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Spectral clustering using a multilevel approach

Kalman Szenes

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Motivation

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- Clustering is one of the main techniques in exploratory data analysis
- Clustering problem can be rewritten as a graph partitioning problem
  - Solving balanced metric is **NP-Hard**
  - Relaxed problem can be solved using spectral methods

Outline

1. Graphs
2. Graclus Framework
3. Clustering Algorithms
4. Results

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1. Graphs

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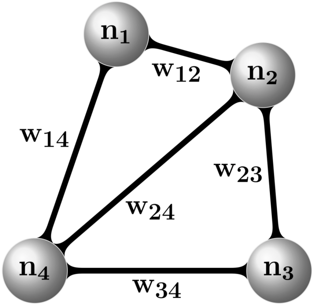
Graph Representation[1]

For a graph $\mathcal{G}(\mathcal{V}$, E, W)

- Adjacency: **W** $\in R^{n*n}$
- Degree: **D** $\in R^{n*n}$
- Graph Laplacian: **L** $\in R^{n*n}$

$$\mathbf{W} = \begin{pmatrix} 0 & w_{12} & 0 & w_{14} \\ w_{12} & 0 & w_{23} & w_{24} \\ 0 & w_{23} & 0 & w_{34} \\ w_{14} & w_{24} & w_{34} & 0 \end{pmatrix}, \qquad d_{ii} = \begin{pmatrix} \sum_j w_{1j} \\ \sum_j w_{2j} \\ \sum_j w_{3j} \\ \sum_j w_{4j} \end{pmatrix}$$



[1] Pasadakis, Alappat, Schenk, and Wellein 2021.

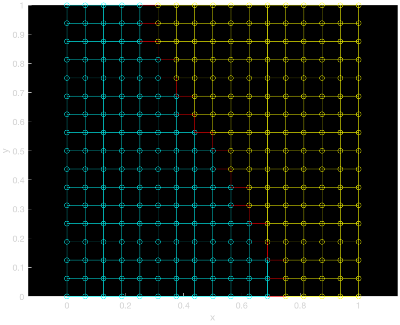
Partition Metric[2]

For subsets $\pi_1, \ldots, \pi_k$

- $cut(\pi, \bar{\pi}) = \sum_{i \in \pi, j \in \bar{\pi}} w_{ij}$
- $vol(\pi) = \sum_{i \in \pi} d_{ii}$

Minimize normalized cut:

$$NCut(\pi_1, \ldots, \pi_k) = \sum_{i=1}^{k} \frac{cut(\pi_i, \bar{\pi}_i)}{vol(\pi_i)}$$



A bi-partitioned graph

[2]Pasadakis, Alappat, Schenk, and Wellein 2021.

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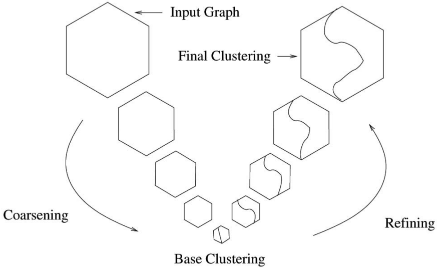
Coarsening and Refinement[3]



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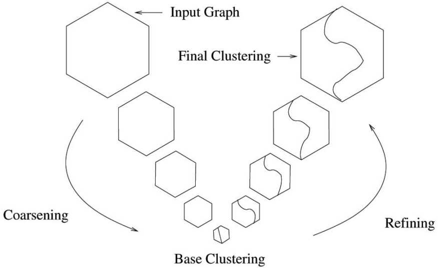
Coarsening and Refinement[3]

Coarsening



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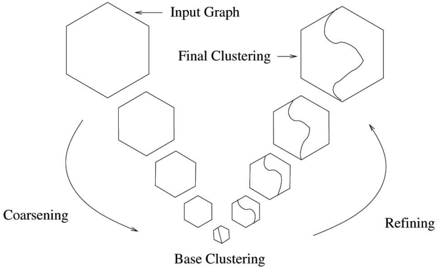
Coarsening and Refinement[3]

Coarsening

- Visit each vertex and merge with neighbor forming supernode

  $\Rightarrow$ Node degree and edge weights are summed



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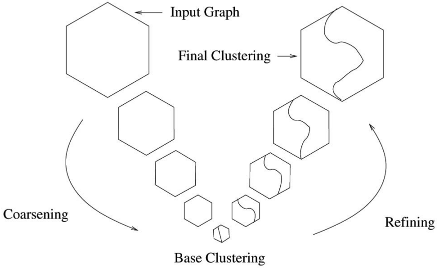
- Obtain successively smaller graphs $\{G, G_{+1}, ..., G_m\}$



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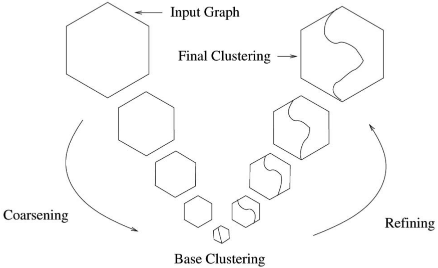

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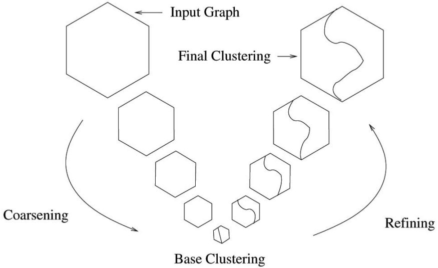

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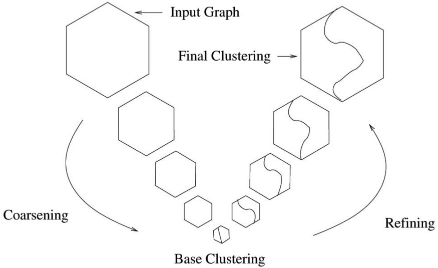
Refining

- Finer graphs inherit coarser partitioning



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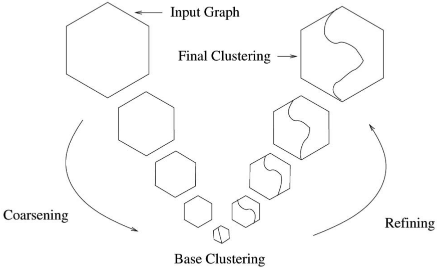
Refining

- Finer graphs inherit coarser partitioning
- Refine partitioning using Weighted Kernel K-Means algorithm



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Weighted Kernel K-Means[4]

- K-means simple clustering algorithm.

  Minimize sum of distances to centroids:

- $\sum_{c=1}^{k} \sum_{x_i \in \pi_c} ||x_i - \mu_c||^2$

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- **Solution** Project to higher dimension (KKM)

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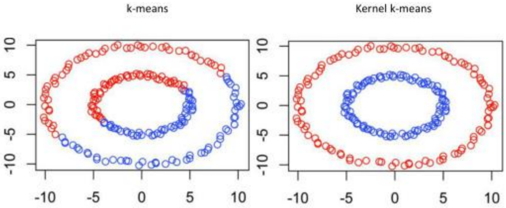

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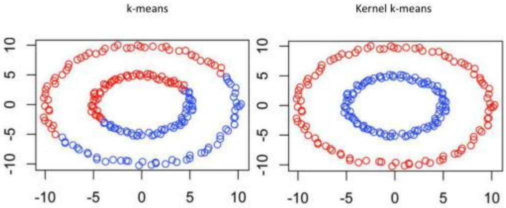

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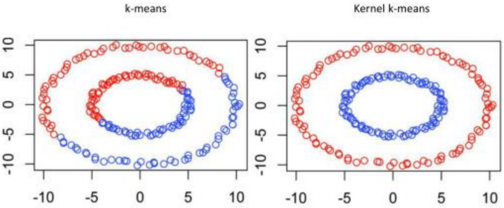
Node Weight	Kernel
Degree of node	$\sigma D^{-1} + D^{-1} W D^{-1}$

Table: Weights and Kernel for minimising NCut



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Outline

Direct Mutliway Spectral Clustering[7]

- **Goal**: Partition graph into k parts
- Compute k smallest eigenvectors of graph Laplacian

  $\Rightarrow U \in R^{n*k}$ containing eigenvectors
- Use k-means algorithm to cluster eigenvectors

[6] Inoue, Li, and Kurata 2010.
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[7] von Luxburg 2007.

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Three Laplacians to study

- Normalized Laplacian: $L_{rw} = I - D^{-1}W$
- β-Laplacian [5]: $L_{\beta} = I - D^{-\beta}W \quad \beta \in [1,2]$
- p-Spectral [6]

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p-Spectral[8]

- Smallest eigenvector computation:

$$\min_{U \in R^{n*k}} Tr(U^T L U) \text{ subject to } U^T U = I$$

$$\text{with } Tr(U^T L U) = \sum_{l}^{k} \sum_{ij}^{n} \frac{w_{ij}(u_i^l - u_j^l)^2}{2||u^l||_2^2}$$

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Unconstrained p-norm optimization on Grassmann

$$\underset{U \in \mathcal{G}r(k,n)}{\text{minimize}} = \sum_{l}^{k} \sum_{ij}^{n} \frac{w_{ij}|u_i^l - u_j^l|^p}{2||u^l||_p^p} \quad p \in [1.1, 2]$$

$$\text{p-norm: } ||u||_p = \sqrt[p]{\sum_{i=1}^{n} |u_i|^p}$$

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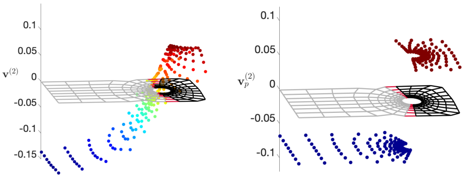

Fiedler vector for p=2 (left) p = 1.1 (right)

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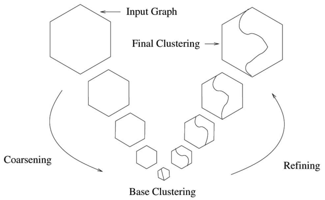
Algorithm: Multilevel spectral clustering algorithm
Input: Adjacency matrix $W \in R^{n*n}$, number k of clusters to construct

1) **Coarsen** graph to produce successively smaller adjacency matrices $\{W, W_1, ..., W_m\}$
   - Merge vertices together, sum up node degree and edge weights
   - Stop once $|V_m| < 5k$
2) Run **base clustering**
   - Compute first k eigenvectors using (RW, Beta, p)-Laplacian
   - Cluster eigenvectors using k-means algorithm
3) **Refine** partition to initial graph
   - Finer graph inherits partitioning of lower level graph
   - Use as initial guess for WKKM

Output: Clusters $A_1, ..., A_k$



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Metrics

Internal Metrics

- Normalized Cut (**minimize**):

$$\sum_{i=1}^{k} \frac{cut(C_i, \bar{C}_i)}{vol(C_i)}$$

External Metrics

- Accuracy (**maximize**)

Simulation Parameters

- Averaged over 10 runs
- Coarsen until $|\mathcal{V}_m| < 5k$
- K-means algorithm run 30 times
- Best beta chosen from 11 values $\in [1, 2]$
- p-Spectral method uses **normalized eigenvectors** as initial guess.
- Best p chosen from 8 values $\in [1.1, 2]$

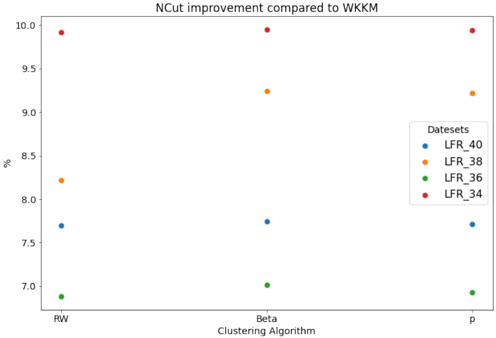
LFR Dataset

Stochastic block model with 10 clusters.

- Increasing **noise**

Coarse Level

Less than **50 vertices**



Original Graph

Metric	RW (%)	Beta (%)	p (%)
NCut	-1.71	-1.45	-1.48
Acc	+1.35	+1.33	+1.41
Runtime (s)	0.2	1.7	55.1

Table: Benchmark of LFR_40 dataset at finest level (**1000 vertices**)

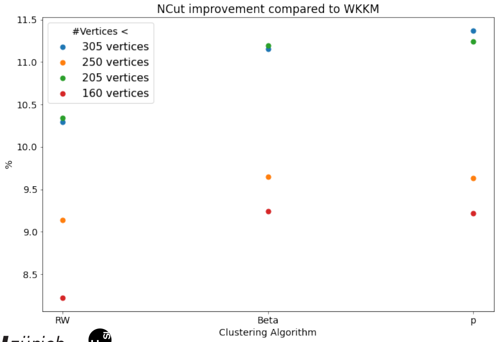
Gauss Dataset

Dataset containing k clusters with 400 points each, sampled from **Gaussian** distribution.
k $\in \{32, 41, 50, 61\}$

- Increasing **size**

Coarse Level

Less than **5k vertices**



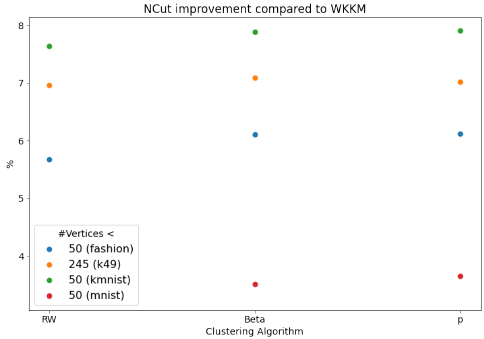
Original Graph

Metric	RW (%)	Beta (%)	p (%)
NCut	0.0	-0.79	+0.03
Acc	+0.06	+1.62	-0.61
Runtime (s)	1.0	7.2	219.7

Table: Benchmark of largest Gauss dataset at finest level (**24400 vertices**)

Real-World Data

Coarse Level



Original Graph

Metric	RW (%)	Beta (%)	p (%)
NCut	-3.58	-5.12	-4.66
Acc	-2.94	-1.38	-1.02
Runtime (s)	0.2	1.0	46.4

Table: Benchmark of Fashion dataset at finest level (**10000 vertices**)

Future Work

- Rewrite Graclus code
- Improve refinement algorithm
- Study the combination of β-Laplacian and p-Spectral

Thank you for your attention!

References

- Dhillon, Inderjit S., Yuqiang Guan, and Brian Kulis (Nov. 2007). "Weighted Graph Cuts without Eigenvectors A Multilevel Approach". In: *IEEE Transactions on Pattern Analysis and Machine Intelligence* 29.11, pp. 1944–1957. ISSN: 1939-3539. DOI: 10.1109/TPAMI.2007.1115.
- Inoue, Kentaro, Weijiang Li, and Hiroyuki Kurata (Sept. 2010). "Diffusion Model Based Spectral Clustering for Protein-Protein Interaction Networks". In: *PLoS ONE* 5.9. Ed. by Ingemar T. Ernberg, e12623. ISSN: 1932-6203. DOI: 10.1371/journal.pone.0012623.
- Pasadakis, Dimosthenis, Christie Louis Alappat, Olaf Schenk, and Gerhard Wellein (Nov. 2021). "Multiway P-Spectral Graph Cuts on Grassmann Manifolds". In: *Machine Learning*. ISSN: 1573-0565. DOI: 10.1007/s10994-021-06108-1.
- von Luxburg, Ulrike (Nov. 2007). "A Tutorial on Spectral Clustering". In: *arXiv:0711.0189 [cs]*. arXiv: 0711.0189 [cs].

LFR Original

Metric	RW %	Beta %	p %	p+beta %
NCut	-1.71	-1.45	-1.48	-1.40
Acc	+1.35	+1.33	+1.41	+1.34
NMI	+1.40	+1.09	+1.21	+1.10

Table: Comparison of Fashion dataset at original graph

Gauss Original

Metric	RW (%)	Beta (%)	p (%)
NCut	0.0	-0.79	+0.03
Acc	+0.06	+1.62	-0.61
NMI	-0.02	+0.47	-0.18
Runtime (s)	1.0	7.2	219.7

Table: Comparison of Gauss_61_55_10NN dataset at original graph with 24400 vertices

Real-World Ncut Coarse

Dataset	RW %	Beta %	p %	p+beta %
Fashion	5.68	6.11	6.12	6.22
k49	6.96	7.09	7.02	7.11
kmnist	7.64	7.89	7.91	7.91
mnist	3.29	3.52	3.65	3.79

Table: Percentage of improvement in NCut when compared to WKKM

Real-World Metrics Original

Metric	RW %	Beta %	p %	p+beta %
NCut	3.58	5.12	4.66	4.01
Acc	-2.94	-1.38	-1.02	-0.93
NMI	-0.79	-0.04	+0.57	+0.08

Table: Comparison of Fashion dataset at original graph

Random Walk Laplacian

Diffusion Laplacian[9]

$$L = I - D^{-\beta}W$$

with beta taking values between 1 and 2.

[9] Inoue, Li, and Kurata 2010.

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