

# Spectral Clustering of Graphs with the Bethe Hessian

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# Clustering by the Laplacian $L = D - A$ <sup>[1]</sup>

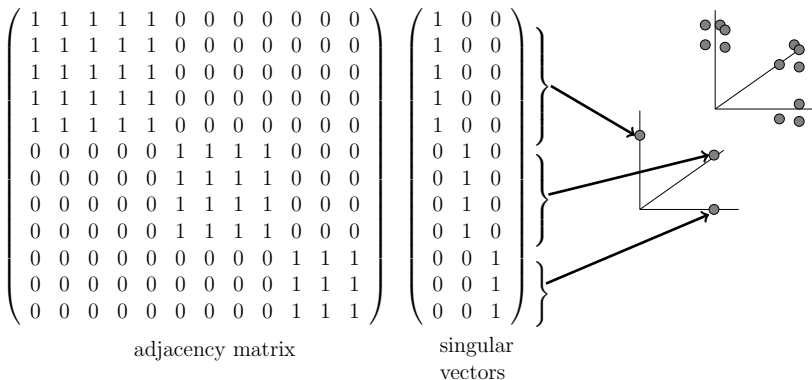
Input: Adjacency matrix  $A \in \mathbb{R}^{n \times n}$ , number of clusters  $q$

- $q = 2$ 
  - 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

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

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



<sup>[2]</sup>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<sup>[3]</sup>
- Corresponding eigenvectors are localized around these vertices<sup>[3]</sup>

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<sup>[3]</sup>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<sup>[4]</sup>

- 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  $-1$

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

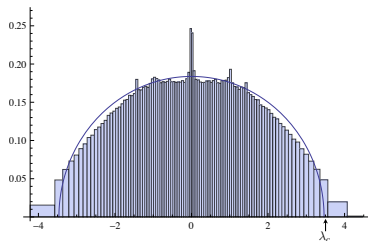
# Stochastic Block Model

- 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

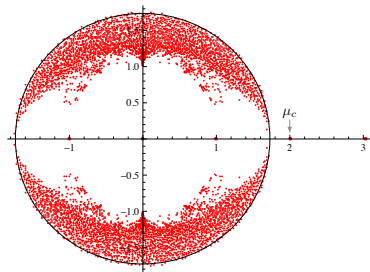
$$\Pr[A_{u,v} = 1] = \begin{cases} c_{\text{in}}/n & g_u = g_v \\ c_{\text{out}}/n & g_u \neq g_v \end{cases}, \text{ where } c_{\text{in}} > c_{\text{out}}$$

- Average degree  $c = (c_{\text{in}} + c_{\text{out}})/2$  when  $q = 2$
- $G$  becomes sparse when  $n$  is large

# Spectrum of $A$ and $B$



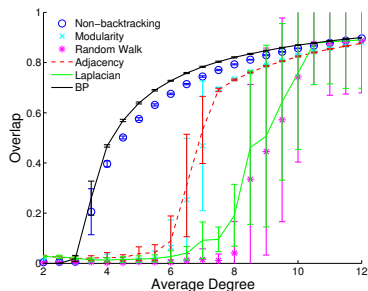
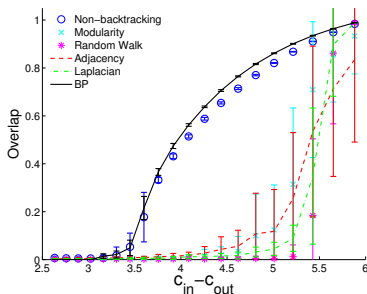
(a) The spectrum of  $A$



(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 $n = 10^5$



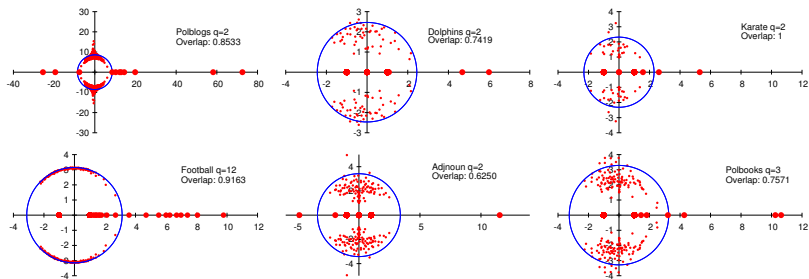
- $\text{Overlap} \triangleq \left( \frac{1}{n} \sum_u \delta_{g_u, \tilde{g}_u} - \frac{1}{q} \right) / \left( 1 - \frac{1}{q} \right)$

- Theoretical threshold<sup>[5]</sup>  $\approx 3.46$

<sup>[5]</sup>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  $\lambda$  of  $B$  not  $\pm 1$  are the roots of the equation<sup>[6]</sup>

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

- By the first companion linearization<sup>[7]</sup>, 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

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<sup>[6]</sup>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.

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

# The Bethe Hessian Matrix

- All eigenvalues  $\lambda$  of  $B$  not  $\pm 1$  are the roots of the equation

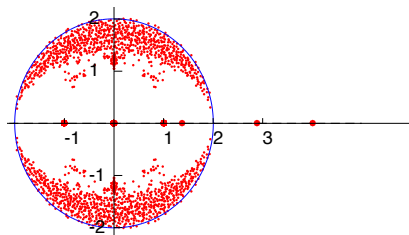
$$\det [\lambda^2 \mathbb{1} - \lambda A + (D - \mathbb{1})] = 0 \quad (1)$$

- The Bethe Hessian matrix  $H(r)$

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

- $\forall$  real eigenvalue  $\lambda$  of  $B$ ,  $H(\lambda)$  has a eigenvalue 0
  - $H(\lambda)$ 's null space  $\longleftrightarrow$   $B$ 's eigenvector corresponding to  $\lambda$
  - Let  $r_c = \sqrt{\rho(B)}$
  - Eigenvectors of  $H(r_c)$ 's negative eigenvalues reveal clustering

# Spectrum of $B$ and $H(r)$

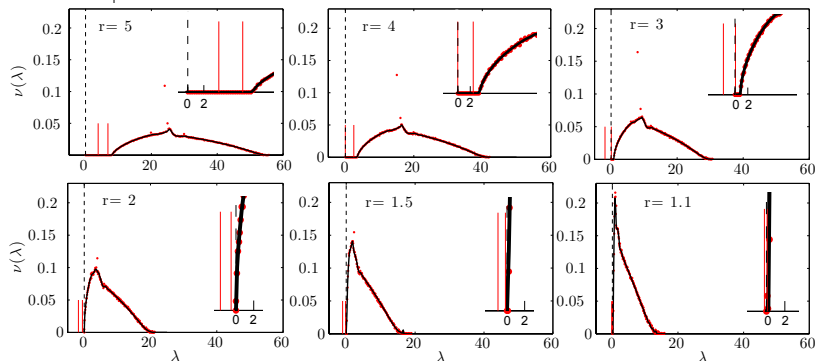


Stochastic block model

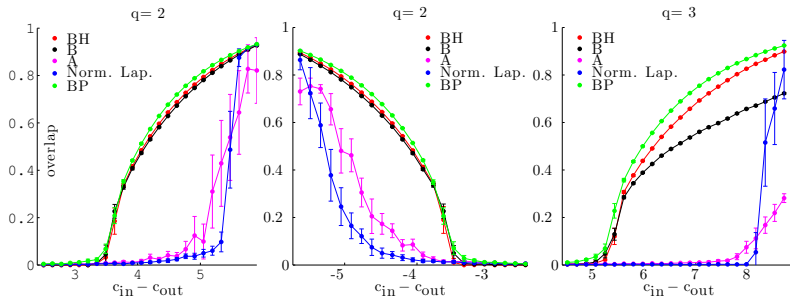
•  $n = 10^4$

•  $c = 4$

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



# 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<sup>[8]</sup>

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

- 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

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

# The End