Heat Kernels in Graphs:

A Journey from Random Walks to Geometry, and Back

He Sun

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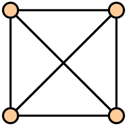

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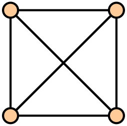

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Matrix $\mathcal{L}$ has eigenvalues $0 = \lambda_1 \leq \ldots \leq \lambda_n$ with corresponding eigenvectors

$$f_1, \ldots, f_n.$$

Heat Kernel: a Fundamental Solution of a PDE

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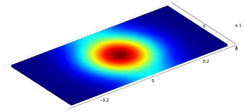

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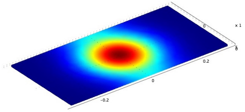

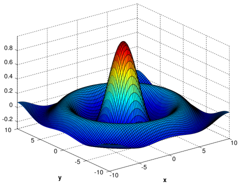

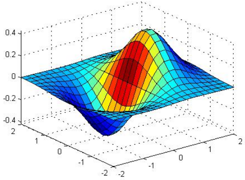

Heat Kernel Defines a Continuous-Time Random Walk

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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Assume that $t \approx$ local mixing time, which can will be found by binary search.

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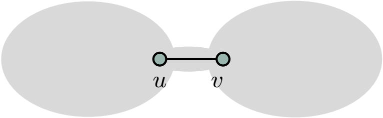

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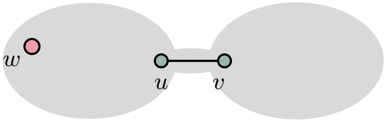

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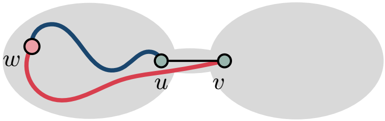

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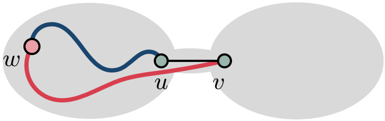

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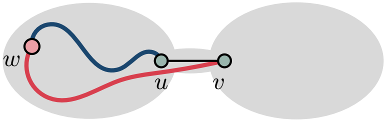

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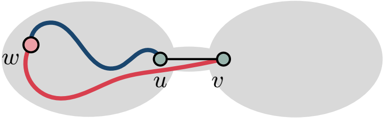

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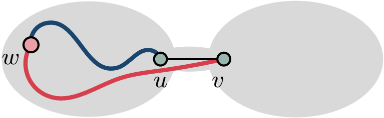

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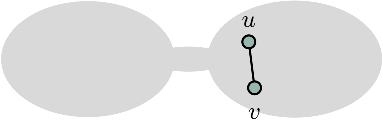

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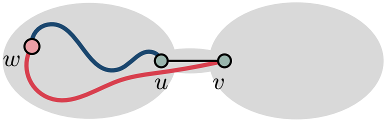

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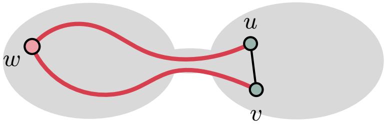

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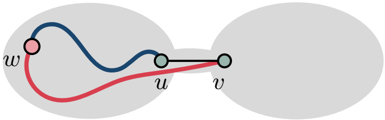

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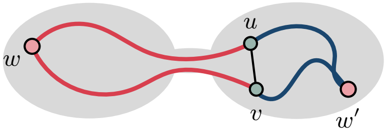

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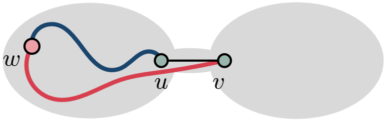

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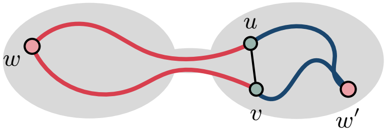

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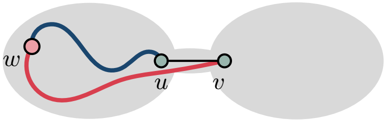

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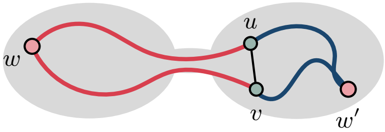

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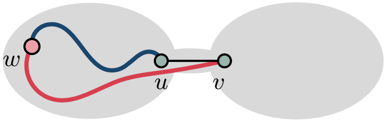

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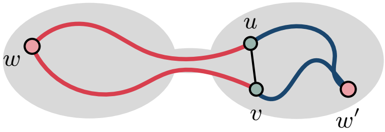

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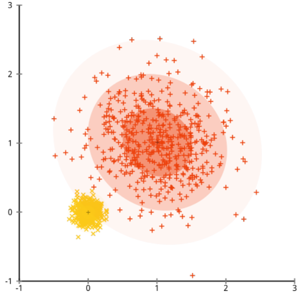
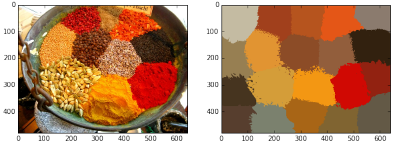
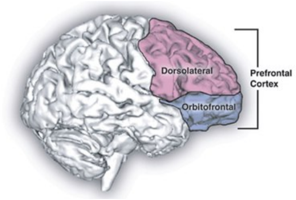
- Do heat kernels give us an entirely new technique to design algorithms for large datasets?

Graph Clustering

Applications in clustering:







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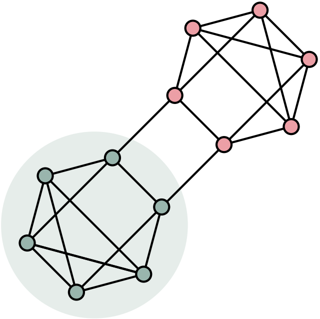

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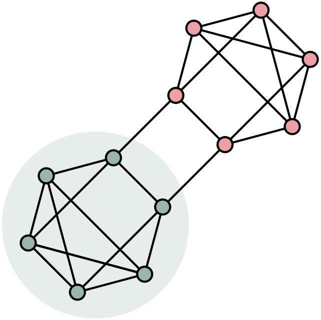

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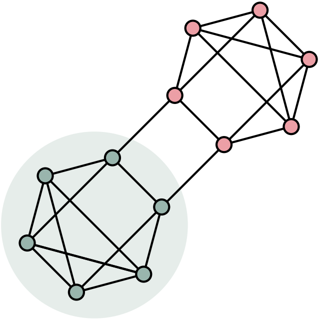
Cheeger's Inequality

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

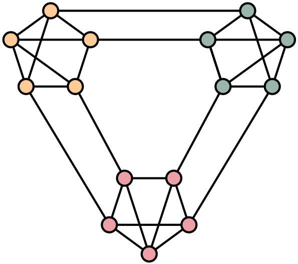


$$\phi_G(S) = \frac{2}{4 \cdot 6} = \frac{1}{12}$$

k-Way Expansion

The k-way expansion constant is defined by

$$\rho(k) = \min_{\text{partition } A_1,\ldots,A_k} \max_{1\le i\le k} \phi_G(A_i).$$



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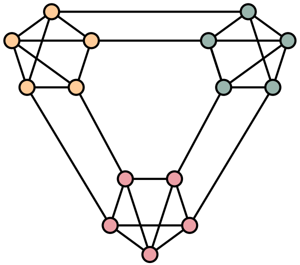

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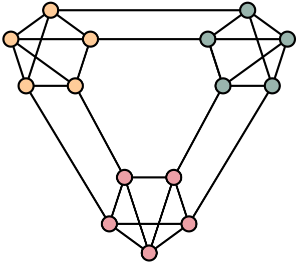

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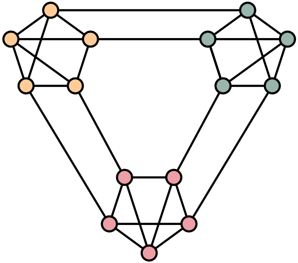

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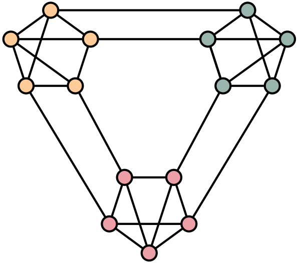

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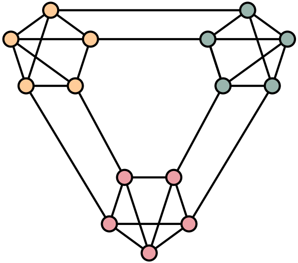

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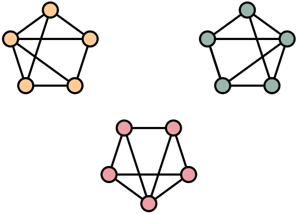
The key parameter: $\Upsilon \triangleq \dfrac{\lambda_{k+1}}{\rho(k)}$.

The Structure Theorem

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



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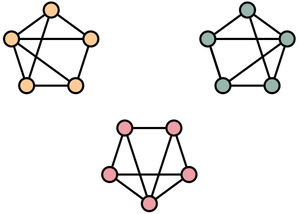

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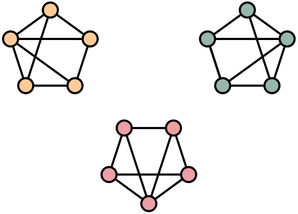

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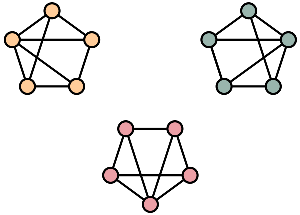

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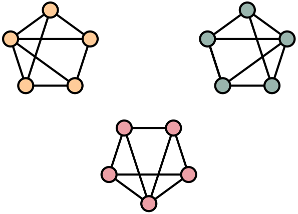

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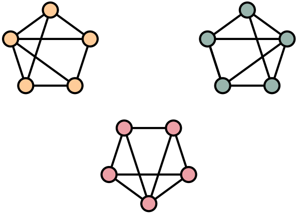

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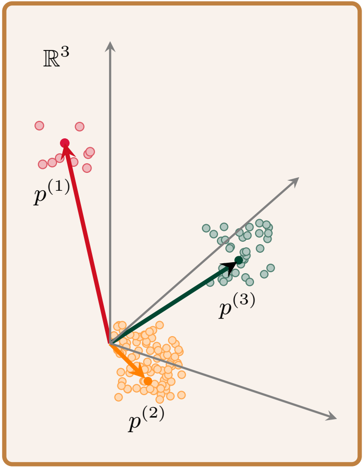
There are points $p^{(1)}, \ldots, p^{(k)}$, s.t. cluster S_i is concentrated around $p^{(i)}$.

Corollaries of the Structure Theorem



$$\sum_{i=1}^{k} \sum_{u \in S_i} \left\| F(u) - p^{(i)} \right\|^2 \leq k^2 / \Upsilon.$$

Points from S_i concentrate around $p^{(i)}s$.

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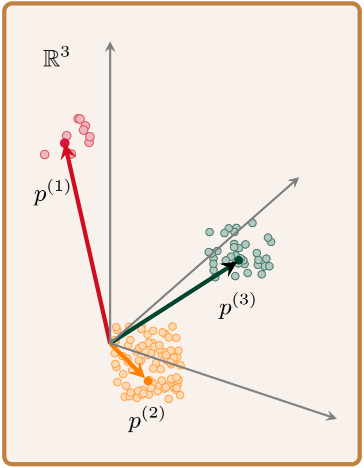

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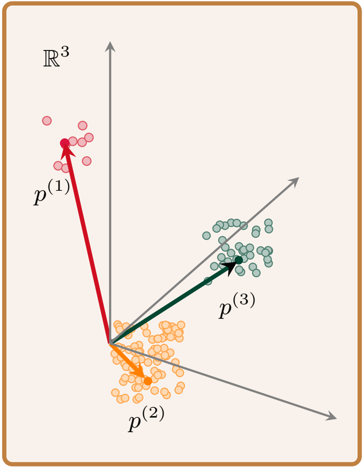

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$$\left\|p^{(i)}-p^{(j)}\right\|^2 \geq \frac{1}{k\min\{|S_i|,|S_j|\}}$$

Distance between different clusters inversely ≈ the smaller cluster.

A Simple Algorithm For Graph Clustering

ASSUME we know the pairwise distances of the points for free!

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1. Obtain a set C of candidate centres.

Algorithm

for $i = 1$ **to** $K = \Theta(k \log k)$ **do**
  set $c_i = v$ with prob. proportional to $\|F(v)\|^2$.
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Runtime is $O(n \cdot \text{poly}\log n)$, 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.

Main Result

Theorem (Peng-S.-Zanetti, 2017)

There is a linear-time algorithm that, for a graph G with k clusters $S_1, \ldots, S_k$ and $\Upsilon = \Omega(k^3)$, outputs a partition $A_1, \ldots, A_k$ such that

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- BUT, our analysis only holds when there is an eigengap.

Beyond Graph Clustering

Could heat kernels be a general tool for designing fast algorithms?

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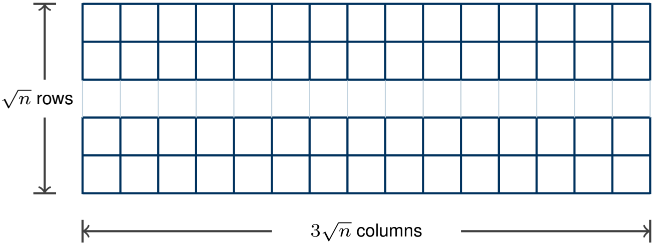
Improve the state-of-the-art algorithm by heat kernels?

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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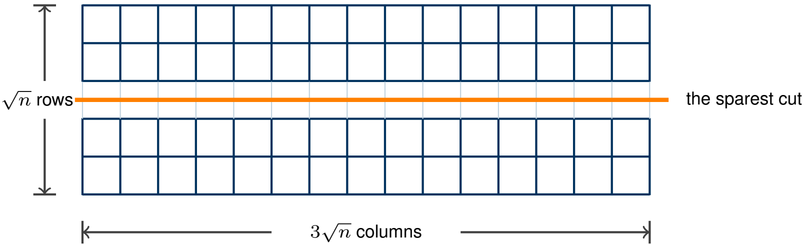

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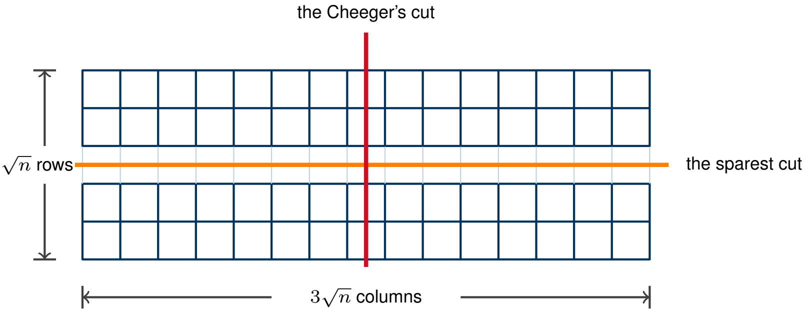
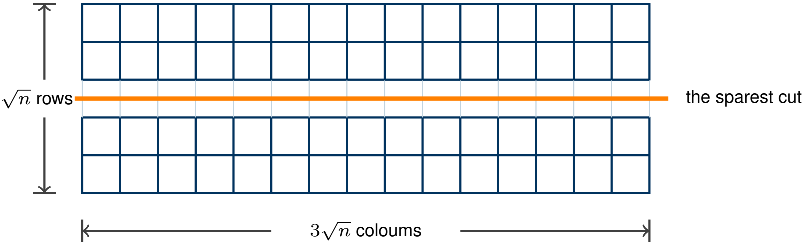
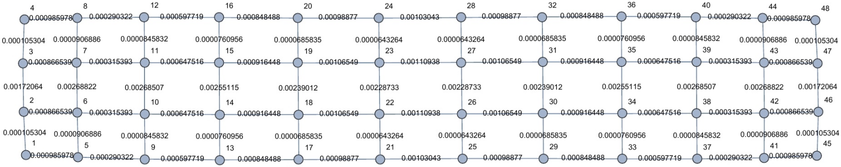


Heat Kernel Distances in the Grid Graphs





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This algorithm finds the optimal cut for the Grid Graph.

The proposed algorithm

Run the following for $t = 2^i, i = 1, 2, \ldots, c \log n$

- Compute heat kernel distances $h_t(u, v)$ for all edges $u \sim v$
- Construct a new graph $Q_t = (V, E, w)$ where $w(u, v) = \exp(-h_t(u, v))$
- Find a sparse cut of Q_t by the sweep set algorithm, i.e. the proof from Cheeger inequality
- Store the set $S \subseteq V$ with minimum conductance found so far.

Output S

This algorithm finds the optimal cut for the Grid Graph.

What is the approximate ratio of this algorithm?

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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.