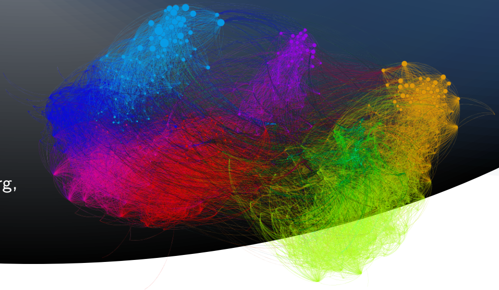
Graphs in Machine Learning

Spectral Clustering: RatioCut NCut

Approximation Algorithms

Michal Valko

Inria & ENS Paris-Saclay, MVA



Partially based on material by: Ulrike von Luxburg,
Miller, Doyle & Schnell, Daniel Spielman

Spectral Clustering: Relaxing Balanced Cuts

objective function of spectral clustering

$$\min_{\mathbf{f}} \mathbf{f}^{\mathsf{T}} \mathbf{L} \mathbf{f} \quad \text{s.t.} \quad f_i \in \mathbb{R}, \quad \mathbf{f} \perp \mathbf{1}_N, \quad \|\mathbf{f}\| = \sqrt{N}$$

Solution:

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$$\text{cluster}_i = \begin{cases} 1 & \text{if } i \in C_1, \\ -1 & \text{if } i \in C_{-1}. \end{cases}$$

Spectral Clustering: Approximating RatioCut

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$$\mathrm{RatioCut}(A, B) = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{|A|} + \frac{1}{|B|} \right)$$

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Normalized Cut

$$\mathrm{NCut}(A, B) = \sum_{i \in A, j \in B} w_{ij} \left(\frac{1}{\mathrm{vol}(A)} + \frac{1}{\mathrm{vol}(B)} \right)$$

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Can we apply Rayleigh-Ritz now?

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$\mathbf{f}$ is a the second eigenvector of $\mathbf{L}_{\mathrm{rw}}$!

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tl;dr: Get the second eigenvector of $\mathbf{L}/\mathbf{L}_{\text{rw}}$ for RatioCut/NCut.

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demo: `https://dominikschmidt.xyz/spectral-clustering-exp/`

Spectral Clustering: Approximation

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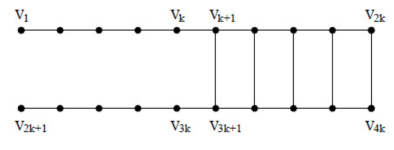
Pretty bad. Example: cockroach graphs



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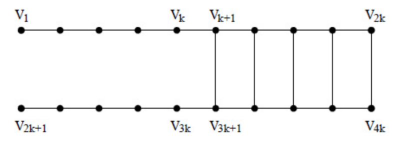
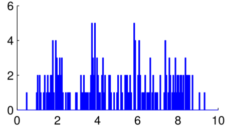


No efficient approximation exist. Other relaxations possible.

https://www.cs.cmu.edu/~glmiller/Publications/Papers/GuMi95.pdf

Spectral Clustering: 1D Example



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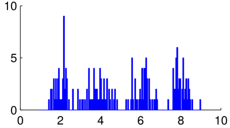

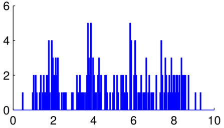

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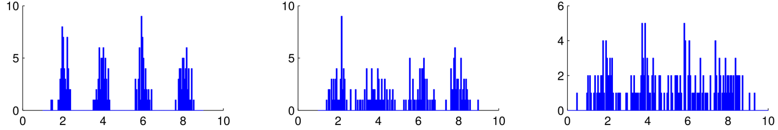

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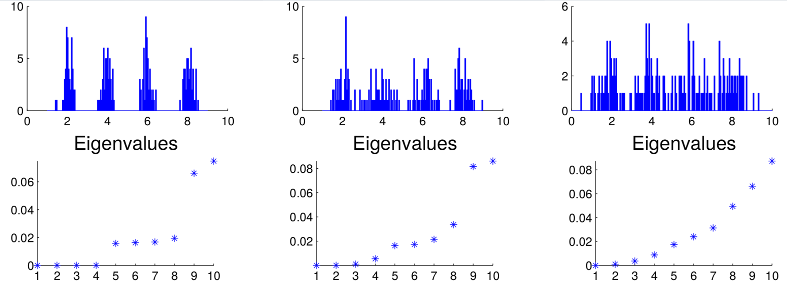

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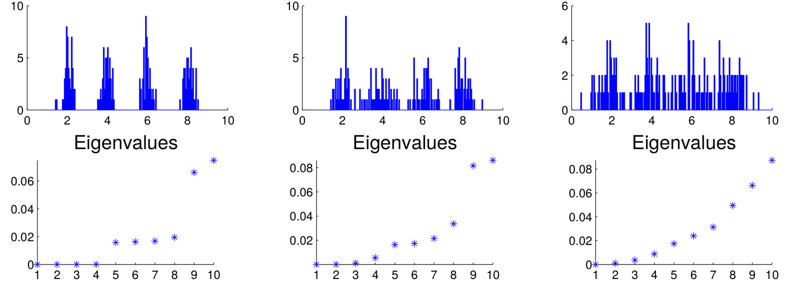
Elbow rule/EigenGap heuristic for number of clusters



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https://misovalko.github.io/mva-ml-graphs.html