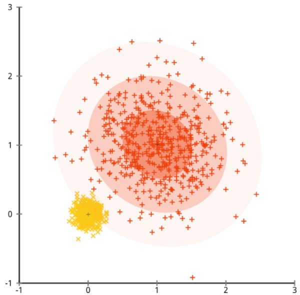

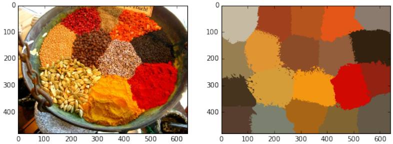

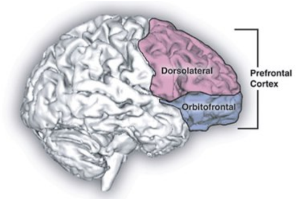

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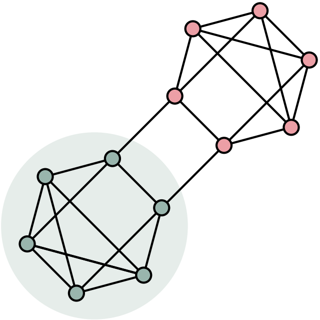

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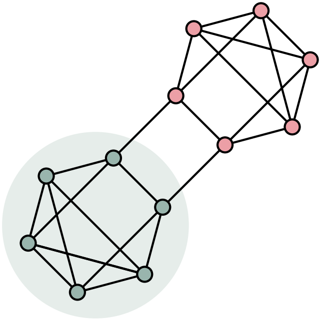

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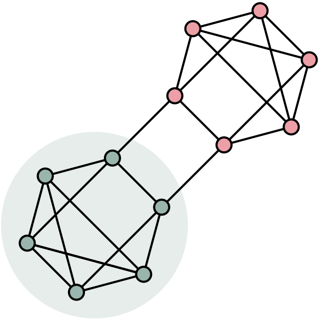
Cheeger's Inequality

$$\frac{\lambda_2}{2} \leq \phi_G \leq \sqrt{2\lambda_2}.$$



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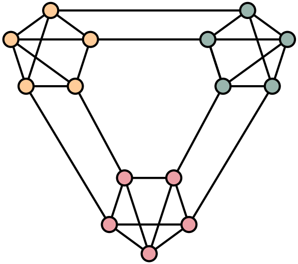

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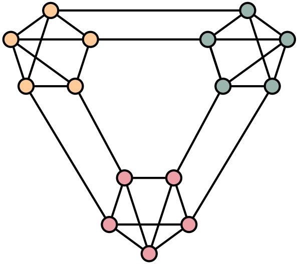

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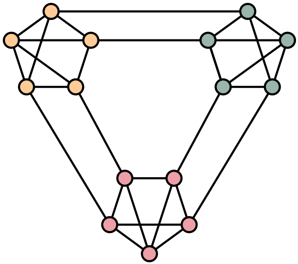

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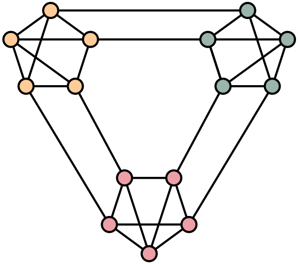

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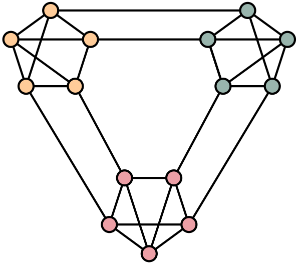

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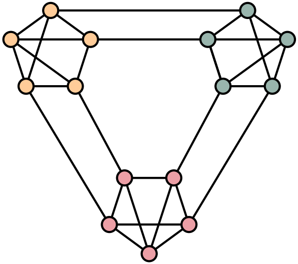

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The key parameter: $\Upsilon \triangleq \dfrac{\lambda_{k+1}}{\rho(k)}.$

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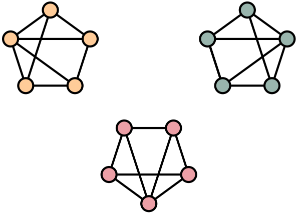
Let G be a d-regular graph with k disjoint components $S_1, \ldots, S_k$.



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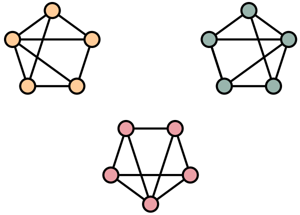

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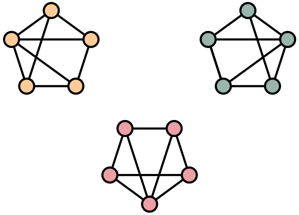

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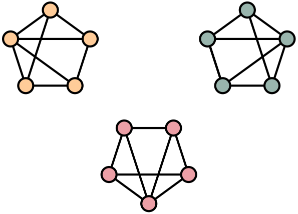

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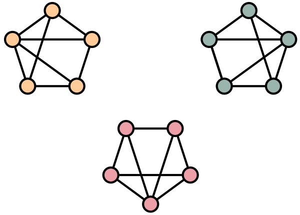

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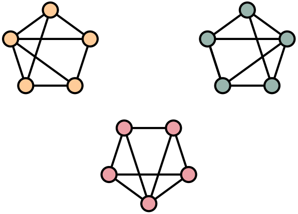

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Define $F(v) = (f_1(v), \ldots, f_k(v))$.

There are points $p^{(1)}, \ldots, p^{(k)}$, s.t. cluster S_i is concentrated around $p^{(i)}$.

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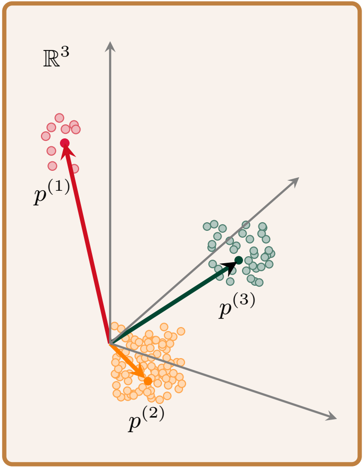

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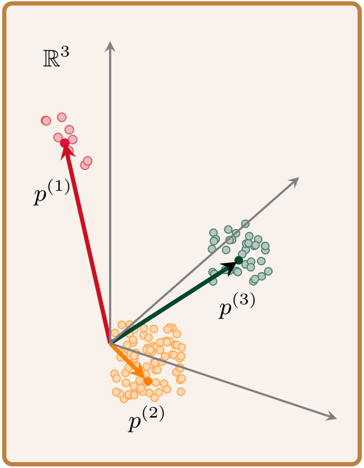

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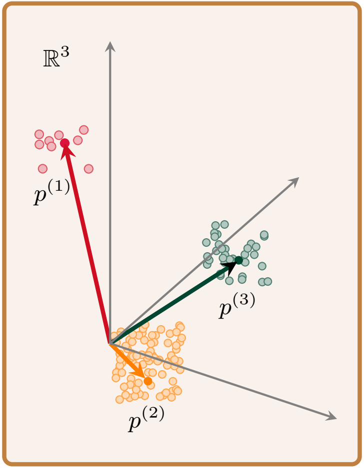

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$$\left\| p^{(i)} - p^{(j)} \right\|^2 \geq \frac{1}{k \min\{|S_i|, |S_j|\}}$$

Distance between different clusters inversely $\approx$ the smaller cluster.

A Simple Algorithm For Graph Clustering

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1. Obtain a set C of candidate centres.

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for $i = 1$ **to** $K = \Theta(k \log k)$ **do**

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Runtime is $O(n \cdot \operatorname{poly} \log n)$, even for a large value of k!

Obtaining the Pairwise Distances via Heat Kernels

Recall the two embeddings discussed so far:

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Proof Sketch

- Johnson-Lindenstrauss transformation
- Algorithm for approximating matrix exponential.

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- A direct proof based on random walks?

Beyond Graph Clustering

What is the limit of this technique?

Revisit the Graph Expansion Problem

Graph Expansion

Given a d-regular graph $G = (V, E)$ as input, find a set $S \subseteq V$ of size $|S| \leq n/2$ of minimum conductance, i.e.,

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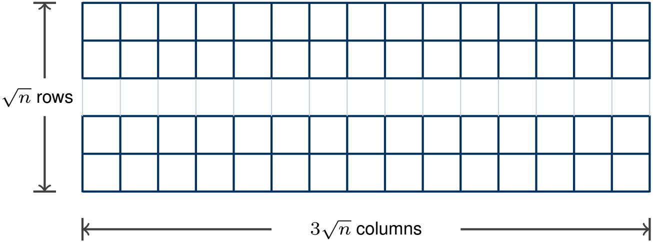
Improve the state-of-the-art algorithm by heat kernels?

Grid Graphs

We define a family of graphs $\{G\}_n$ as follows:

- Every G_n has $3n$ vertices, which form a grid of size $\sqrt{n} \times 3\sqrt{n}$.
- The weight of every edge in the middle row has weight $1/\sqrt{n}$, and all the other edges have weight 1.



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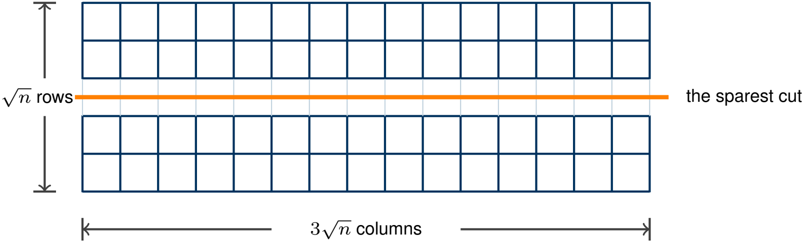

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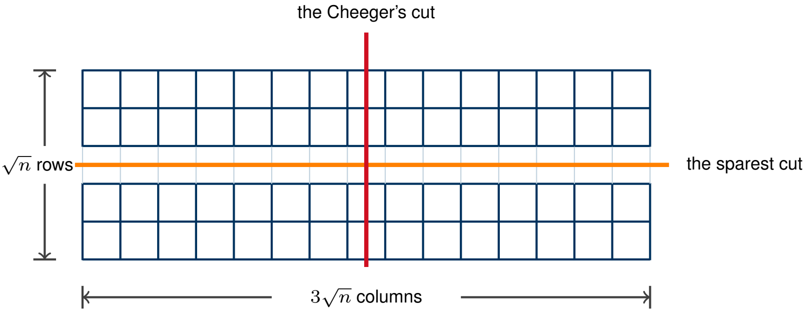
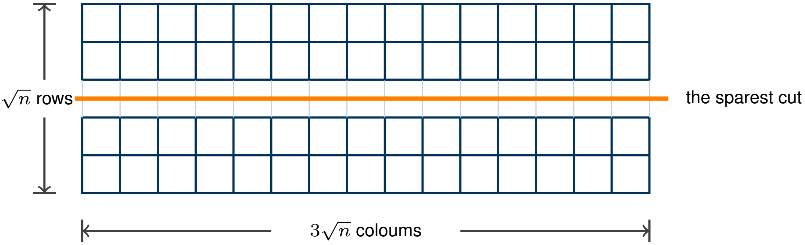
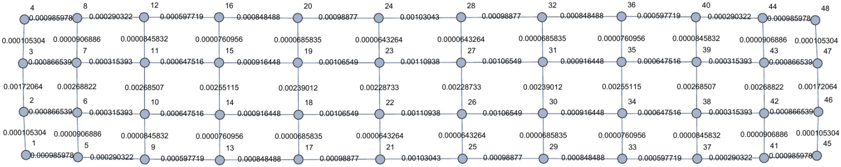


Heat Kernel Distances in the Grid Graphs





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THANK YOU!

Reference: Richard Peng, He Sun, and Luca Zanetti: Partitioning Well-Clustered Graphs: Spectral Clustering Works! SIAM Journal on Computing, 46(2):710-743, 2017.