

Spectral clustering in sparse heterogeneous networks

Lorenzo Dall'Amico
Romain Couillet, Nicolas Tremblay

Laboratoire Gipsa-lab, UMR 5216, CNRS, UGA
11 rue des mathématiques 38420 Grenoble, France
lorenzo.dall-amico@gipsa-lab.fr

May 10, 2019



Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_{\alpha}$?

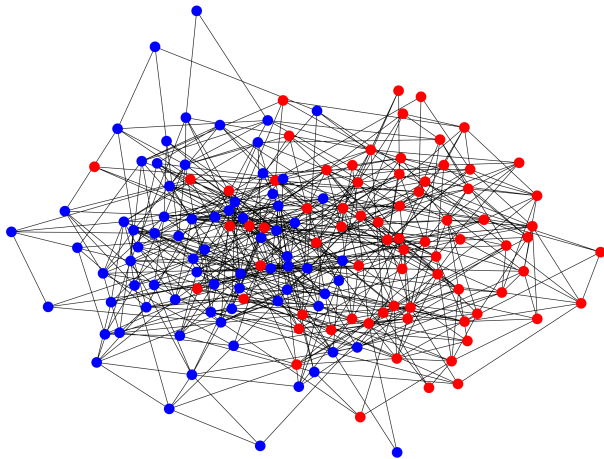
Results

More than two classes

Conclusion

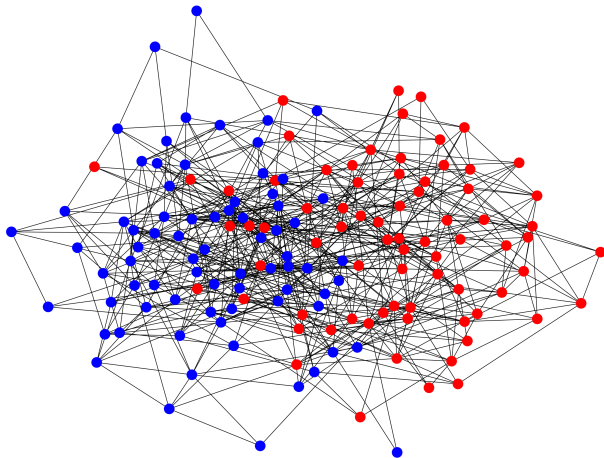


What and why



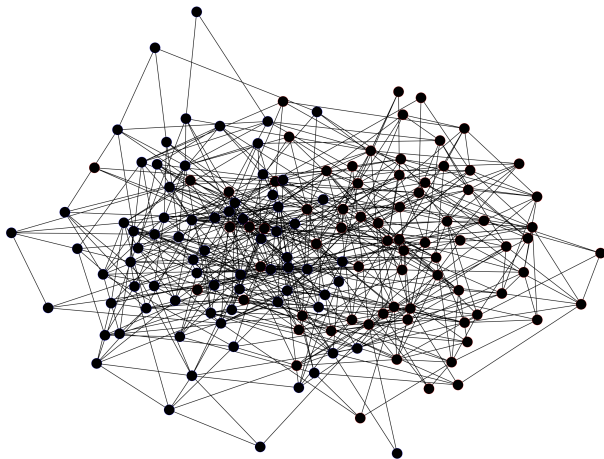
What and why

The solution...



What and why

The problem



The spectral techniques

Information inside the eigenvectors



The spectral techniques

Information inside the eigenvectors



FAST



The spectral techniques

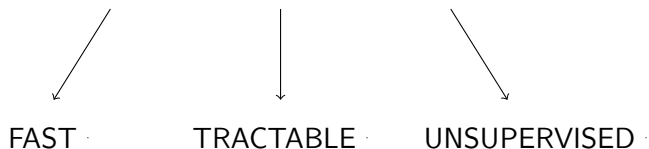
Information inside the eigenvectors

↙
FAST

↘
UNSUPERVISED

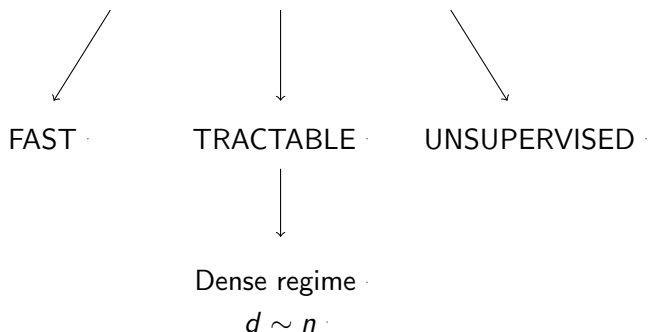
The spectral techniques

Information inside the eigenvectors



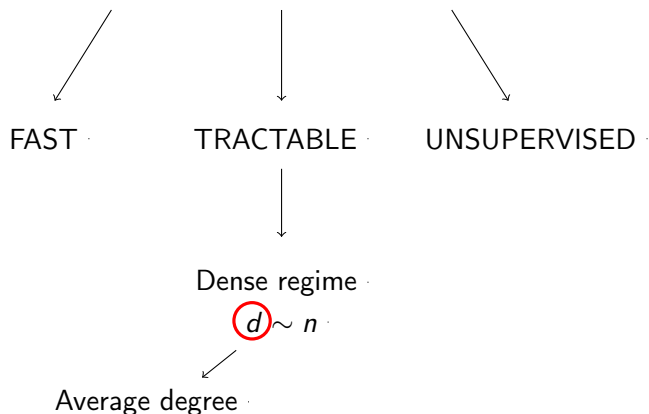
The spectral techniques

Information inside the eigenvectors



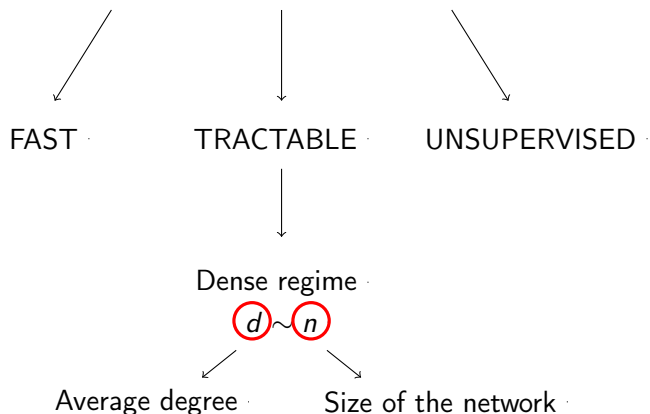
The spectral techniques

Information inside the eigenvectors



The spectral techniques

Information inside the eigenvectors



Example

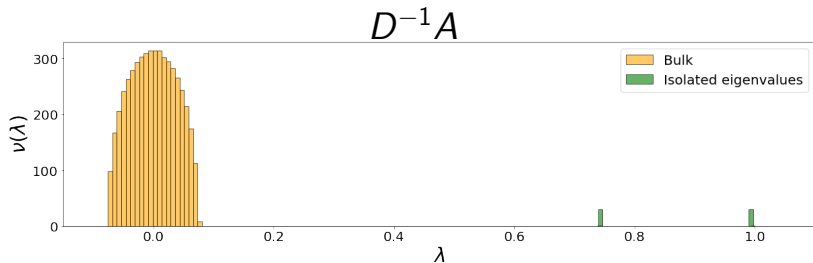
- ▶ A : adjacency matrix, $A_{ij} = 1$ if (ij) are connected, zero else

Example

- ▶ A : adjacency matrix, $A_{ij} = 1$ if (ij) are connected, zero else
- ▶ D : degree matrix $D = \text{diag}(A\mathbf{1})$

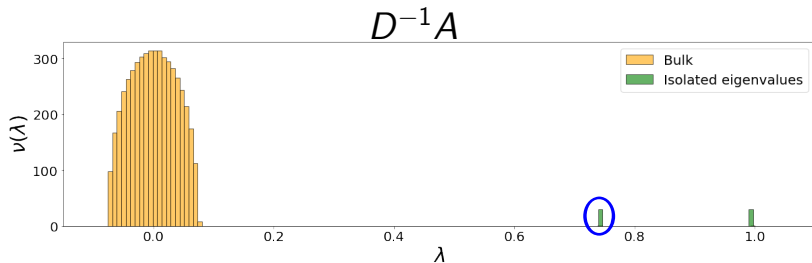
Example

- ▶ A : adjacency matrix, $A_{ij} = 1$ if (ij) are connected, zero else
- ▶ D : degree matrix $D = \text{diag}(A\mathbf{1})$

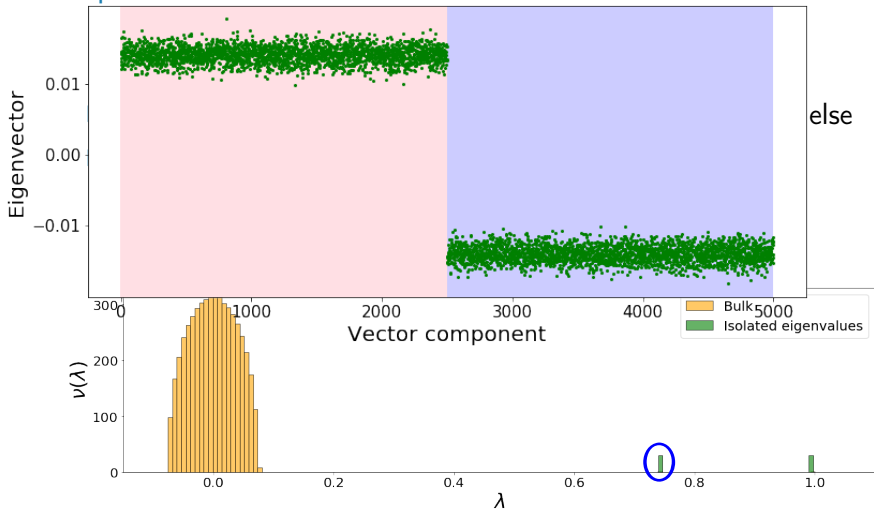


Example

- ▶ A : adjacency matrix, $A_{ij} = 1$ if (ij) are connected, zero else
- ▶ D : degree matrix $D = \text{diag}(A\mathbf{1})$



Example



Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_{\alpha}$?

Results

More than two classes

Conclusion

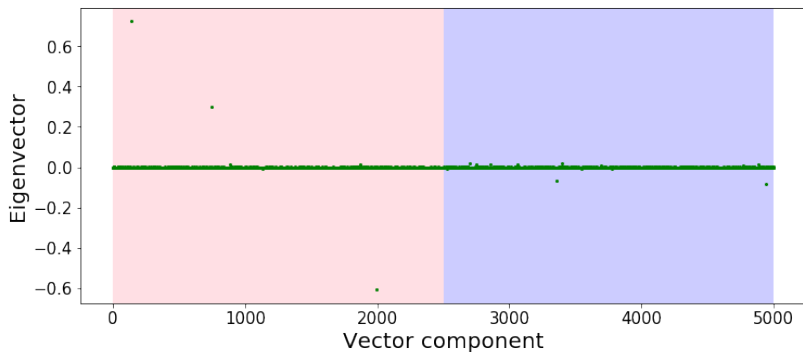
Real networks are sparse

$$d \approx \text{const}$$



Real networks are sparse

$$d \approx \text{const}$$



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$

¹Krzakala et al, Spectral redemption in clustering sparse networks, PNAS 2013 



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

Important theoretical results:

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

Important theoretical results:

1. Work in the sparse regime

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

Important theoretical results:

1. Work in the sparse regime
2. Work asymptotically down to the detectability threshold

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Two solutions

- ▶ Non-backtracking matrix¹ $B \in \{0, 1\}^{2|\mathcal{E}| \times 2|\mathcal{E}|}$
 $B_{(ij),(kl)} = \delta_{jk}(1 - \delta_{il})$
- ▶ Bethe-Hessian matrix²
 $H_r = (r^2 - 1)I_n + D - rA, r \in \mathbb{R}$

Important theoretical results:

1. Work in the sparse regime
2. Work asymptotically down to the detectability threshold

Only for homogeneous degree distribution

¹Krzakala et al., Spectral redemption in clustering sparse networks, PNAS 2013

²Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014



Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_{\alpha}$?

Results

More than two classes

Conclusion



The DC-SBM

$$\mathbb{P}(A_{ij} = 1 | \sigma_i, \sigma_j, \mathbf{q}_i, \mathbf{q}_j) = \mathbf{q}_i \mathbf{q}_j \frac{C(\sigma_i, \sigma_j)}{n}$$



The DC-SBM

$$\mathbb{P}(A_{ij} = 1 | \sigma_i, \sigma_j, q_i, q_j) = q_i q_j \frac{C(\sigma_i, \sigma_j)}{n}$$

$$\mathbb{E}[q] = 1, \quad \mathbb{E}[q^2] = \Phi, \quad C = \begin{pmatrix} c_{\text{in}} & c_{\text{out}} \\ c_{\text{out}} & c_{\text{in}} \end{pmatrix}, \quad c = \frac{c_{\text{in}} + c_{\text{out}}}{2}$$



The DC-SBM

$$\mathbb{P}(A_{ij} = 1 | \sigma_i, \sigma_j, q_i, q_j) = q_i q_j \frac{C(\sigma_i, \sigma_j)}{n}$$

$$\mathbb{E}[q] = 1, \quad \mathbb{E}[q^2] = \Phi, \quad C = \begin{pmatrix} c_{\text{in}} & c_{\text{out}} \\ c_{\text{out}} & c_{\text{in}} \end{pmatrix}, \quad c = \frac{c_{\text{in}} + c_{\text{out}}}{2}$$

Detectability threshold³ :

$$\alpha := \frac{c_{\text{in}} - c_{\text{out}}}{\sqrt{c}} \geq \frac{2}{\sqrt{\Phi}}$$

³Gulikers et al. An impossibility result for reconstruction in the degree-corrected stochastic block model, The Annals of Applied Probability 2018



Goal

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \in \mathbb{R}$$

Second smallest eigenvector of H_r for:



Goal

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \in \mathbb{R}$$

Second smallest eigenvector of H_r for:

- ▶ Community detection in sparse and heterogeneous networks



Goal

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \in \mathbb{R}$$

Second smallest eigenvector of H_r for:

- ▶ Community detection in sparse and heterogeneous networks
- ▶ Reach the detectability threshold



Goal

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \in \mathbb{R}$$

Second smallest eigenvector of H_r for:

- ▶ Community detection in sparse and heterogeneous networks
- ▶ Reach the detectability threshold

Pick the good value of r to:



Goal

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \in \mathbb{R}$$

Second smallest eigenvector of H_r for:

- ▶ Community detection in sparse and heterogeneous networks
- ▶ Reach the detectability threshold

Pick the good value of r to:

- ▶ Retrieve σ regardless of \mathbf{q}



Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_\alpha$?

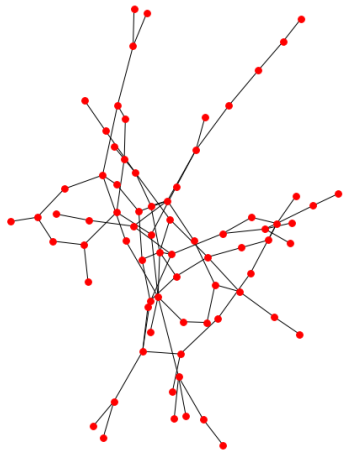
Results

More than two classes

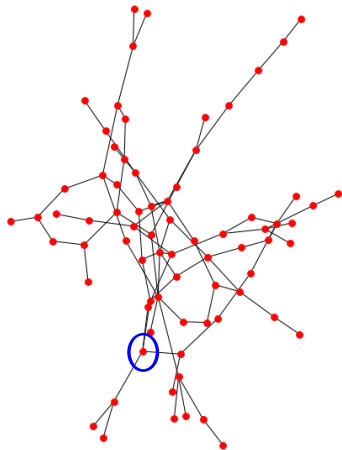
Conclusion



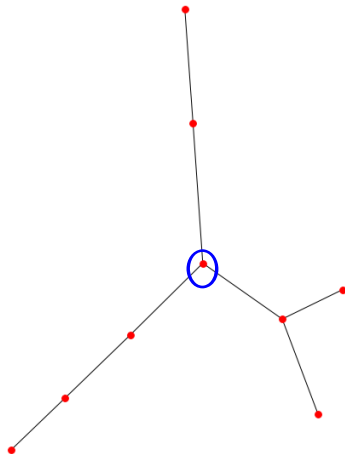
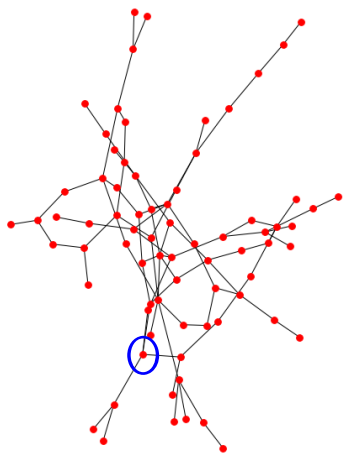
Tree like approximation



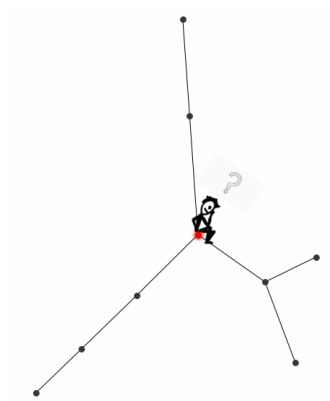
Tree like approximation



Tree like approximation



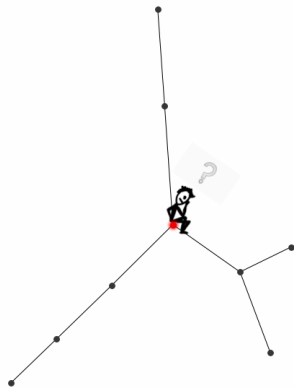
Tree like approximation



Tree like approximation

$$\mathbb{P}(\sigma_i = \sigma_j | A_{ij} = 1) = \frac{c_{in}}{c_{in} + c_{out}}$$

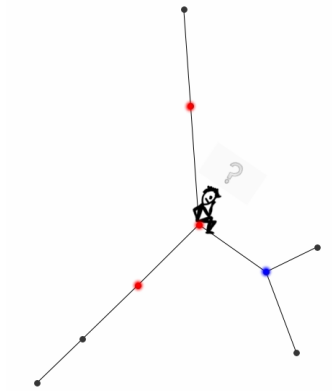
$$\mathbb{P}(\sigma_i \neq \sigma_j | A_{ij} = 1) = \frac{c_{out}}{c_{in} + c_{out}}$$



Tree like approximation

$$\mathbb{P}(\sigma_i = \sigma_j | A_{ij} = 1) = \frac{c_{in}}{c_{in} + c_{out}}$$

$$\mathbb{P}(\sigma_i \neq \sigma_j | A_{ij} = 1) = \frac{c_{out}}{c_{in} + c_{out}}$$

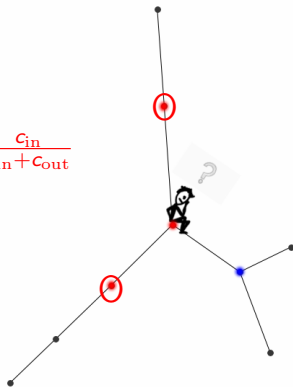


Tree like approximation

$$\mathbb{P}(\sigma_i = \sigma_j | A_{ij} = 1) = \frac{c_{in}}{c_{in} + c_{out}}$$

$$\mathbb{P}(\sigma_i \neq \sigma_j | A_{ij} = 1) = \frac{c_{out}}{c_{in} + c_{out}}$$

$$\mathbb{E}[|\partial_i^{(s)}|] = d_i \frac{c_{in}}{c_{in} + c_{out}}$$



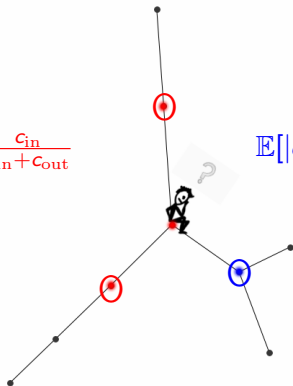
Tree like approximation

$$\mathbb{P}(\sigma_i = \sigma_j | A_{ij} = 1) = \frac{c_{in}}{c_{in} + c_{out}}$$

$$\mathbb{P}(\sigma_i \neq \sigma_j | A_{ij} = 1) = \frac{c_{out}}{c_{in} + c_{out}}$$

$$\mathbb{E}[|\partial_i^{(s)}|] = d_i \frac{c_{in}}{c_{in} + c_{out}}$$

$$\mathbb{E}[|\partial_i^{(o)}|] = d_i \frac{c_{out}}{c_{in} + c_{out}}$$



Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_{\alpha}$?

Results

More than two classes

Conclusion



The optimal choice of r

What is the informative eigenvector of H_r ?

The optimal choice of r

What is the informative eigenvector of H_r ?

What is r such that : $H_r \sigma \approx \lambda \sigma$?



The optimal choice of r

What is the informative eigenvector of H_r ?

What is r such that : $H_r \sigma \approx \lambda \sigma$?

$$\mathbb{E}[\left[\left((r^2 - 1)I_n + D - rA \right) \sigma \right]_i]$$



The optimal choice of r

What is the informative eigenvector of H_r ?

What is r such that : $H_r \sigma \approx \lambda \sigma$?

$$\mathbb{E}[\left[((r^2 - 1)I_n + D - rA)\sigma \right]_i] = \sigma_i \left[(r^2 - 1) + d_i \left(1 - r \frac{c_{in} - c_{out}}{c_{in} + c_{out}} \right) \right]$$



The optimal choice of r

What is the informative eigenvector of H_r ?

What is r such that : $H_r \sigma \approx \lambda \sigma$?

$$\mathbb{E}[\left[((r^2 - 1)I_n + D - rA)\sigma \right]_i] = \sigma_i \left[(r^2 - 1) + d_i \left(1 - r \frac{c_{in} - c_{out}}{c_{in} + c_{out}} \right) \right]$$

$$r_{\text{opt}} = \zeta \equiv \frac{c_{in} + c_{out}}{c_{in} - c_{out}} \equiv \zeta_{\alpha} = \frac{2\sqrt{c}}{\alpha}$$



From heuristics arguments...

$$O_V = 2 \left(\frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i, \tilde{\sigma}_i} - \frac{1}{2} \right)$$

Explicit expression of the overlap

$$\mathbb{E}[O_V] \simeq \frac{1}{n} \sum_{i=1}^n \operatorname{erf} \left[\sqrt{\frac{\alpha^2 d_i}{8c - 2\alpha^2} \left(\frac{c\Phi - \zeta_\alpha^2}{c\Phi - 1} \right)} \right]$$



From heuristics arguments...

$$O_V = 2 \left(\frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i, \tilde{\sigma}_i} - \frac{1}{2} \right)$$

Explicit expression of the overlap

$$\mathbb{E}[O_V] \simeq \frac{1}{n} \sum_{i=1}^n \operatorname{erf} \left[\sqrt{\frac{\alpha^2 d_i}{8c - 2\alpha^2} \left(\frac{c\Phi - \zeta_\alpha^2}{c\Phi - 1} \right)} \right]$$



From heuristics arguments...

$$O_V = 2 \left(\frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i, \tilde{\sigma}_i} - \frac{1}{2} \right)$$

Explicit expression of the overlap

$$\mathbb{E}[O_V] \simeq \frac{1}{n} \sum_{i=1}^n \operatorname{erf} \left[\sqrt{\frac{\alpha^2 d_i}{8c - 2\alpha^2} \left(\frac{c\Phi - \zeta_\alpha^2}{c\Phi - 1} \right)} \right]$$

$$\lim_{c_{\text{out}} \rightarrow 0} 8c - 2\alpha^2 = 0$$



From heuristics arguments...

$$O_V = 2 \left(\frac{1}{n} \sum_{i=1}^n \delta_{\sigma_i, \tilde{\sigma}_i} - \frac{1}{2} \right)$$

Explicit expression of the overlap

$$\mathbb{E}[O_V] \simeq \frac{1}{n} \sum_{i=1}^n \operatorname{erf} \left[\sqrt{\frac{\alpha^2 d_i}{8c - 2\alpha^2} \left(\frac{c\Phi - \zeta_\alpha^2}{c\Phi - 1} \right)} \right]$$

$$\lim_{\alpha \rightarrow \alpha_c} c\Phi - \zeta_\alpha^2 = 0$$



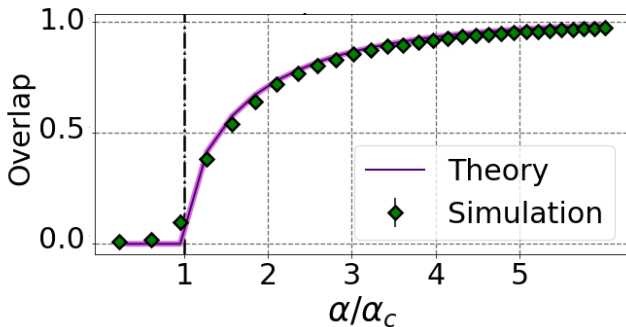


Figure: Simulated versus theoretical overlap for q_i distributed according to a power law. Average over 10 realizations. Both figures : The following parameters were used: $n = 5000$, $c_{\text{out}} = 8$, $c_{\text{in}} = 9 \rightarrow 61$.

Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_{\alpha}$?

Results

More than two classes

Conclusion



How to estimate $r_{\text{opt}} = \zeta_\alpha$?

From linearisation of BP

$$B\mathbf{w} = \zeta_\alpha \mathbf{w}$$



How to estimate $r_{\text{opt}} = \zeta_\alpha$?

From linearisation of BP

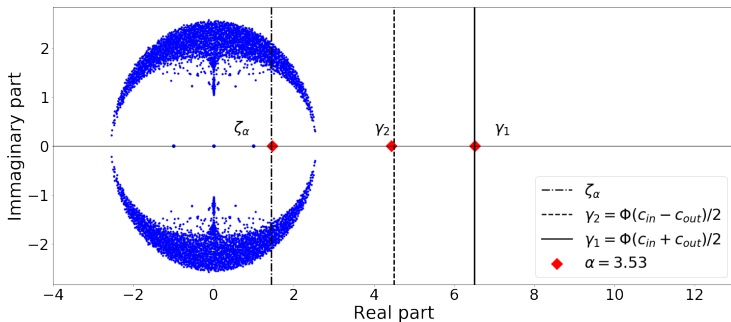
$$B\mathbf{w} = \zeta_\alpha \mathbf{w}$$



How to estimate $r_{\text{opt}} = \zeta_\alpha$?

From linearisation of BP

$$B\mathbf{w} = \zeta_\alpha \mathbf{w}$$



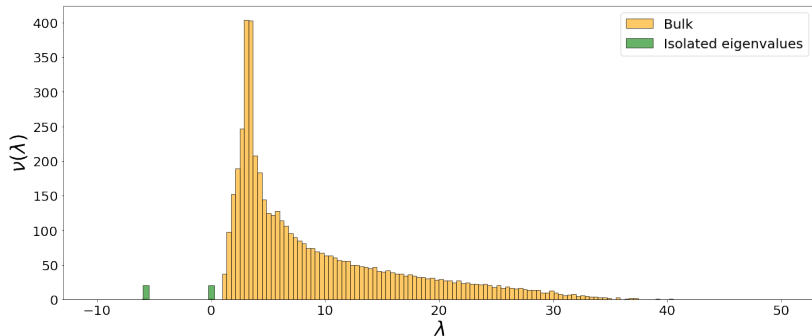
Property

$$B\mathbf{w} = \zeta_\alpha \mathbf{w} \rightarrow \det[H_{\zeta_\alpha}] = 0$$



Property

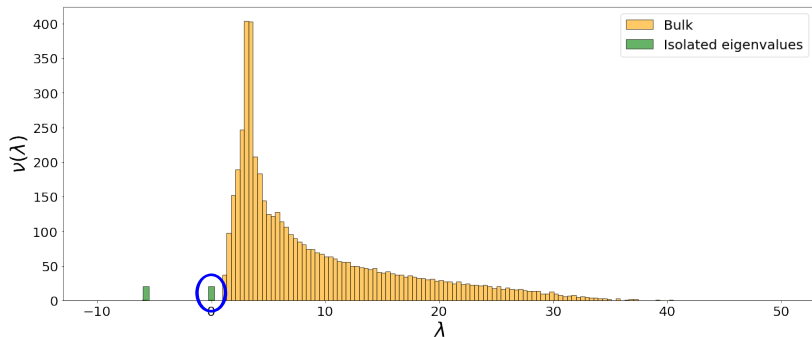
$$Bw = \zeta_\alpha w \rightarrow \det[H_{\zeta_\alpha}] = 0$$



Spectrum of H_{ζ_α}

Property

$$Bw = \zeta_\alpha w \rightarrow \det[H_{\zeta_\alpha}] = 0$$



Spectrum of H_{ζ_α}

Framework

Motivation

Sparse networks

Sparse and heterogeneous networks

Analysis

The tree like approximation

The optimal choice of r

How to estimate $r_{\text{opt}} = \zeta_\alpha$?

Results

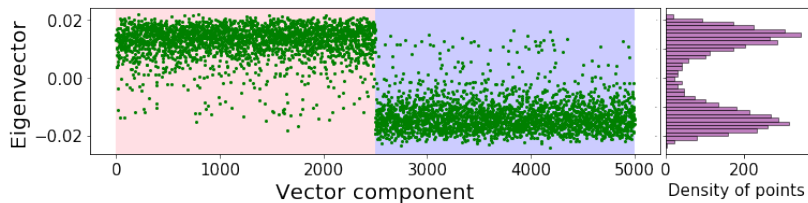
More than two classes

Conclusion



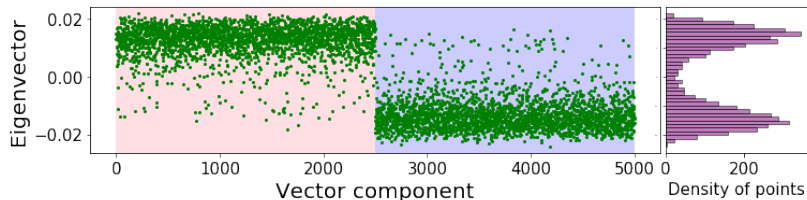
The eigenvector

$$\text{Optimal value } r = \zeta_\alpha = \frac{c_{\text{in}} + c_{\text{out}}}{c_{\text{in}} - c_{\text{out}}}$$

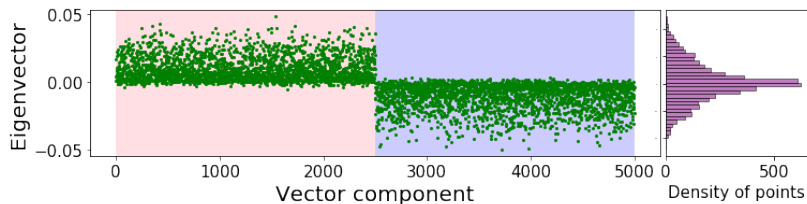


The eigenvector

$$\text{Optimal value } r = \zeta_\alpha = \frac{c_{\text{in}} + c_{\text{out}}}{c_{\text{in}} - c_{\text{out}}}$$



$$\text{Initially proposed}^4 \text{ value } r = \frac{\sum_i d_i^2}{\sum_i d_i}$$

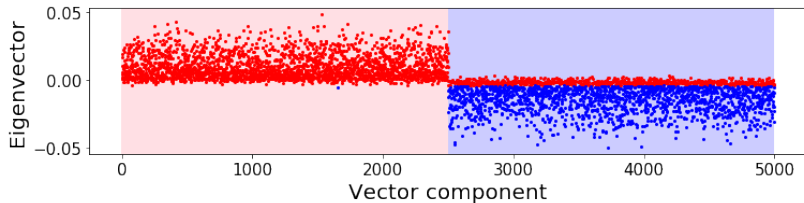
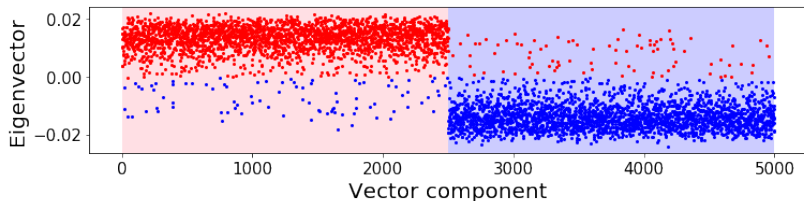


⁴Saade et al., Spectral clustering of graphs with the Bethe-Hessian, NIPS 2014.



k - means

$$\text{Optimal value } r = \zeta_\alpha = \frac{c_{\text{in}} + c_{\text{out}}}{c_{\text{in}} - c_{\text{out}}}$$



The overlap

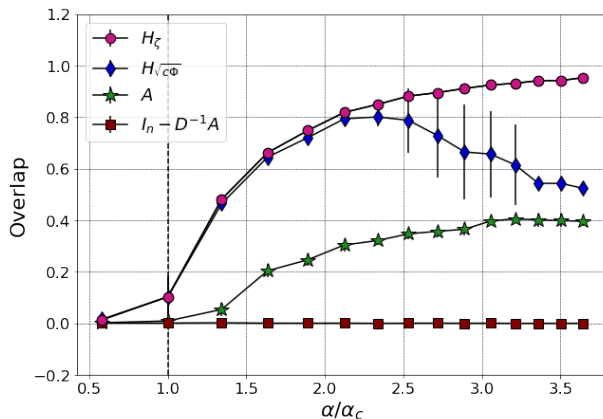


Figure: Overlap as a function of α/α_c for a power law degree distribution

More than two classes

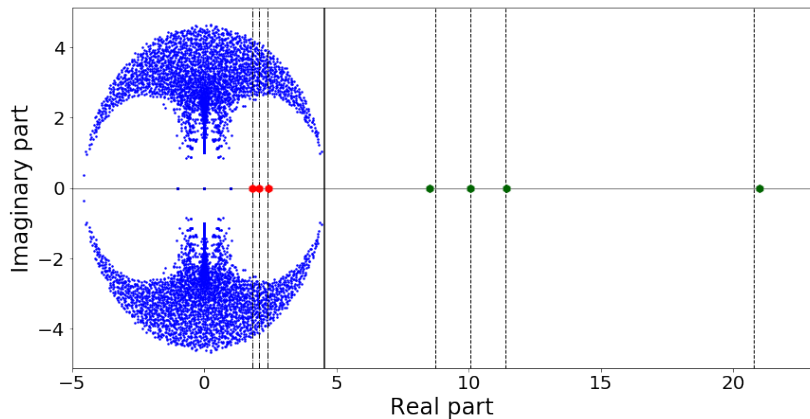


Figure: Spectrum of B for 4 classes

Future steps

- ▶ Theoretical support for our findings



Future steps

- ▶ Theoretical support for our findings
- ▶ Algorithmic optimization (eigencounts techniques)



Thank you!

