Spectral Clustering of Graphs with the Bethe Hessian

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Clustering by the Laplacian $L=D-A^{{\scriptsize \scriptsize [1]}}$

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

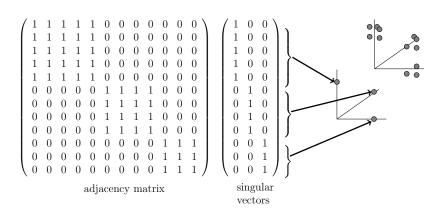
- q = 2
 - ullet Cluster by the signs of the 2nd eigenvector of L
- q > 2
 - ullet Let u_1,\cdots,u_q be the first q eigenvectors of L
 - Let $U=(u_1,\cdots,u_q)\in\mathbb{R}^{n imes q}$

• Let
$$\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} = U$$

• Cluster the points $y_1, \cdots, y_n \in \mathbb{R}^q$ with k-means

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

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



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

Spectral Clustering in Sparse Networks

- ullet Clustering based on A fails to detect communities
- Locally tree-like structure
- Leading eigenvalues of A are dictated by the vertices of highest ${\rm degree}^{{\rm [3]}}$
- 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]

ullet The 2m imes 2m non-backtracking matrix B

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

- ullet The spectrum of B is not sensitive to high-degree vertices
- ullet Properties of B
 - A tree contributes zero eigenvalues to the spectrum
 - ullet 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.

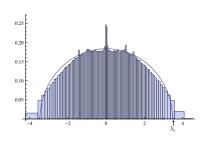
Stochastic Block Model

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

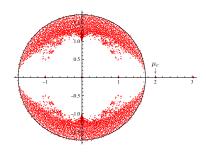
$$\Pr[A_{u,v}=1] = egin{cases} c_{
m in}/n & g_u=g_v \ c_{
m out}/n & g_u
eq g_v \end{cases}$$
 , where $c_{
m in} > c_{
m out}$

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

Spectrum of \boldsymbol{A} and \boldsymbol{B}



(a) The spectrum of ${\cal A}$

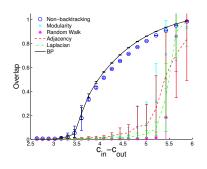


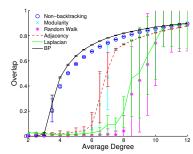
(b) The spectrum of ${\cal B}$

•
$$n = 4000$$
, $c_{\rm in} = 5$, $c_{\rm out} = 1$

- The radius of the bulk
 - For A, $2\sqrt{c} = 3.46$
 - For B, $\sqrt{c} = \sqrt{3}$

Experiments $n=10^{51}$

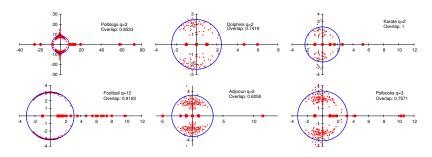




- Overlap $\triangleq \left(\frac{1}{n} \sum_{u} \delta_{g_{u}, \tilde{g}_{u}} \frac{1}{q}\right) / \left(1 \frac{1}{q}\right)$
- Theoretical threshold $^{\text{[5]}} pprox 3.46$

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

Detecting Number of Clusters



- \bullet Each circle's radius is $\sqrt{\rho(B)}$
- $\bullet\,$ 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]

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

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

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

ullet Clustering by a 2n imes 2n matrix rather than a 2m imes 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

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

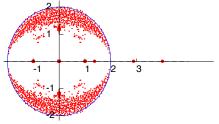
$$\det \left[\mu^2 \mathbb{1} - \mu A + (D - \mathbb{1}) \right] = 0 \tag{1}$$

• The Bethe Hessian matrix H(r)

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

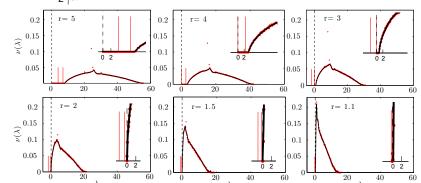
- \forall real eigenvalue μ of B, $H(\mu)$ has a eigenvalue 0
 - Let $r_c = \sqrt{\rho(B)}$
 - ullet Eigenvectors of $H(r_c)$'s negative eigenvalues reveal clustering

Spectrum of ${\cal B}$ and ${\cal H}(r)$

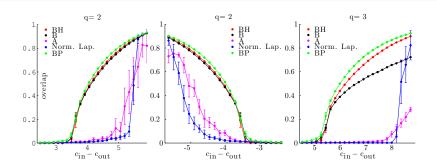


Stochastic block model

- $n = 10^4$
- c = 4
- $c_{\mathrm{out}}/c_{\mathrm{in}} = \frac{1}{7}$



Experiments



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

Conclusions and Perspectives

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

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

- 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