Graphs in Machine Learning

Spectral Clustering: RatioCut & NCut

Relaxation & Approximation Algorithms

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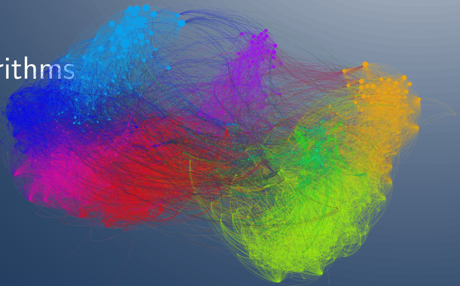

Partially based on material by: Ulrike von Luxburg, Gary Miller, Doyle & Schnell, Daniel Spielman

Spectral Clustering: Relaxing Balanced Cuts

Relaxation for (simple) balanced cuts for 2 sets

$$\min_{A,B} \operatorname{cut}(A, B) \quad \text{s.t.} \quad |A| = |B|$$

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What is the relationship with the **smoothness** of a graph function?

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objective function of spectral clustering

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

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$$\cancel{f_i = \pm 1} \quad \rightarrow \quad f_i \in \mathbb{R}$$

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Rayleigh-Ritz theorem

If $\lambda_1 \leq \cdots \leq \lambda_N$ are the eigenvalues of real symmetric $\mathbf{L}$ then

$$\lambda_1 = \min_{\mathbf{x} \neq 0} \frac{\mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}}{\mathbf{x}^{\mathsf{T}}\mathbf{x}} = \min_{\mathbf{x}^{\mathsf{T}}\mathbf{x}=1} \mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}$$

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How can we use it?

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Generalized Rayleigh-Ritz theorem (Courant-Fischer-Weyl)

If $\lambda_1 \leq \cdots \leq \lambda_N$ are the eigenvalues of real symmetric $\mathbf{L}$ and $\mathbf{v}_1, \ldots, \mathbf{v}_N$ the corresponding orthogonal eigenvectors, then for $k = 1 : N - 1$

$$\lambda_{k+1} = \min_{\mathbf{x} \neq 0, \mathbf{x} \perp \mathbf{v}_1, \ldots \mathbf{v}_k} \frac{\mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}}{\mathbf{x}^{\mathsf{T}}\mathbf{x}} = \min_{\mathbf{x}^{\mathsf{T}}\mathbf{x} = 1, \mathbf{x} \perp \mathbf{v}_1, \ldots \mathbf{v}_k} \mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}$$

$$\lambda_{N-k} = \max_{\mathbf{x} \neq 0, \mathbf{x} \perp \mathbf{v}_n, \ldots \mathbf{v}_{N-k+1}} \frac{\mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}}{\mathbf{x}^{\mathsf{T}}\mathbf{x}} = \max_{\mathbf{x}^{\mathsf{T}}\mathbf{x} = 1, \mathbf{x} \perp \mathbf{v}_N, \ldots \mathbf{v}_{N-k+1}} \mathbf{x}^{\mathsf{T}}\mathbf{L}\mathbf{x}$$

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Solution:

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

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objective function of spectral clustering (same - it's magic!)

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Spectral Clustering: Approximating NCut

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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$$(\mathbf{Df})^\mathsf{T}\mathbf{1}_n = 0$$

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$$(\mathbf{Df})^\mathsf{T} \mathbf{1}_n = 0 \qquad \mathbf{f}^\mathsf{T} \mathbf{Df} = \mathrm{vol}(\mathcal{V})$$

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objective function of spectral clustering (NCut)

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Can we apply Rayleigh-Ritz now?

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Spectral Clustering: Approximating NCut

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

Spectral Clustering: Approximating NCut

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

Spectral Clustering: Approximation

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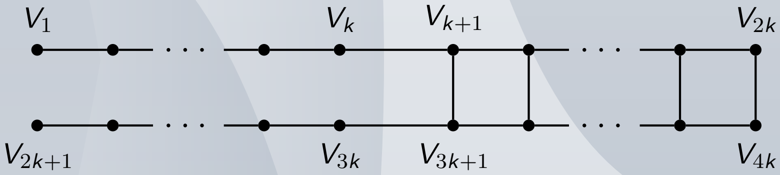

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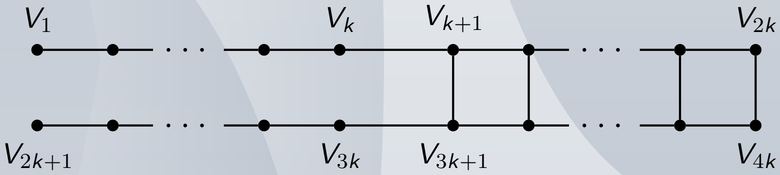
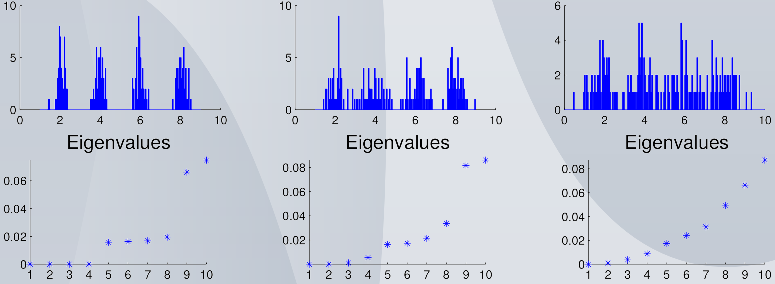


No efficient approximation exist. Other relaxations possible.

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

Spectral Clustering: 1D Example



Source: von Luxburg (2007)

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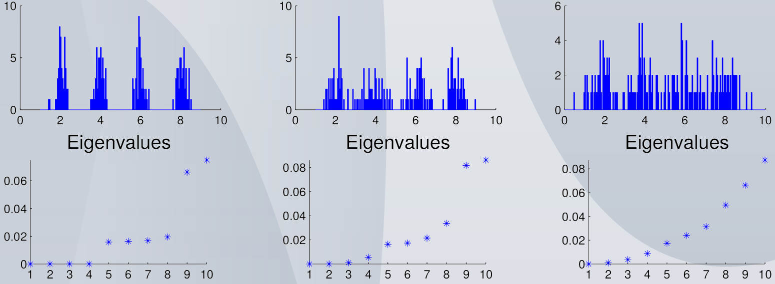

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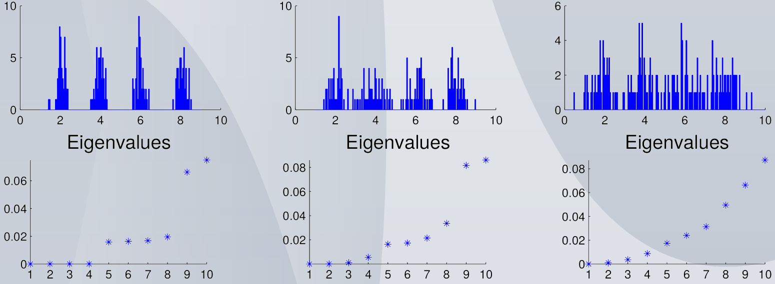

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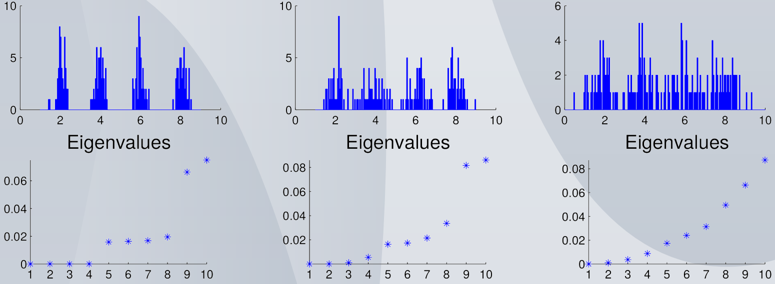

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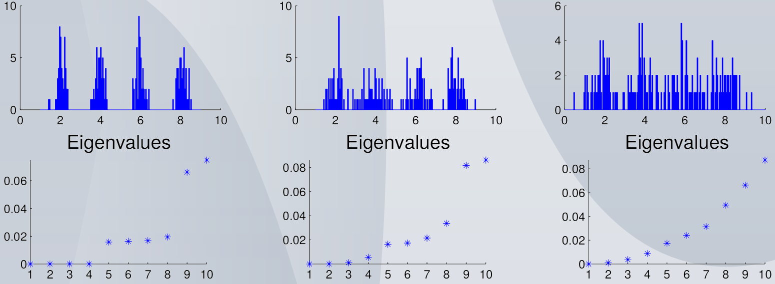
Spectral Clustering: 1D Example

Elbow rule/EigenGap heuristic for number of clusters



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