Spectral methods for graph clustering

Ph.D. defence

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INTRODUCTION

- Graph clustering
- Community detection
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Clustering

Unsupervised methods for data **categorization**

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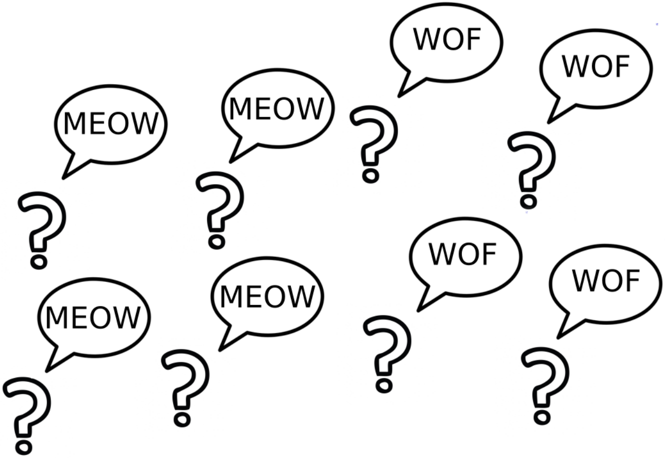

Clustering

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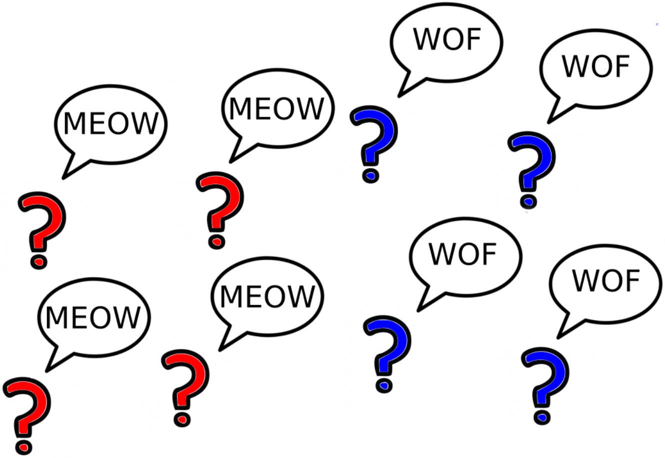

Clustering

Feature extraction and clustering paradigm

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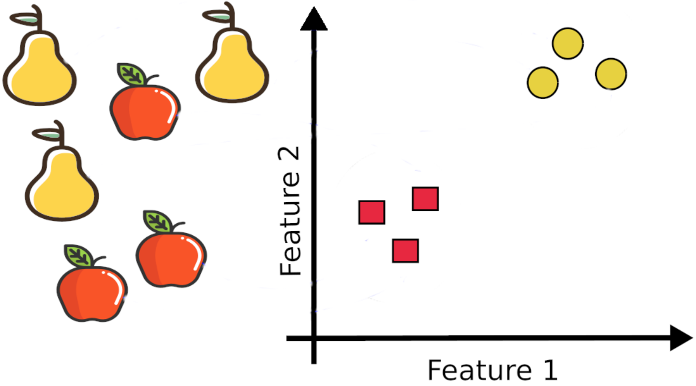

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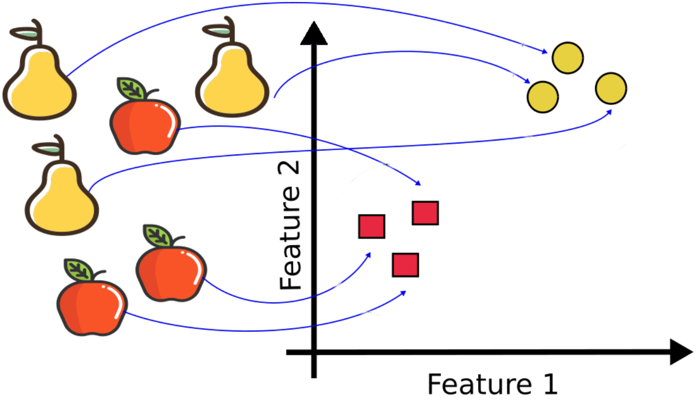

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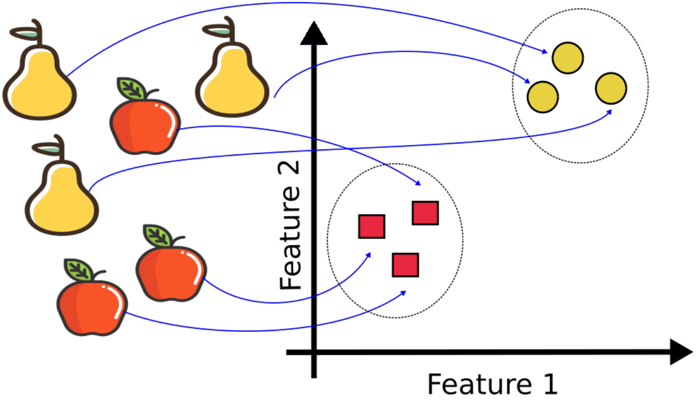
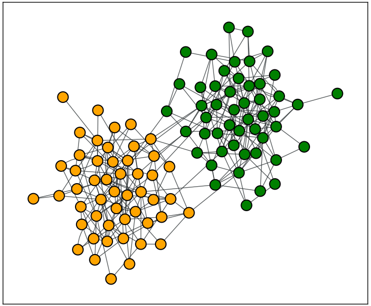
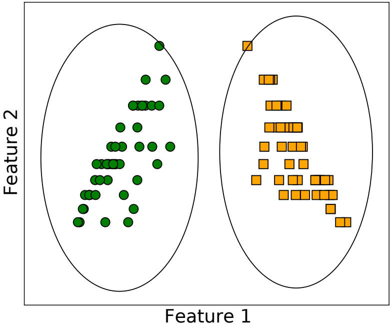


The relevant features define the concept of categories

Graph clustering

A **graph representation** for **pairwise "affinity"**





Graph matrix representation

$\mathcal{G}(\mathcal{V}, \mathcal{E})$, is a graph with $|\mathcal{V}| = n$ nodes.

Definition: adjacency matrix

$$\forall\, 1 \leq i < j \leq n, \quad A_{ij} = \mathbb{1}_{(ij) \in \mathcal{E}}$$

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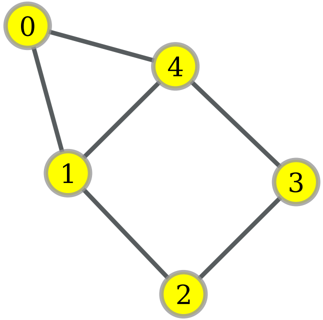
Definition: diagonal degree matrix

$$\forall\, 1 \leq i \leq j \leq n, \quad D_{ij} = \delta_{ij} \sum_{k \in \mathcal{V}} A_{ij}$$

Graph matrix representation



$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix}$$

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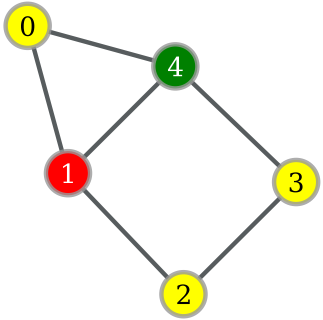

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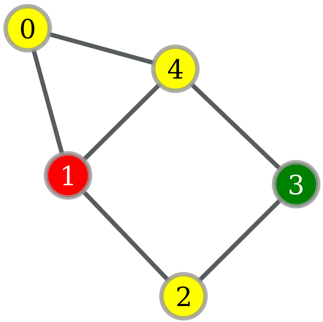

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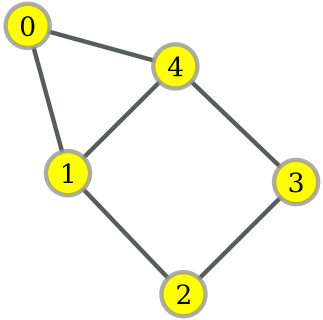

$$D = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{pmatrix}$$

Spectral clustering

Graph $\rightarrow$ Matrix $\rightarrow$ Eigenvectors embedding

Spectral clustering

Graph $\to$ Matrix $\to$ Eigenvectors embedding

Typical spectral clustering algorithm

Input: $\mathcal{G}(\mathcal{V}, \mathcal{E}), k$

- $M \in \mathbb{R}^{n \times n}$: graph matrix representation
- k eigenvectors of M in the columns of $X \in \mathbb{R}^{n \times k}$
- Clustering in k-dimensions (k-means)

Output: $\ell \in \{1, \ldots, k\}^n$, labelling vector

3 years in 40 minutes...

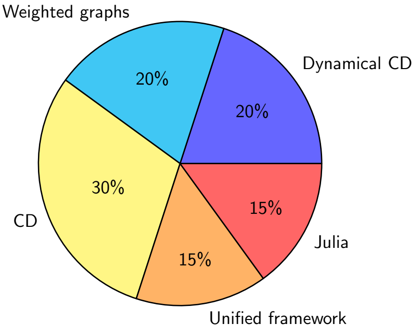

Figure: My PhD

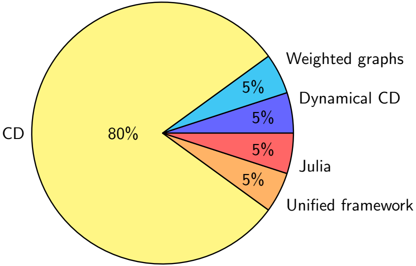

Figure: My presentation

Community detection: problem position

Problem: given $\mathcal{G}(\mathcal{V}, \mathcal{E})$, find a partition of $\mathcal{V}$ to recover the community labels

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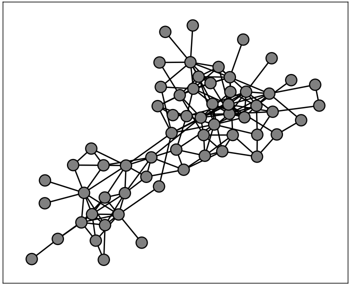

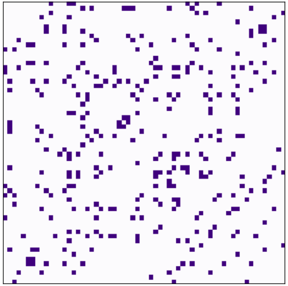

Figure: The dolphin network (Lusseau 2003)

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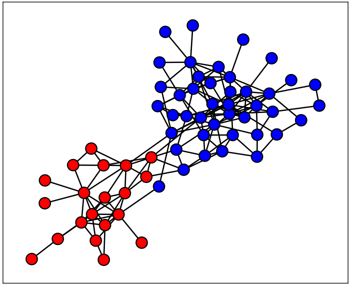

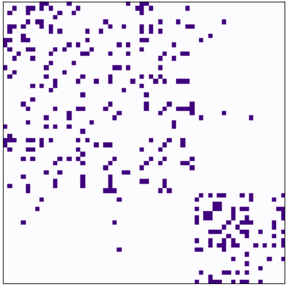

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Spectral clustering for community detection

Recall: compute k eigenvectors of M to embed the nodes in $\mathbb{R}^k$

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Popular choices for M in community detection are

- A, adjacency matrix
- $D - A$, graph Laplacian matrix
- $D^{-1}A, D^{-1/2}AD^{-1/2}$, normalized Laplacian matrices

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Poor performances on **sparse** and **heterogeneous** graphs

Sparsity

Real graphs are typically **sparse**

Dataset	Size	Average degree
Dolphins	62	5
Polbooks	105	8,4
Football	115	10,7
Polblogs	1.222	27,4
Facebook	4.039	43,7
GNutella P2P	6.301	6,6
Astrophysics	18.775	21,1
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Source : Stanford Large Network Dataset Collection

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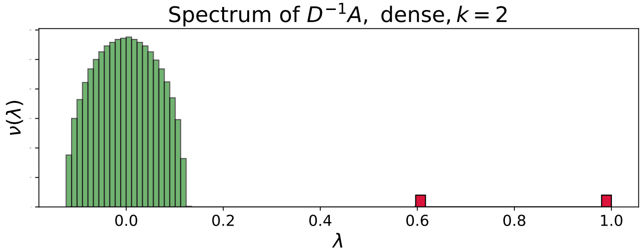
Spectral clustering in sparse graphs



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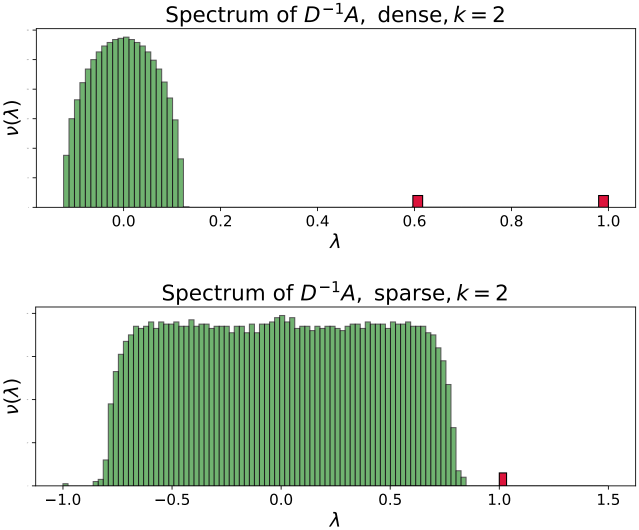

Real graphs typically have a **broad degree distribution**

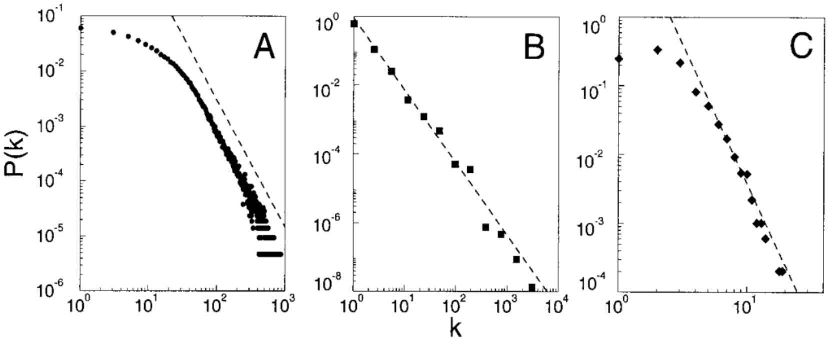

Figure: Degree distribution for various networks. Source: Barabasi, *Emergence of Scaling in Random Networks*, Science 1999

Spectral clustering in heterogeneous graphs

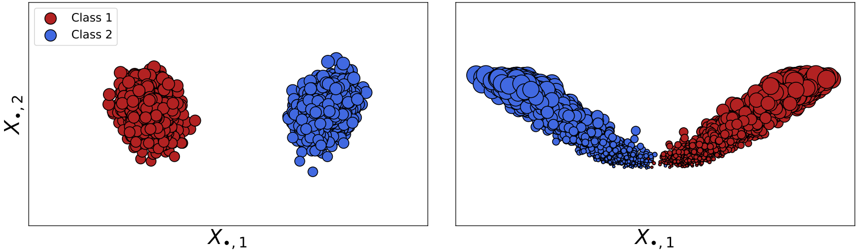

Figure: Spectral node embedding. **Left**: homogeneous degree distribution. **Right**: power law degree distribution

The Degree-corrected stochastic block model (DCSBM)

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$$\mathbb{P}(A_{ij} = 1) = \theta_i \theta_j \cdot \frac{C_{\ell_i \ell_j}}{n}$$

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- $\boldsymbol{\theta} \in \mathbb{R}^n$: intrinsic "probability" of connection
  - $\frac{1}{n} \sum_{i \in \mathcal{V}} \theta_i = 1$
  - $\frac{1}{n} \sum_{i \in \mathcal{V}} \theta_i^2 = \Phi = O_n(1)$: broadness of the degree distribution

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Objective: infer ℓ from A

Detectability threshold

Detectability threshold

- k classes of equal size
- $C = \begin{pmatrix} c_{\text{in}} & c_{\text{out}} & c_{\text{out}} & \cdots \\ c_{\text{out}} & c_{\text{in}} & c_{\text{out}} & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ \cdots & c_{\text{out}} & c_{\text{out}} & c_{\text{in}} \end{pmatrix}$

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Detection in polynomial time if

$$\alpha = f(c_{\text{in}}, c_{\text{out}}, \Phi, k) > \alpha_{\text{c}}$$

Detectability threshold

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Typical choices of M do not achieve the $\alpha_{\rm c}$ threshold

Objectives

Define a new spectral clustering algorithm

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- Inspired by the DCSBM but applicable to **any** input graph

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Define a new spectral clustering algorithm

- Inspired by the DCSBM but applicable to **any** input graph
- Dealing with **sparsity** and **degree heterogeneity**
- Reaching the **detectability threshold** on sparse DCSBM graphs

Contents

PHYSICS INSPIRED METHODS

- The Bethe-Hessian
- The non-backtracking
- Challenges

The Bethe-Hessian

Ising Hamiltonian on $\mathcal{G}$ for $\boldsymbol{s} \in \{-1, 1\}^n$

$$\mathcal{H}(\boldsymbol{s}) = -\boldsymbol{s}^T A \boldsymbol{s} = -\sum_{(ij) \in \mathcal{E}} s_i s_j$$

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Low energetic configurations with all spins in the same class are aligned

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$$\mathcal{H}(\boldsymbol{s}) = -\boldsymbol{s}^T A \boldsymbol{s} = -\sum_{(ij)\in\mathcal{E}} s_i s_j$$

Low energetic configurations with all spins in the same class are aligned

Free energy for $\boldsymbol{m} \in \mathbb{R}^n$

$$F(\boldsymbol{m}) = \underbrace{U(\boldsymbol{m})}_{\text{internal energy}} - T \underbrace{S(\boldsymbol{m})}_{\text{entropy}}$$

The minima of $F(\boldsymbol{m})$ are informative

The Bethe-Hessian

- Ising Hamiltonian $\mathcal{H}(\boldsymbol{s})$

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Definition: Bethe-Hessian family of matrices

$$H_r = (r^2 - 1)I_n + D - rA, \quad r \geq 1$$

The Bethe-Hessian

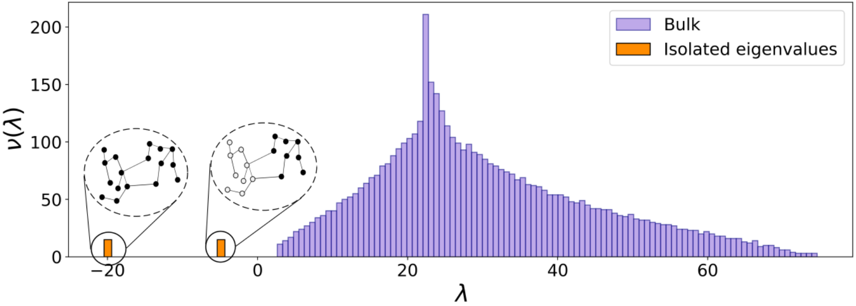

Figure: Spectrum of H_r for r fixed and $k = 2$

The non-backtracking

Definition: non-backtracking matrix

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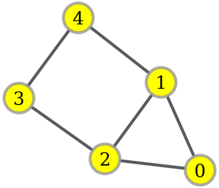

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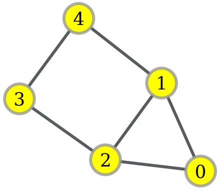

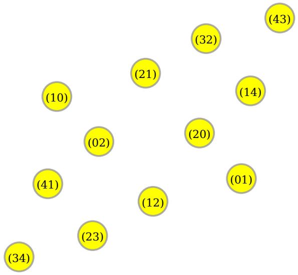

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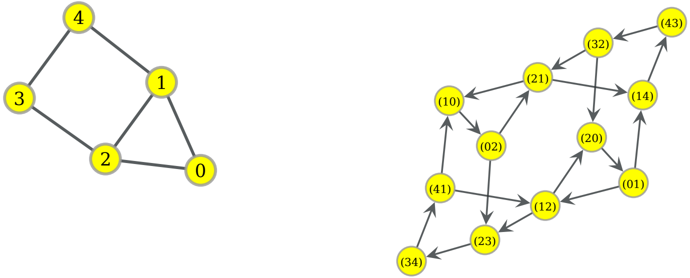

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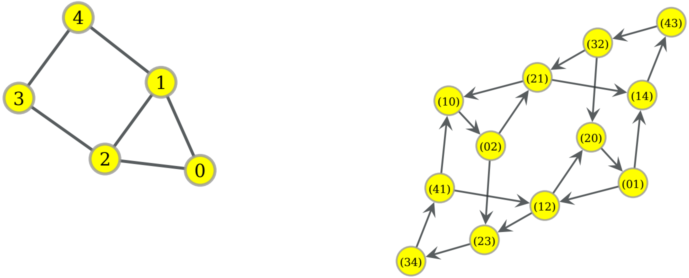

$$\det(B - rI_{|\mathcal{E}_\mathrm{d}|}) \propto \det(H_r)$$

Spectrum of B (DCSBM)

- For $\alpha > \alpha_c$, k real isolated eigenvalues
- All complex eigenvalues satisfy $|\lambda_i(B)| \leq \sqrt{\rho(B)} + o_n(1)$

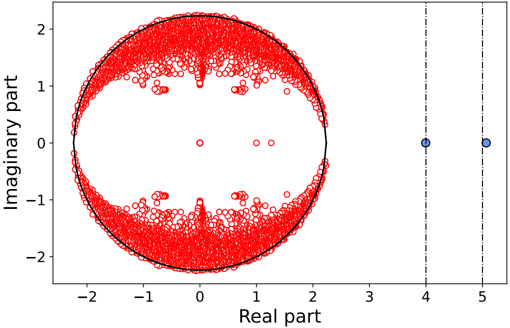

Figure: Spectrum of B for $k = 2$, sparse DCSBM

Spectrum of H_r (DCSBM)

For $r = \sqrt{\rho(B)}$ (Saade 2014)

- If $\alpha > \alpha_c$, k isolated negative eigenvalues
- All bulk eigenvalues are positive

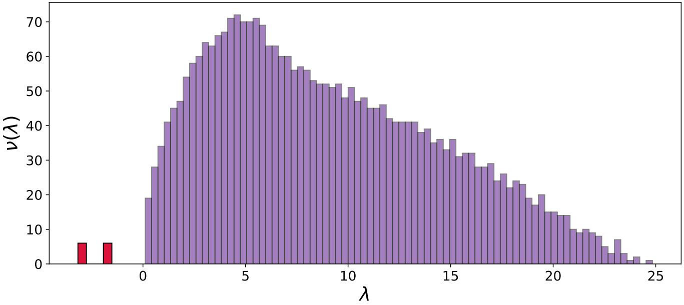

Figure: Spectrum of $H_{\sqrt{\rho(B)}}$ for $k = 2$, sparse DCSBM

Challenges

Both $H_{\sqrt{\rho(B)}}$ and B

✔ achieve **detectability** when $\alpha > \alpha_{\rm c}$

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Q1 : deal with **sparsity** and **heterogeneity** at once

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Q2 : find the optimal $r \neq \sqrt{\rho(B)}$ for H_r

Challenges

Both $H_{\sqrt{\rho(B)}}$ and B

✔ achieve **detectability** when $\alpha > \alpha_c$

✘ do not deal with **heterogeneity**

Q1 : deal with **sparsity** and **heterogeneity** at once

Q2 : find the optimal $r \neq \sqrt{\rho(B)}$ for H_r

Q3 : efficiently estimate the optimal r

Contents

MAIN CONTRIBUTION

- Optimal Bethe-Hessian
- DCSBM
- Algorithm
- Performance
- A unified framework

The definition of ζ_p

Contribution: definition of optimal value of r

$$H_r = (r^2 - 1)I_n + D - rA$$

The definition of ζ_p

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Let $\lambda_p^{\uparrow}(M)$ be the p-th smallest eigenvalue of M

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Definition: ζ_p

For each connected component of $\mathcal{G}$

$$\zeta_p = \min_{r \geq 1}\{r \; : \; \lambda_p^{\uparrow}(H_r) = 0\}$$

The definition of ζ_p

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- Well defined for any $\mathcal{G}$

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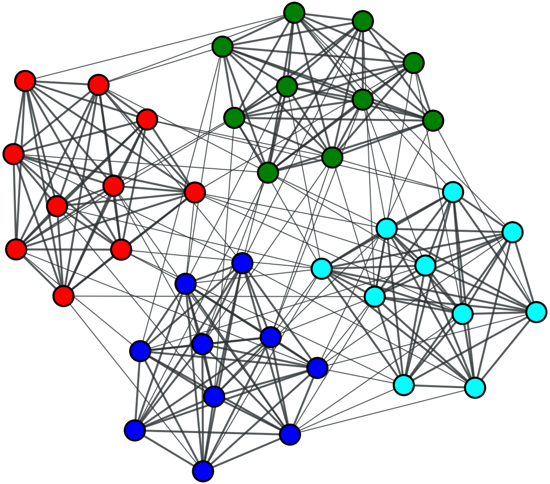
- Well defined for any $\mathcal{G}$
- A "property" of the graph

The definition of ζ_p



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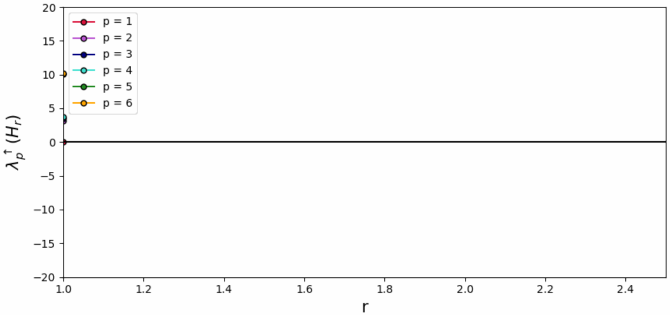

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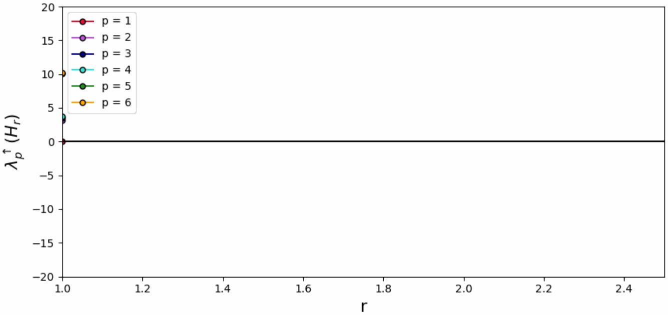

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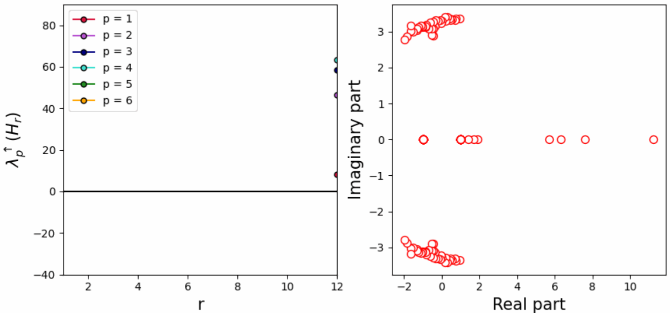

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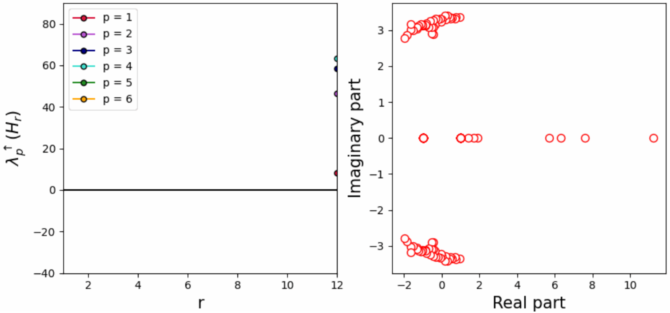

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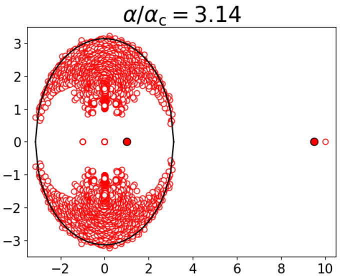

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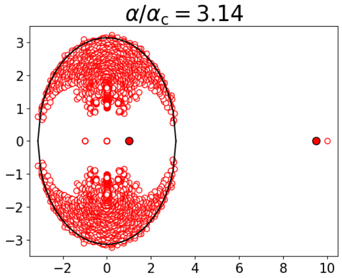

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Valid also for $k > 2$

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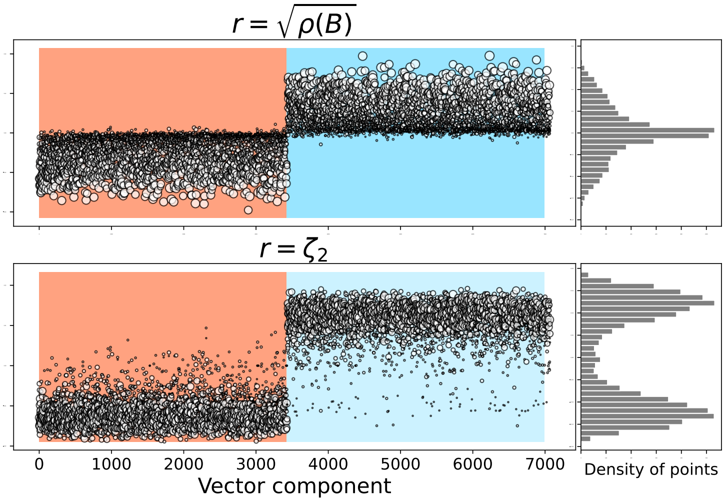

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Input: connected graph $\mathcal{G}$, k

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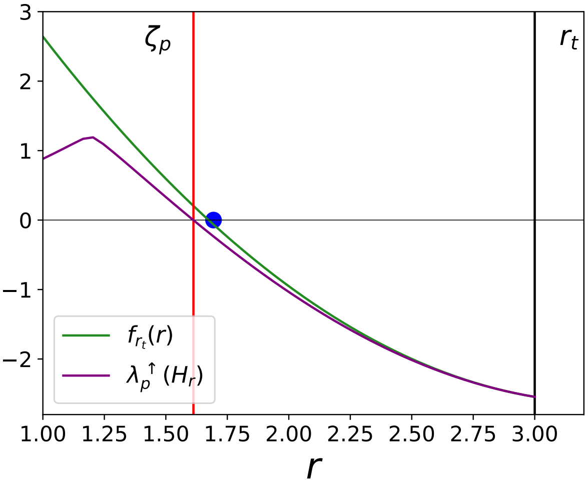

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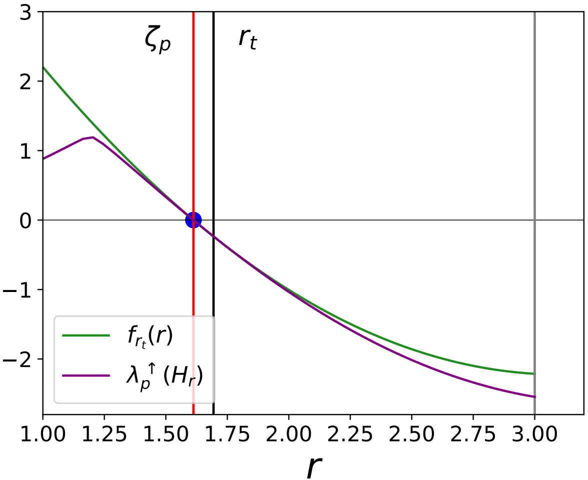

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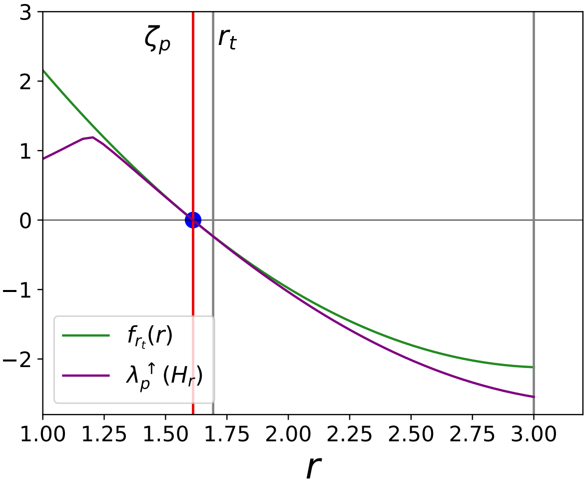

DCSBM graphs

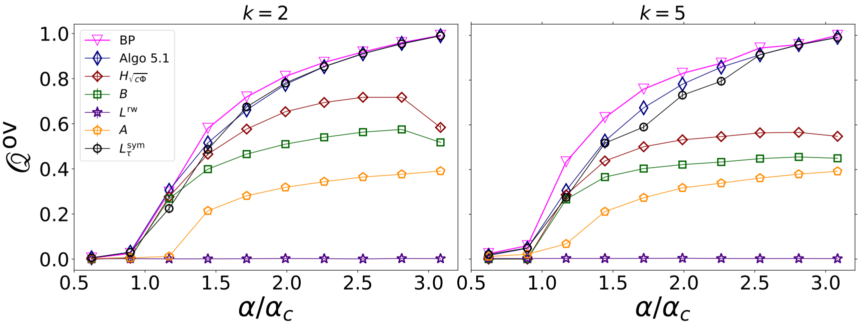

Figure: Performance vs competing methods on DCSBM synthetic graphs. $n = 50.000$, $c = 5$.

Real graphs

Dataset	n	c	k	H_{ζ_p}	A	$H_{\sqrt{c\Phi}}$	B	L^{rw}	L_{τ}^{sym}
Karate	34	4.6	2	**0.37**	**0.37**	**0.37**	**0.37**	0.36	**0.37**
Dolphins	62	5	2	**0.38**	0.21	0.34	0.22	**0.38**	**0.38**
Polbooks	105	8.4	3	**0.50**	0.47	**0.50**	0.45	**0.50**	**0.50**
Football	115	10.7	12	**0.60**	**0.60**	**0.60**	**0.60**	**0.60**	**0.60**
Mail	1133	9.6	21	**0.52**	0.32	0.40	0.37	0.48	**0.52**
Polblogs	1222	27,4	2	**0.43**	0.25	0.27	0.23	0.00	**0.43**
Tv	3892	8.9	41	**0.85**	0.60	0.56	0.55	0.55	0.80
Facebook	4039	43.7	55	**0.76**	0.42	0.49	0.48	0.70	0.58
GrQc	4158	6.5	29	**0.80**	0.52	0.51	0.51	0.34	**0.80**
Power grid	4941	2.7	25	**0.92**	0.18	0.33	0.31	**0.92**	0.85
Politicians	5908	14.1	62	**0.82**	0.48	0.54	0.51	0.74	0.74
GNutella P2P	6299	6.6	4	**0.40**	0.20	0.14	0.14	0.00	0.35
Wikipedia	7066	28.3	22	0.27	0.14	0.18	0.16	**0.34**	0.27
HepPh	11204	21.0	60	**0.57**	0.46	0.42	0.42	0.27	0.52
Vip	11565	11.6	53	**0.62**	0.28	0.32	0.32	0.16	0.54

Table: Modularity (no ground truth) comparison on real networks

A unified framework

- Ising Hamiltonian $\rightarrow$ Bethe approximation $\rightarrow$ Hessian $\rightarrow$ H_r

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Naïve mean field vs Bethe approximation

- Unsuited for sparse graphs
- Does not reach α_c threshold on DCSBM graphs
- Does not keep heterogeneity into account

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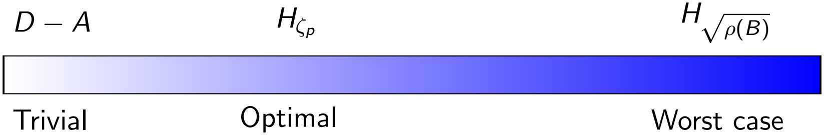

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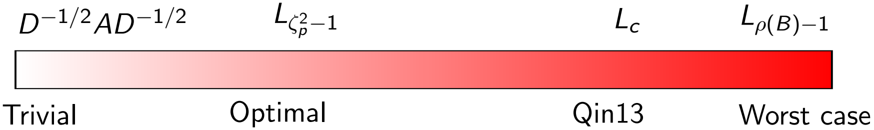

$\tau = \zeta_p^2 - 1$ is the hardness-dependent optimal regularization

Contents

CONCLUSION

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- Between "classical" and "physics-based" methods

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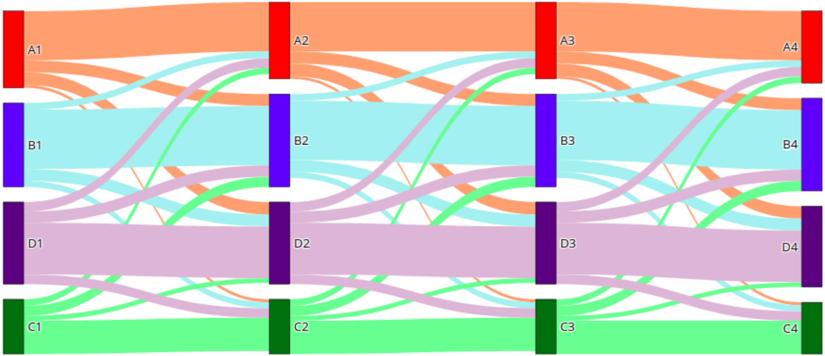
A question

How to find the “right temperature” for a given ML problem?

Extensions: CD in dynamical graphs



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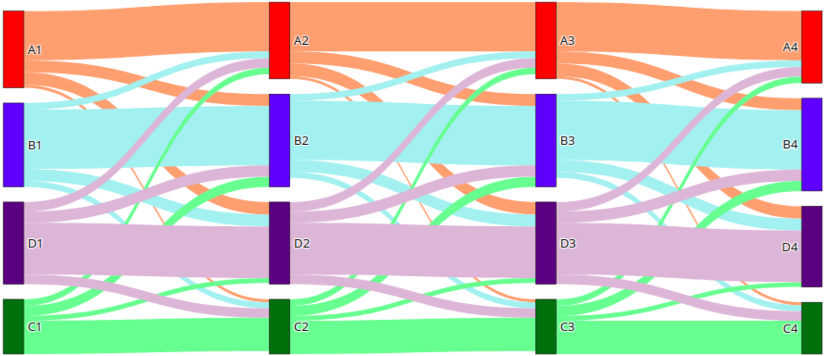

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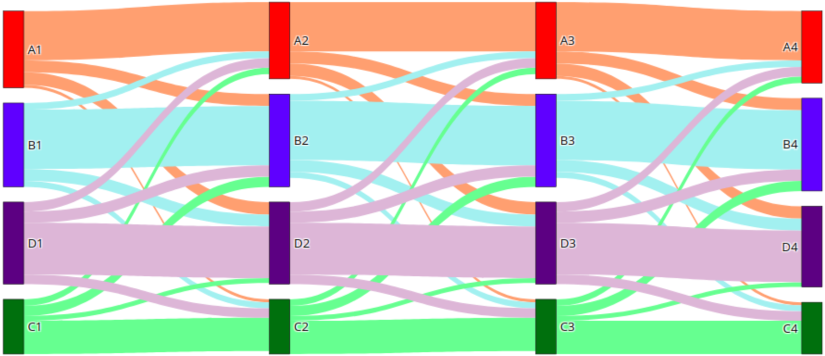

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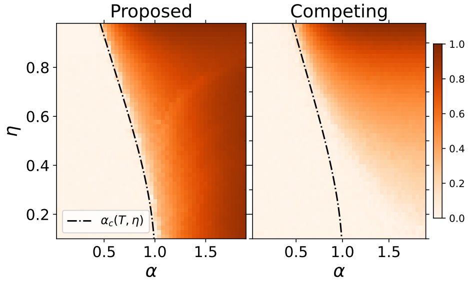

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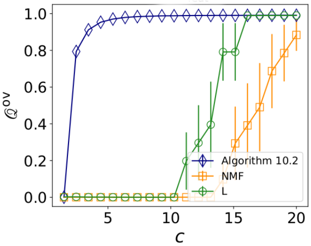

Cost-efficient **data** clustering

Publications

Journal papers

- **LD**, Romain Couillet Nicolas Tremblay: *Nishimori meets Bethe: a spectral method for node classification in sparse weighted graphs*, in Journal of statistichal mechanics
- **LD**, Romain Couillet, Nicolas Tremblay: *A unified framework for spectral clustering in sparse graphs*, in JMLR

Conference papers

- **LD**, Romain Couillet Nicolas Tremblay: *Community detection in sparse time-evolving graphs with a dynamical Bethe-Hessian*, in NeurIPS 2020
- **LD**, Romain Couillet, Nicolas Tremblay: *Optimal Laplacian regularization for sparse spectral community detection*, in ICASSP 2020
- **LD**, Romain Couillet, Nicolas Tremblay: *Classification spectrale par la laplacienne déformée dans des graphes réalistes*, in GRETSI 2019
- **LD**, Romain Couillet, Nicolas Tremblay: *Revisiting the Bethe-Hessian: improved community detection in sparse heterogeneous graphs*, in NeurIPS 2019
- **LD**, Romain Couillet: *Community Detection in Sparse Realistic Graphs: Improving the Bethe Hessian*, in ICASSP 2019