

Spectral Clustering of Graphs with the Bethe Hessian

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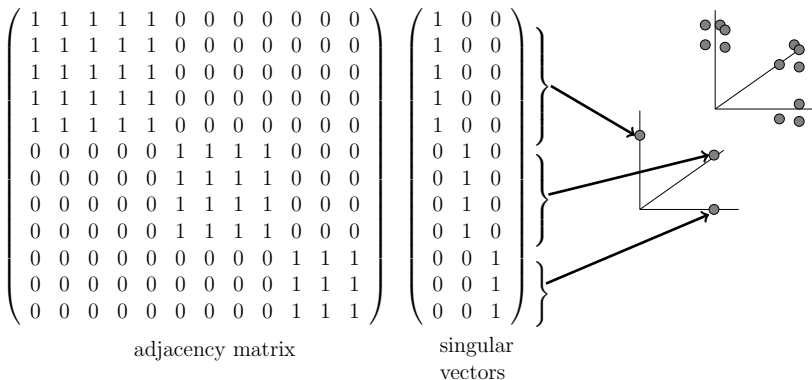
Clustering by the Laplacian $L = D - A$ ^[1]

Input: Adjacency matrix $A \in \mathbb{R}^{n \times n}$, number of clusters q

- $q = 2$
 - Cluster by the signs of the 2nd eigenvector of L
- $q > 2$
 - Let u_1, \dots, u_q be the first q eigenvectors of L
 - Let $U = (u_1, \dots, u_q) \in \mathbb{R}^{n \times q}$
 - Let $\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} = U$
 - Cluster the points $y_1, \dots, y_n \in \mathbb{R}^q$ with k -means

^[1]Ulrike Luxburg (2007). A tutorial on spectral clustering. Statistics and Computing, 17(4):395-416.

Clustering by the Adjacency Matrix $A^{[2]}$



^[2]Avrim Blum, John Hopcroft, and Ravindran Kannan (2016). Foundations of Data Science (pp. 275-281).

Spectral Clustering in Sparse Networks

- Clustering based on A fails to detect communities
- Locally tree-like structure
- Leading eigenvalues of A are dictated by the vertices of highest degree^[3]
- Corresponding eigenvectors are localized around these vertices^[3]

^[3]Michael Krivelevich and Benny Sudakov (2003). The largest eigenvalue of sparse random graphs. *Combinatorics, Probability and Computing*, 12(01):61-72.

Clustering by the Non-Backtracking Matrix^[4]

- The $2m \times 2m$ non-backtracking matrix B

$$B_{(u \rightarrow v), (x \rightarrow y)} = \begin{cases} 1 & \text{if } v = x \text{ and } u \neq y \\ 0 & \text{otherwise.} \end{cases}$$

- The spectrum of B is not sensitive to high-degree vertices
- Properties of B
 - A tree contributes zero eigenvalues to the spectrum
 - Unicyclic components yield eigenvalues either 1 or -1

^[4]Florent Krzakala, Cristopher Moore, et al (2013). Spectral redemption in clustering sparse networks. Proceedings of the National Academy of Sciences, 110(52):20935–20940.

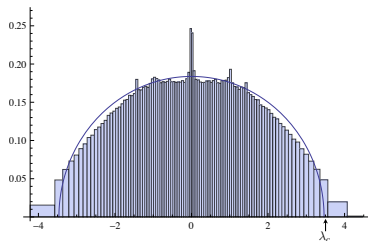
Stochastic Block Model

- Stochastic block model
 - q groups of vertices with size n/q
 - Each vertex v has a group label $g_v \in \{1, \dots, q\}$
 - Adjacency matrix A is generated according to the distribution

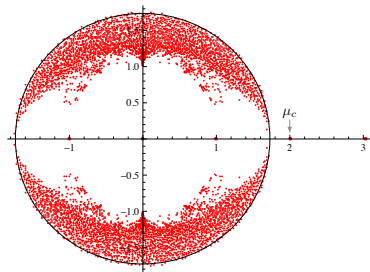
$$\Pr[A_{u,v} = 1] = \begin{cases} c_{\text{in}}/n & g_u = g_v \\ c_{\text{out}}/n & g_u \neq g_v \end{cases}, \text{ where } c_{\text{in}} > c_{\text{out}}$$

- Average degree $c = (c_{\text{in}} + c_{\text{out}})/2$ when $q = 2$
 - $L = D - A \approx c\mathbf{1} - A$
 - Clustering by the second largest eigenvector of A
- G becomes sparse when n is large

Spectrum of A and B



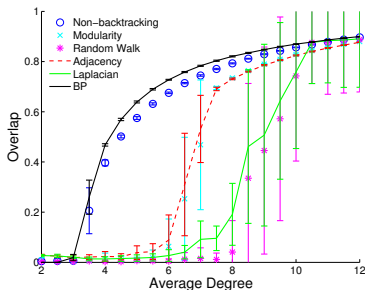
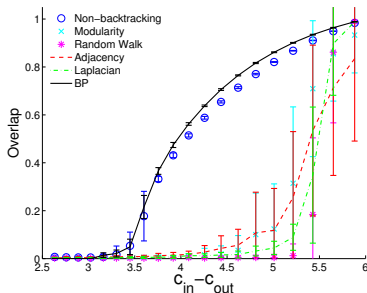
(a) The spectrum of A



(b) The spectrum of B

- $n = 4000, c_{\text{in}} = 5, c_{\text{out}} = 1$
- The radius of the bulk
 - For $A, 2\sqrt{c} = 3.46$
 - For $B, \sqrt{c} = \sqrt{3}$

Experiments $n = 10^5$

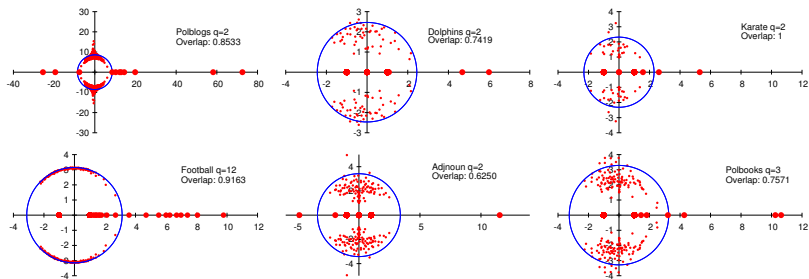


- $\text{Overlap} \triangleq \left(\frac{1}{n} \sum_u \delta_{g_u, \tilde{g}_u} - \frac{1}{q} \right) / \left(1 - \frac{1}{q} \right)$

- Theoretical threshold^[5] ≈ 3.46

^[5]Elchanan Mossel, Joe Neeman, and Allan Sly (2012). Stochastic block models and reconstruction. arXiv preprint, arXiv:1202.1499.

Detecting Number of Clusters



- Each circle's radius is $\sqrt{\rho(B)}$
- The number of real eigenvalues outside the circle indicates the number q of clusters

Reducing the Computational Complexity

- All eigenvalues μ of B not ± 1 are the roots of the equation^[6]

$$\det [\mu^2 \mathbf{1} - \mu A + (D - \mathbf{1})] = 0 \quad (1)$$

- By the first companion linearization^[7], roots of eq. (1) are eigenvalues of

$$B' = \begin{pmatrix} 0 & D - \mathbf{1} \\ -\mathbf{1} & A \end{pmatrix}$$

- Clustering by a $2n \times 2n$ matrix rather than a $2m \times 2m$ one

^[6]Omer Angel, Joel Friedman, and Shlomo Hoory (2015). The non-backtracking spectrum of the universal cover of a graph. Trans. Amer. Math. Soc., 367(6):4287-4318.

^[7]Francoise Tisseur and Karl Meerbergen (2001). The quadratic eigenvalue problem. SIAM Review, 43(2):235-286.

The Bethe Hessian Matrix

- All eigenvalues μ of B not ± 1 are the roots of the equation

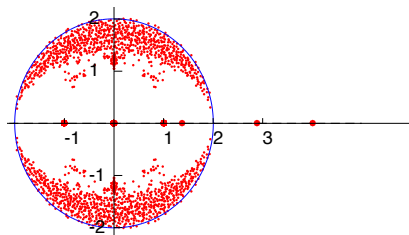
$$\det [\mu^2 \mathbb{1} - \mu A + (D - \mathbb{1})] = 0 \quad (1)$$

- The Bethe Hessian matrix $H(r)$

$$H(r) := r^2 \mathbb{1} - rA + (D - \mathbb{1})$$

- \forall real eigenvalue μ of B , $H(\mu)$ has a eigenvalue 0
 - Let $r_c = \sqrt{\rho(B)}$
 - Eigenvectors of $H(r_c)$'s negative eigenvalues reveal clustering

Spectrum of B and $H(r)$

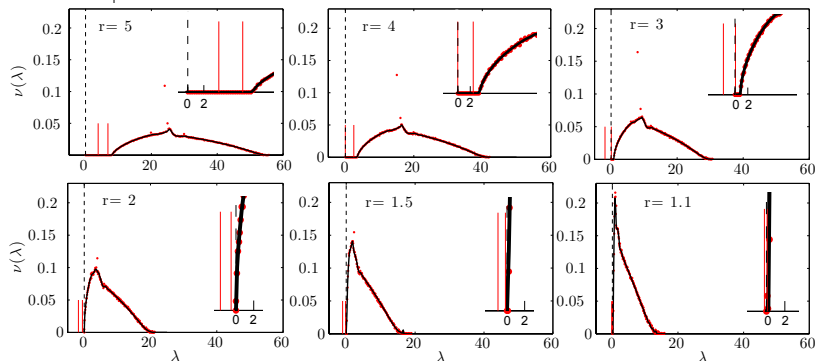


Stochastic block model

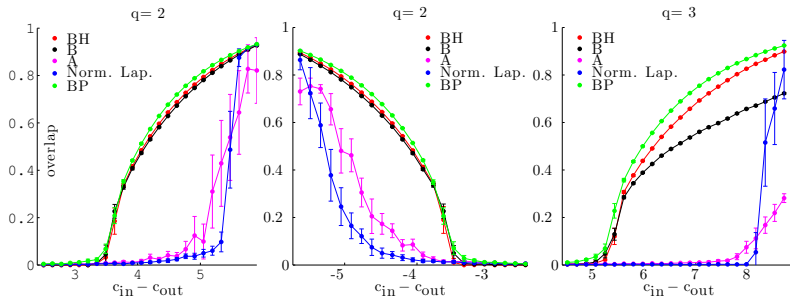
• $n = 10^4$

• $c = 4$

• $c_{\text{out}}/c_{\text{in}} = \frac{1}{7}$



Experiments



PART	Non-backtracking [9]	Bethe Hessian
Polbooks ($q = 3$) [1]	0.742857	0.757143
Polblogs ($q = 2$) [10]	0.864157	0.865794
Karate ($q = 2$) [24]	1	1
Football ($q = 12$) [6]	0.924111	0.924111
Dolphins ($q = 2$) [16]	0.741935	0.806452
Adjnoun ($q = 2$) [8]	0.625000	0.660714

Conclusions and Perspectives

- Comparing to non-backtracking clustering
 - $H(r_c)$ is $n \times n$ symmetric, while B' is $2n \times 2n$ non-symmetric
 - Need to compute $\rho(B)$ to calculate $r_c = \sqrt{\rho(B)}$
 - By solving quadratic eigenproblem (2) using a SLP algorithm^[8]

$$\det H(\lambda) = \det [\lambda^2 \mathbb{1} - \lambda A + (D - \mathbb{1})] = 0 \quad (2)$$

- Detecting the communities in sparse network
 - All the way down to the threshold in SBM
- The number of negative eigenvalues indicating the number of clusters

^[8] Axel Ruhe (1973). Algorithms for the nonlinear eigenvalue problem. SIAM Journal on Numerical Analysis, 10(4):674–689.

The End