Institute of Theoretical Physics
Chinese Academy of Sciences

Spectral detection of global structures in the noisy data

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IoP 11.30 2016

Ref: PZ, *Advances In Neural Information Processing Systems 29*, 541 (2016)


RIP
34
13
17
MOLES

Machine Learning and Physics

Machine Learning and Physics

- **Machine learning —> physics**
  (Why? learn complex features by machines!)

Machine Learning and Physics

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  - Classification of matter using DNN

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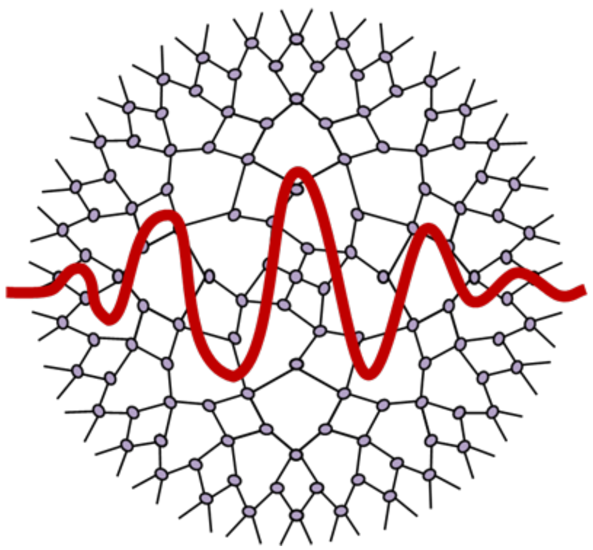

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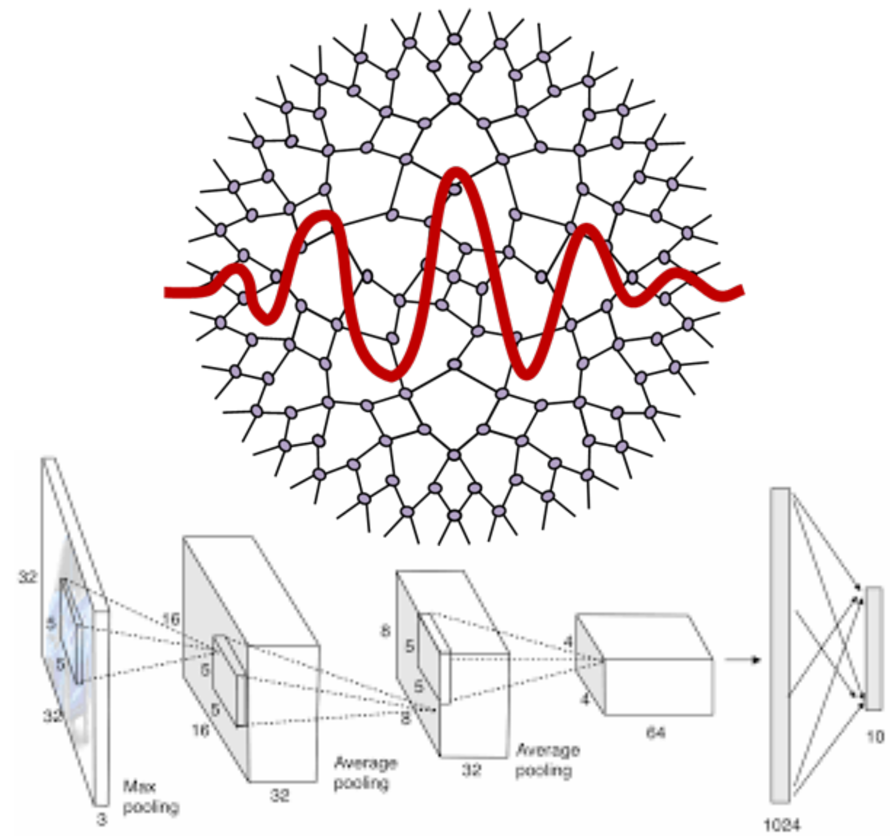

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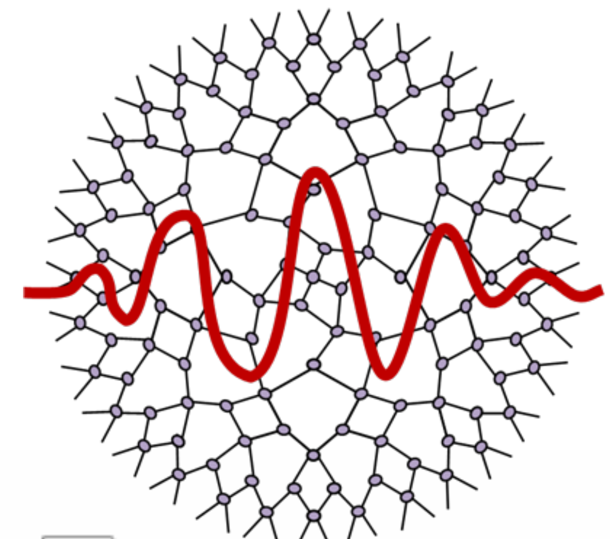

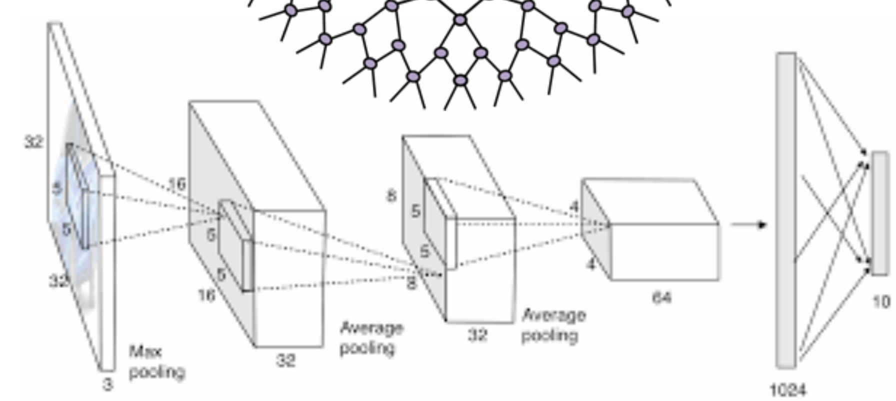

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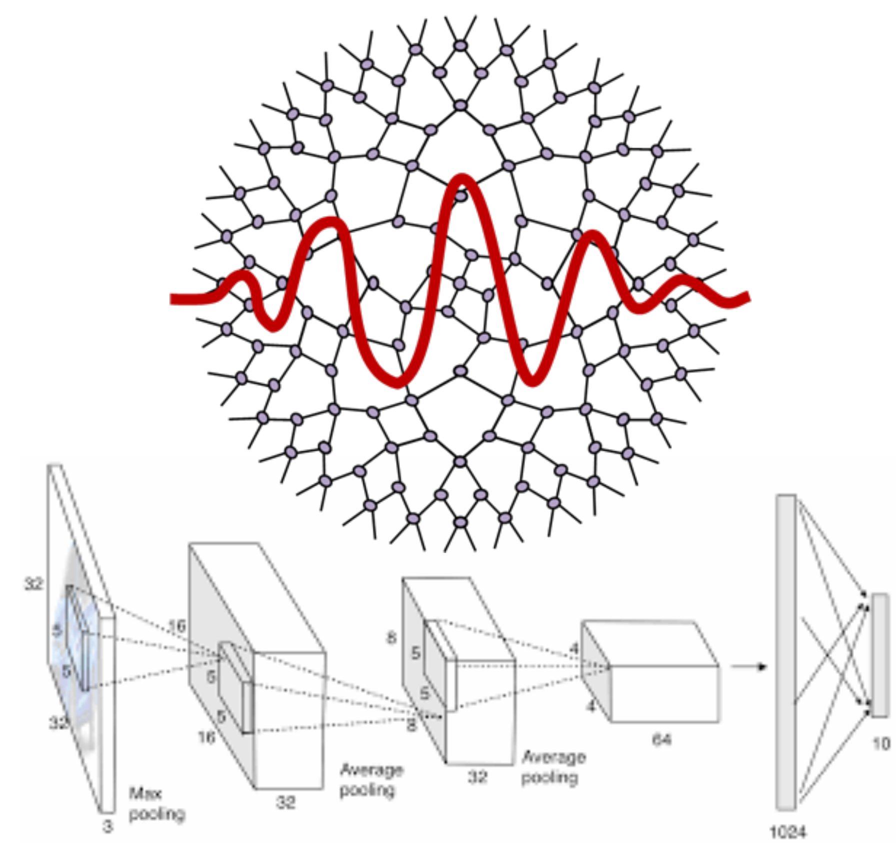
  - Quantum information/computation



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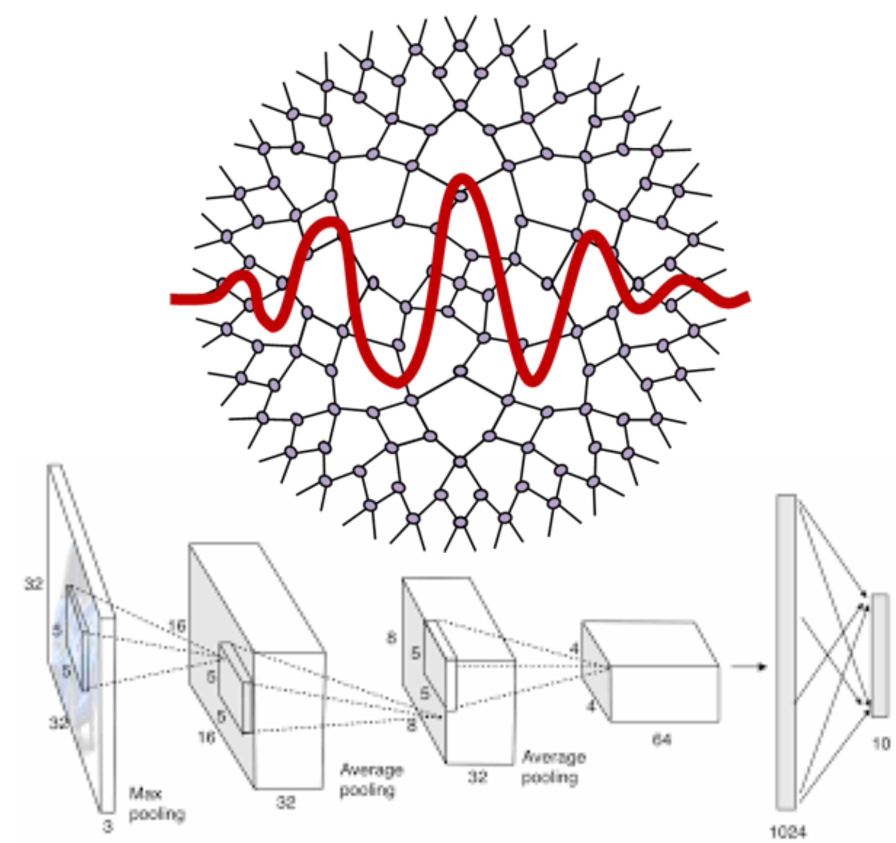

- **Physics —> machine learning**
  - Quantum information/computation
  - Spin Glass Theory, Various transitions, Approximate Bayesian inference

Machine Learning

- Supervised learning

- Unsupervised learning

Machine Learning

- Supervised learning
  - Classification
  - Regression
  - … …
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    - Classification
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    - … …
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    - Clustering
    - Dimensionality reduction
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- Semi-supervised Learning
- Active Learning
- Transfer Learning

Machine Learning Methods

- Supervised learning

- Unsupervised learning

Machine Learning Methods

- Supervised learning
  - Deep neural networks
  - Support Vector Machines
  - Logistic Regression
  - … …
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Machine Learning Methods

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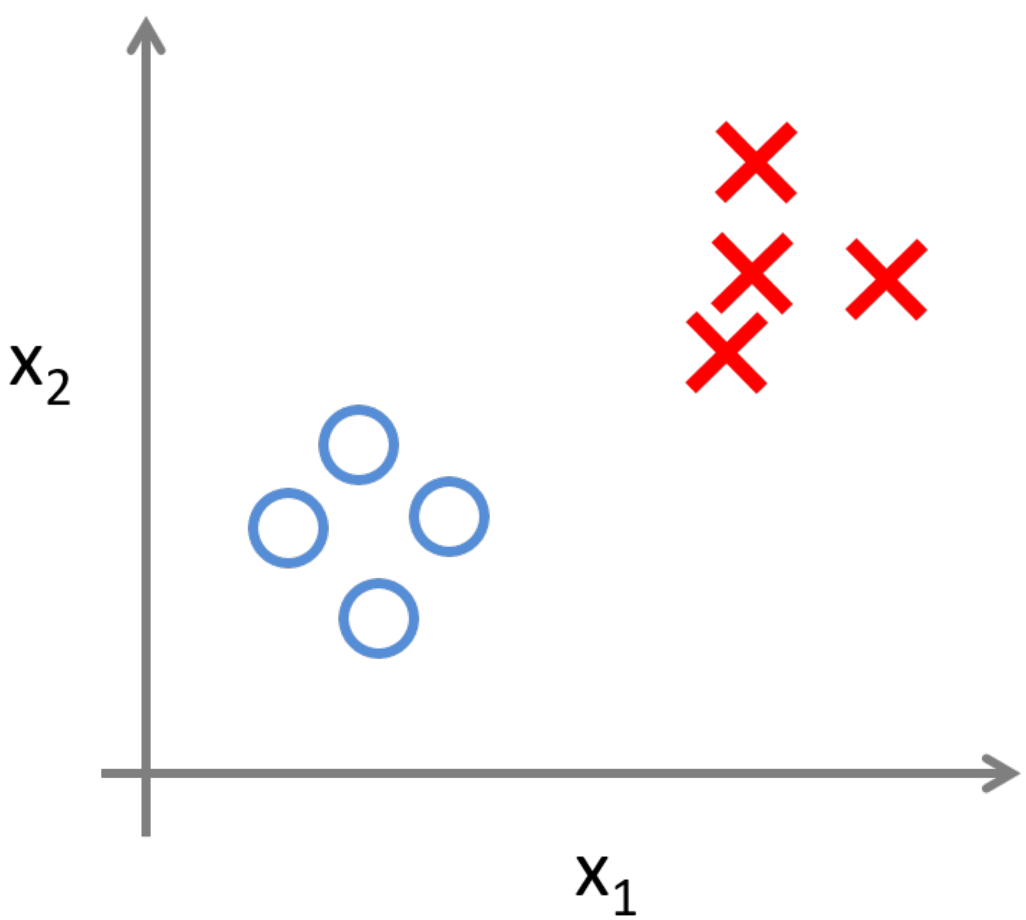
- Unsupervised learning
  - Principled Component Analysis
  - Singular Value Decompositions
  - Hidden Markov Models
  - Expectation-Maximization
  - Graphical Models
  - … …

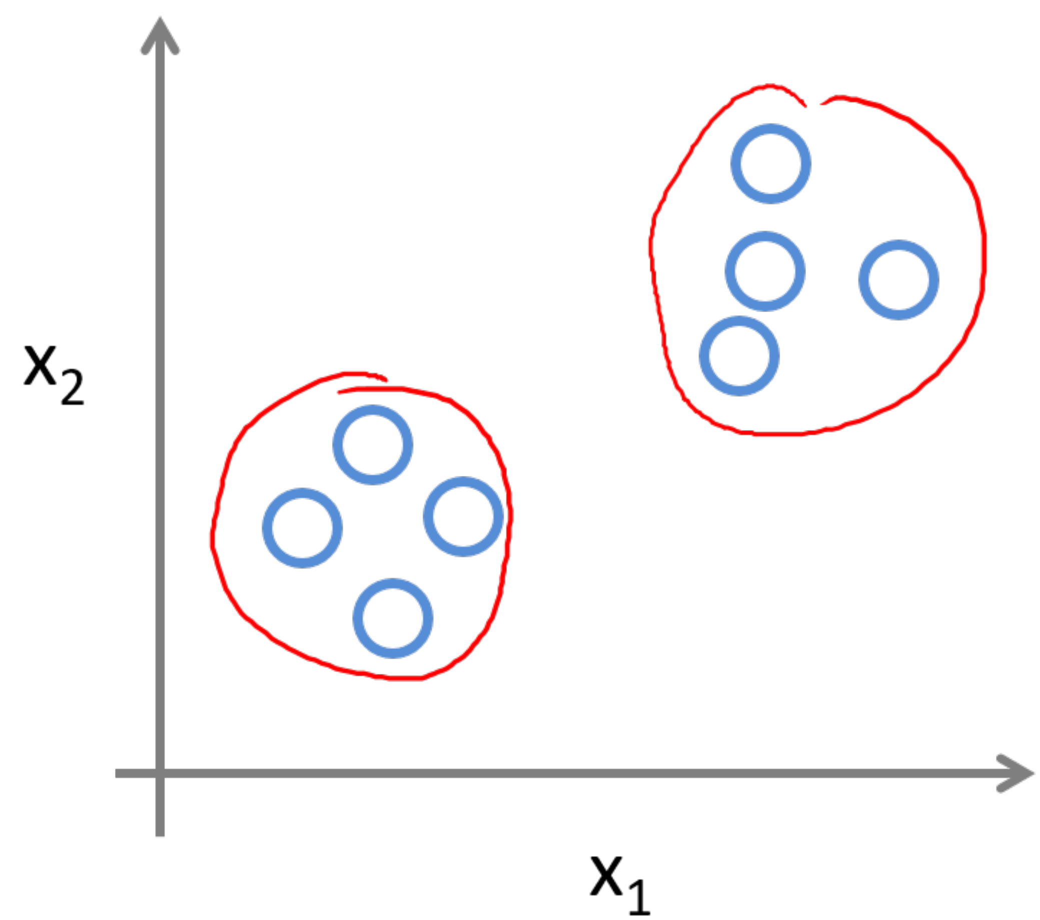
Supervised vs. Unsupervised learning

Supervised Learning



Predicting Labels

Unsupervised Learning



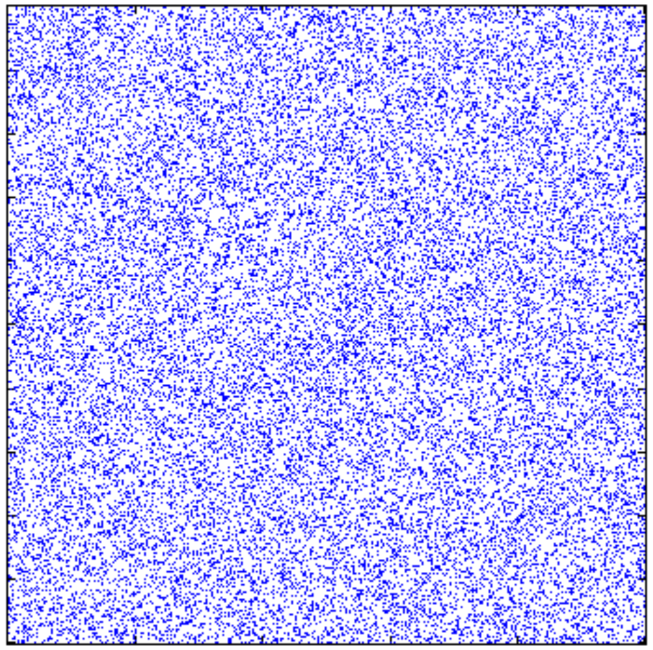
Finding structures in the data

Topic of today

Unsupervised learning: finding structures in the data matrix

Data matrices

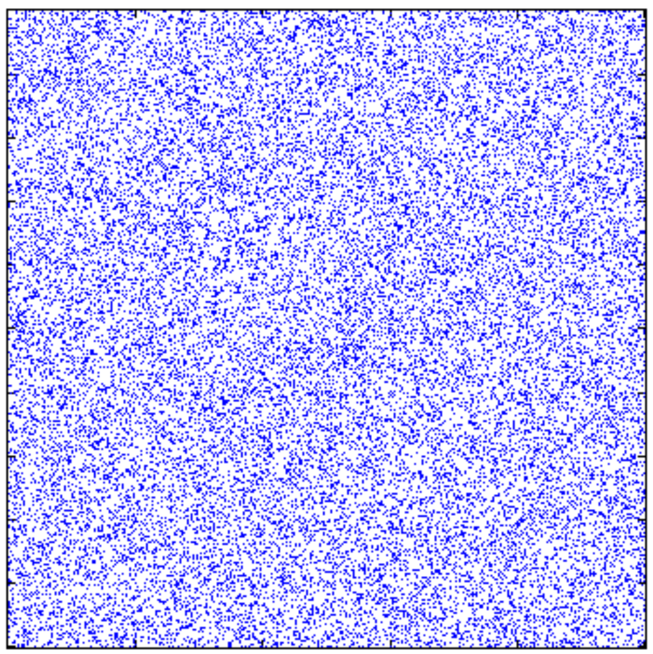
Data matrices

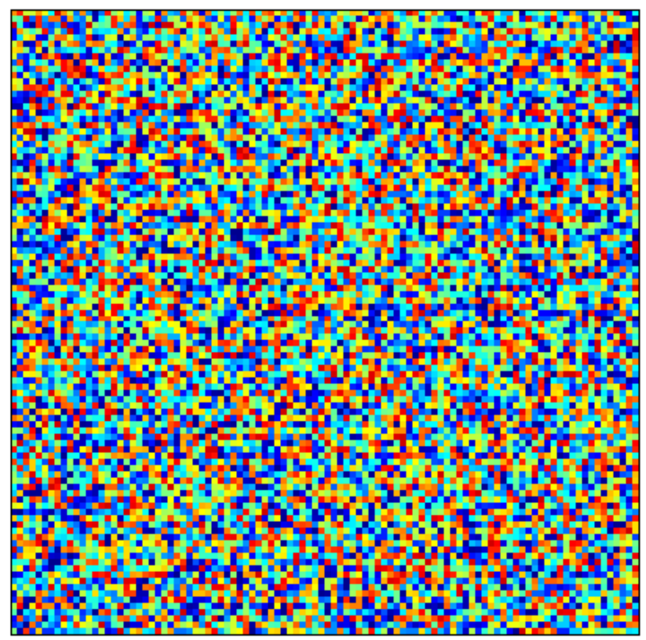


Network:
Adjacency matrix

$A \in \{0,1\}^{n \times n}$

Data matrices





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Clustering:
Similarity matrix

$A \in \mathbb{R}^{n \times n}$

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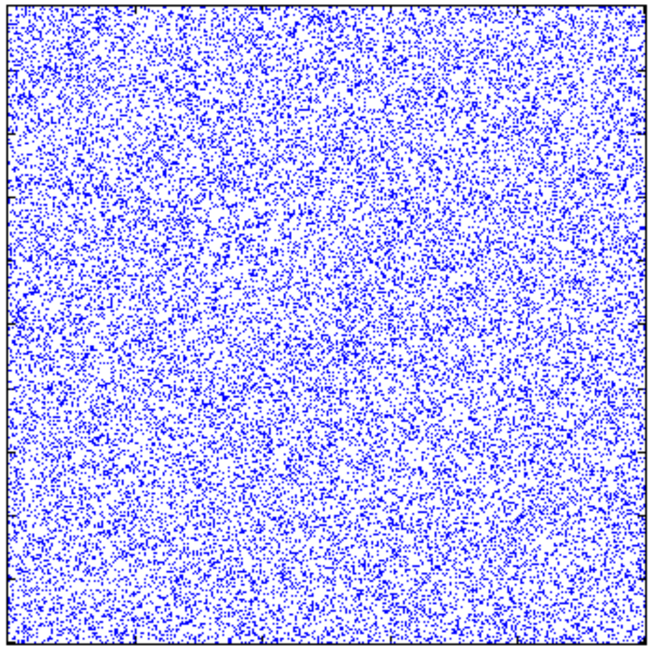

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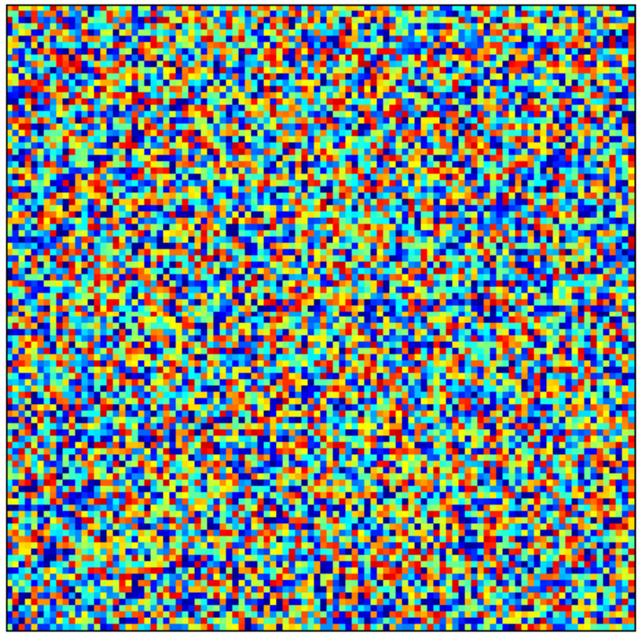

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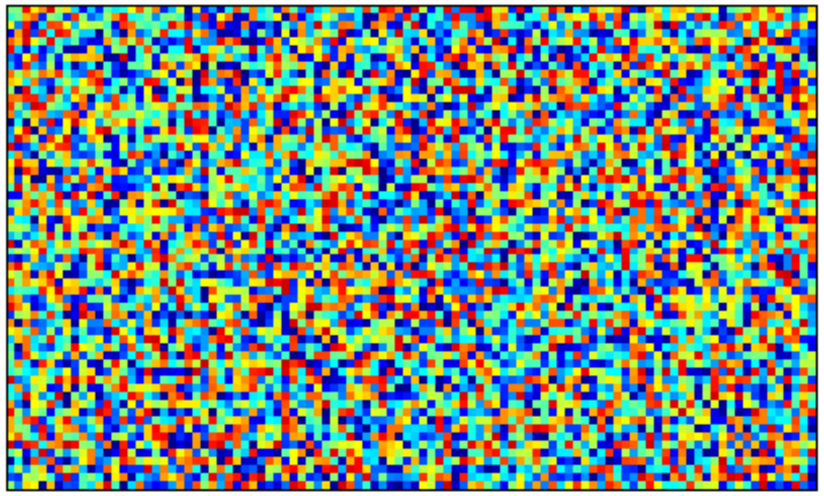
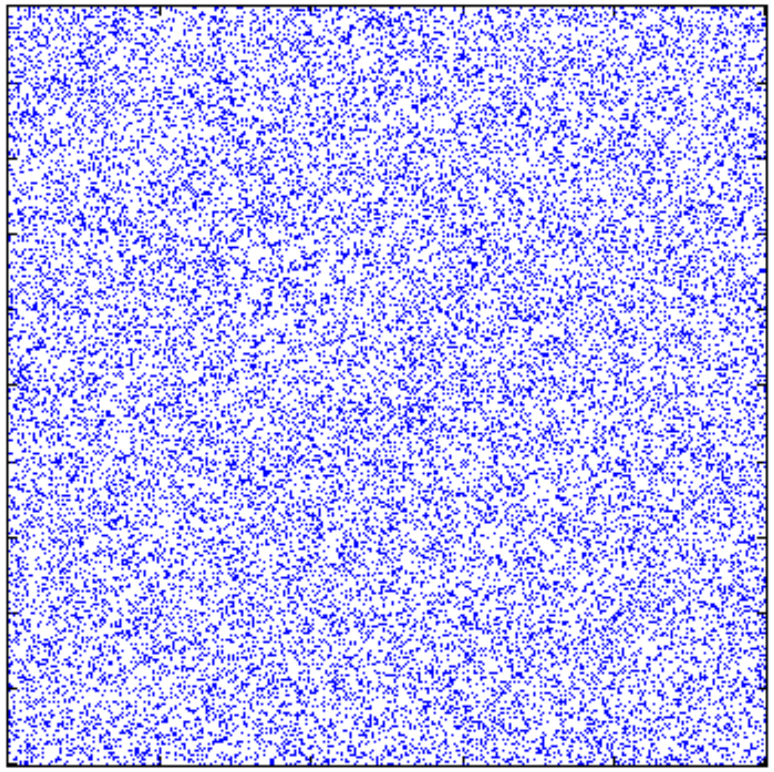


Recommendation:
Rating matrix

$A \in \mathbb{R}^{m \times n}$

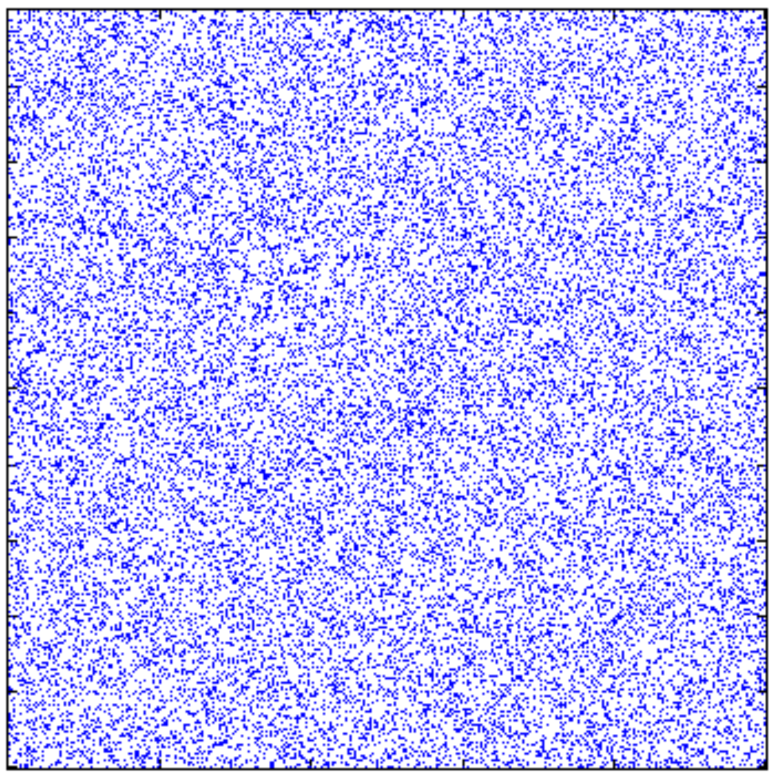
Community detection

Community detection



What you have:
DATA

Community detection



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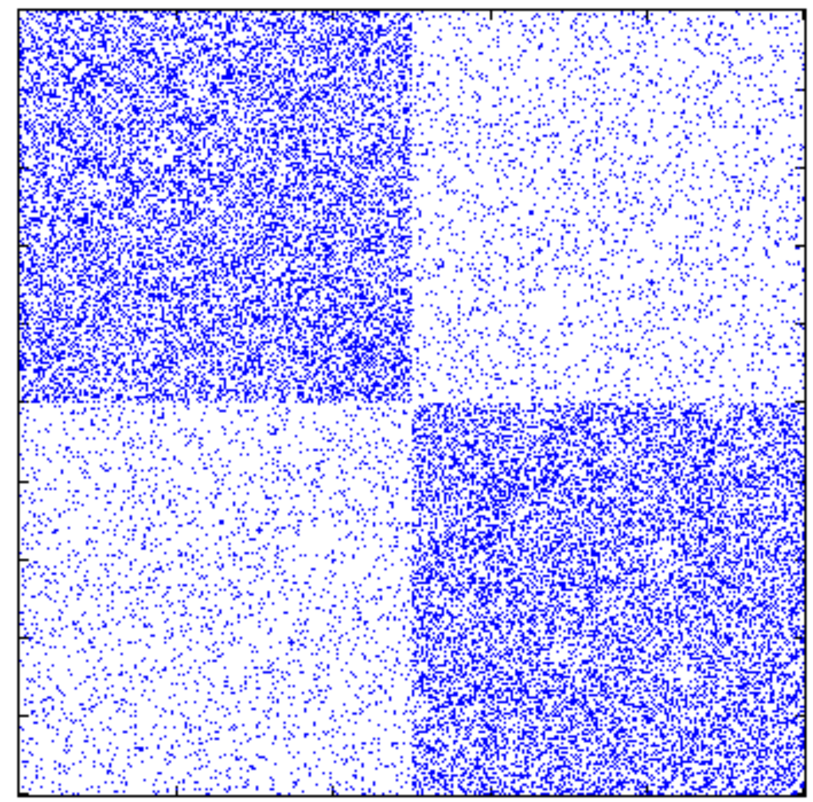


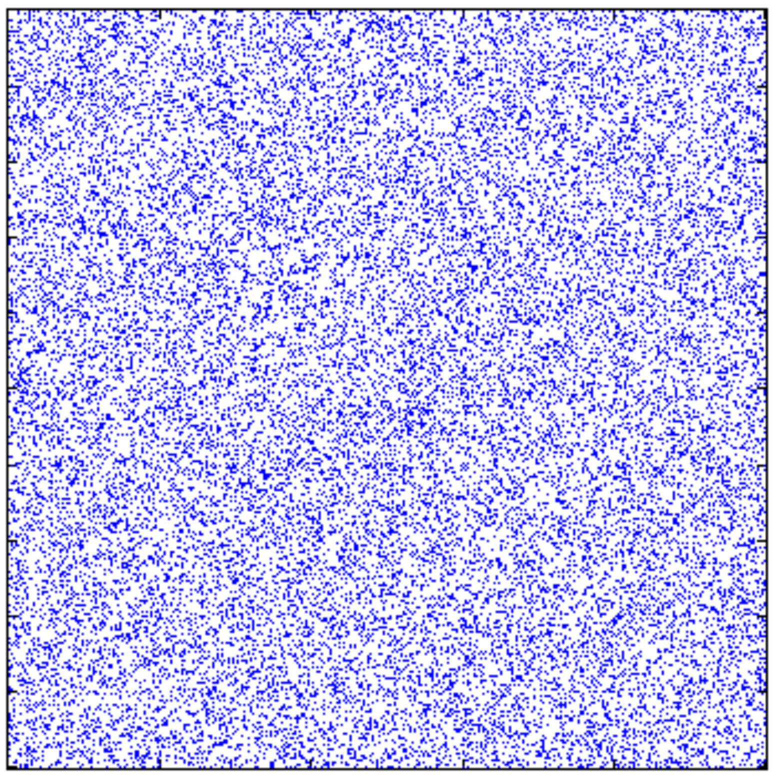
What you want:

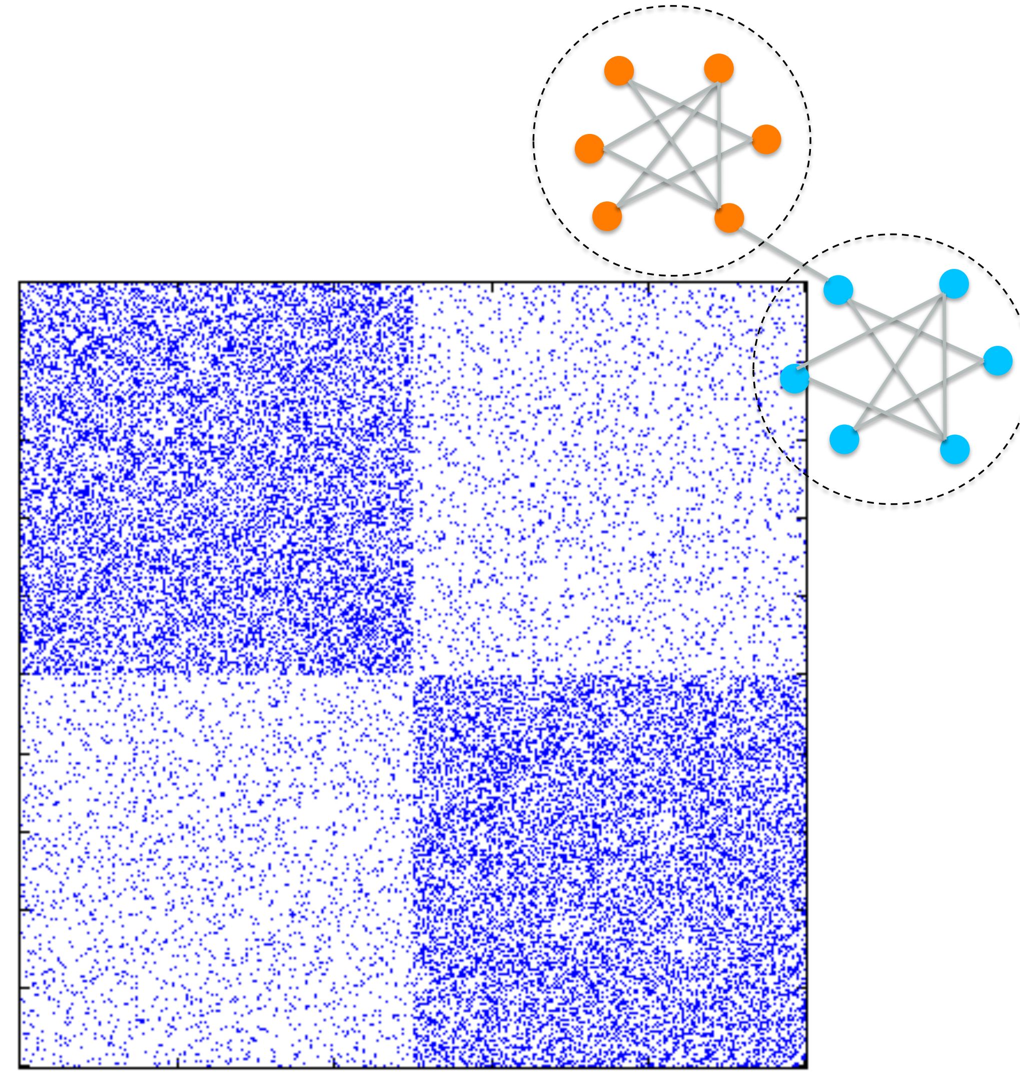
significant structure

which makes data different from noise

or different from ***random graphs***

Community detection





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Clustering from similarities

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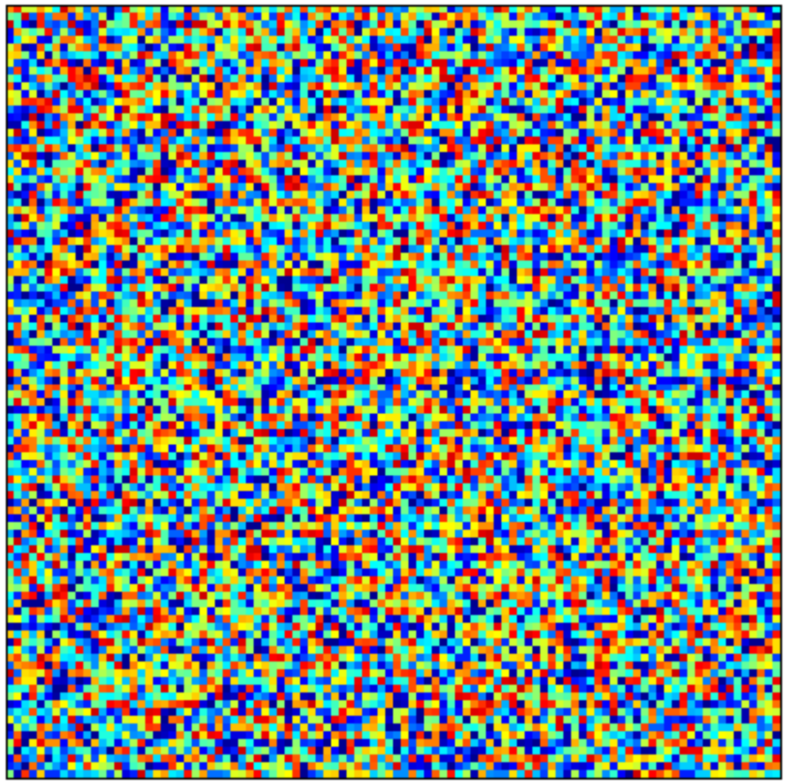
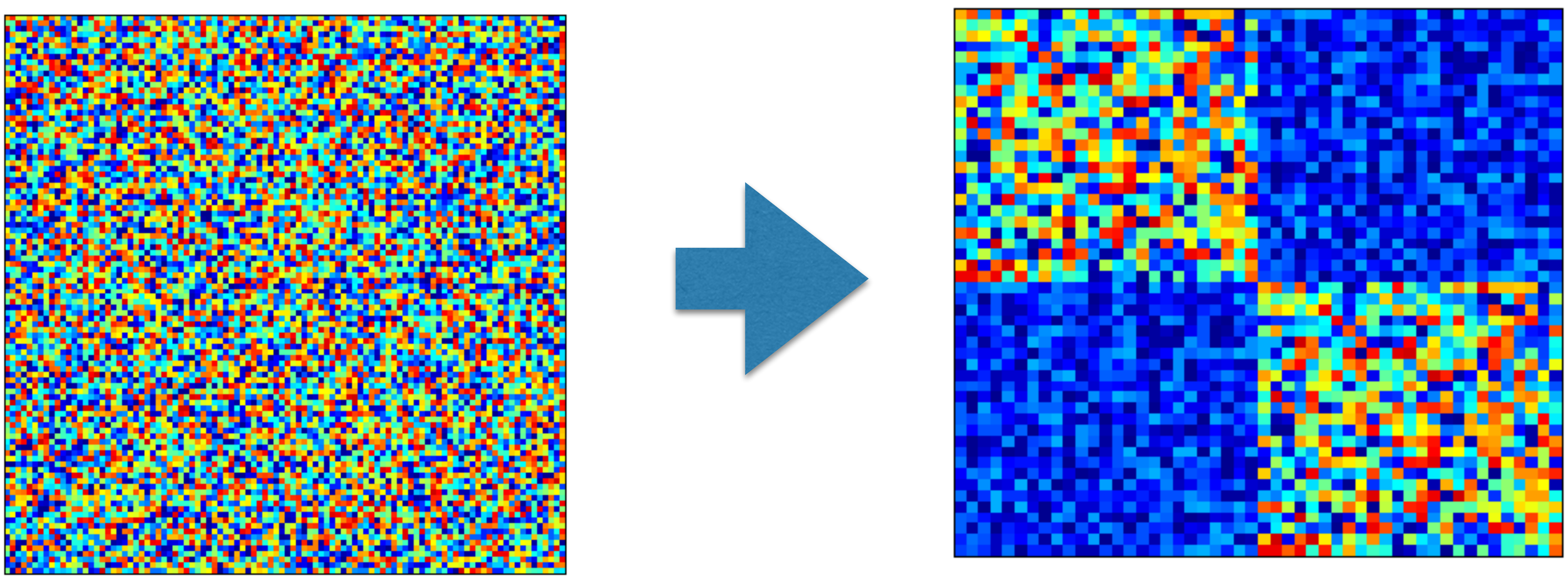
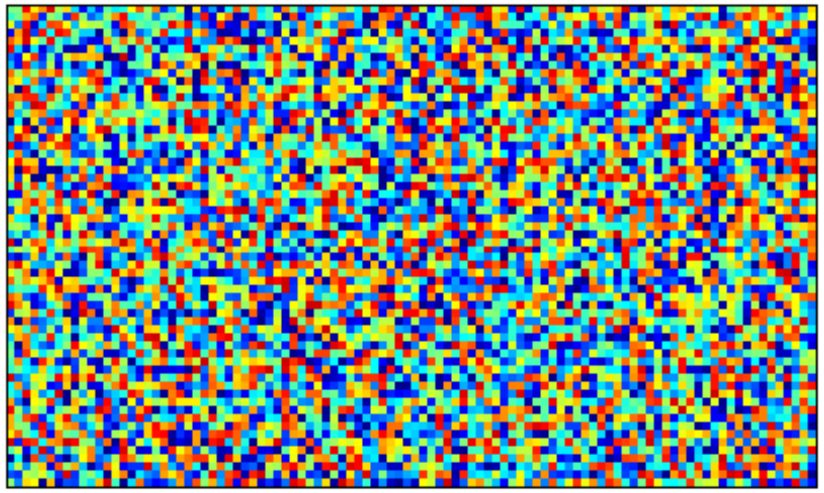


Clustering from similarities



Low-rank matrix factorization

Low-rank matrix factorization



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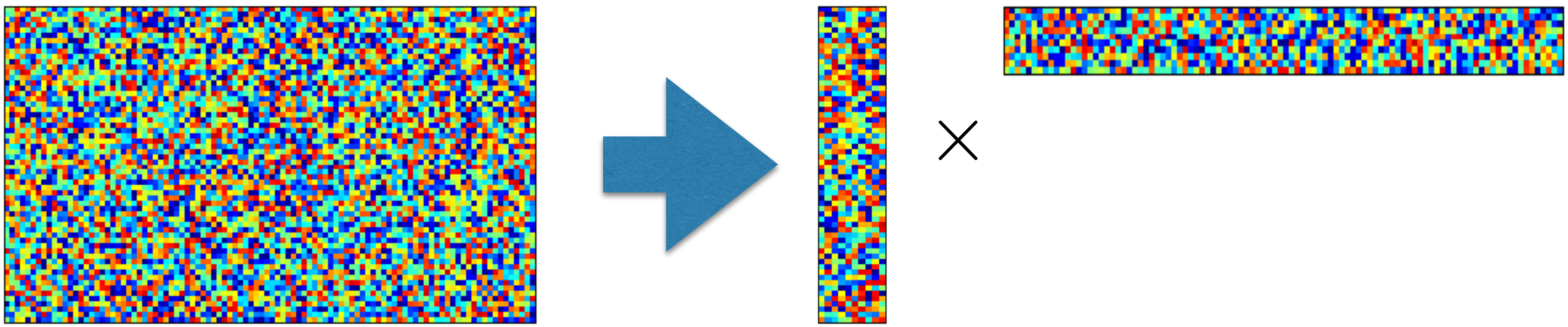

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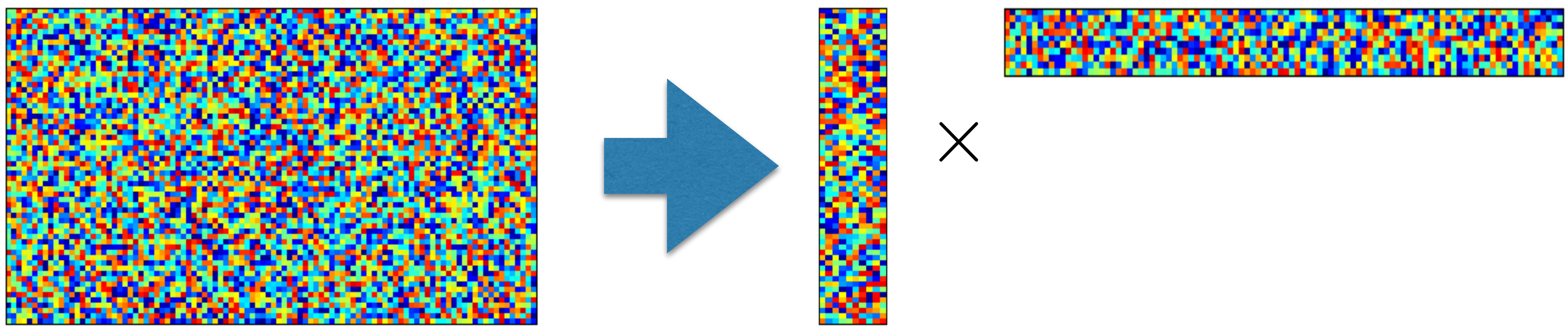
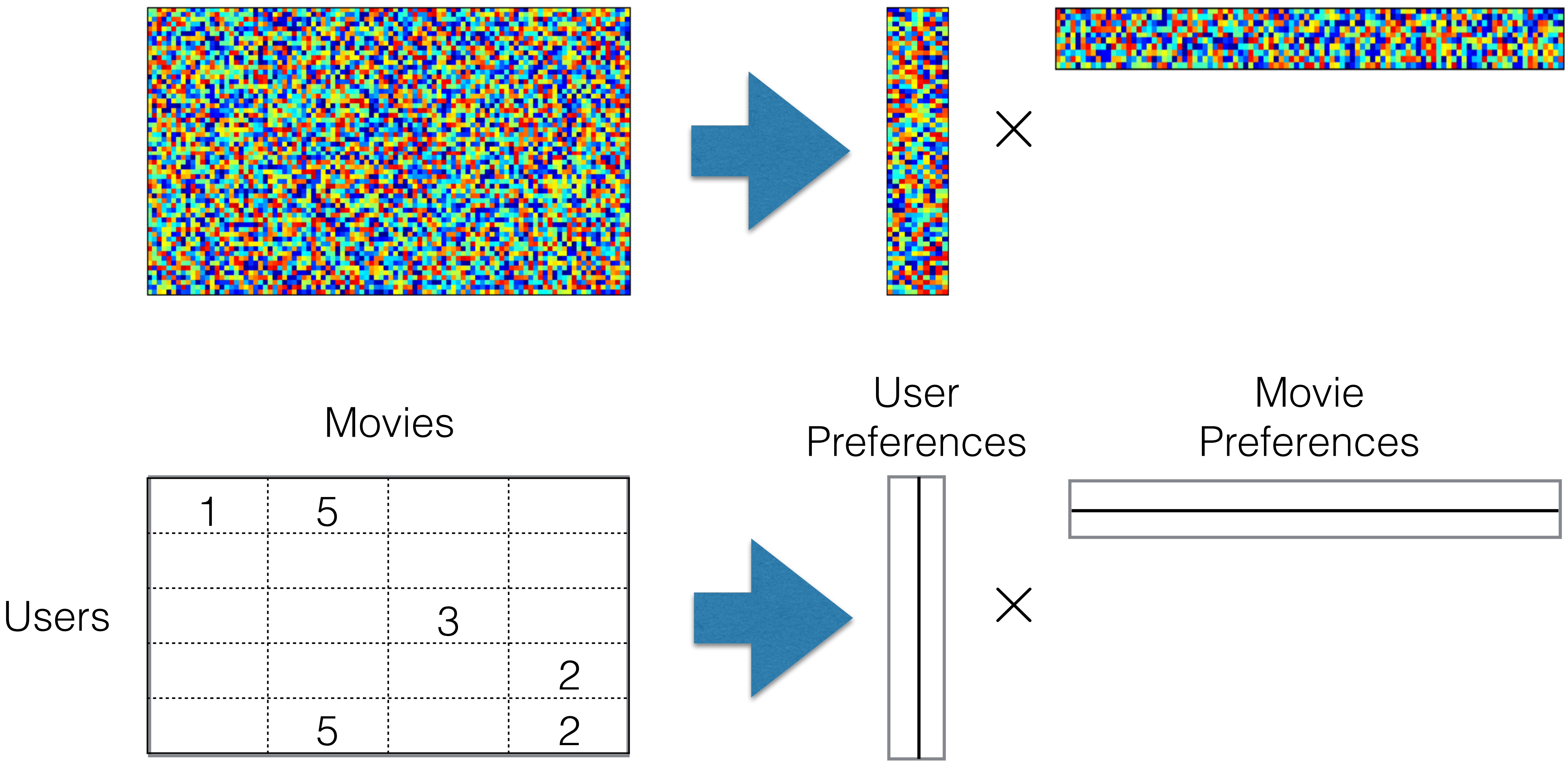


Movies

	1	5		
Users			3	
				2
		5		2

Low-rank matrix factorization

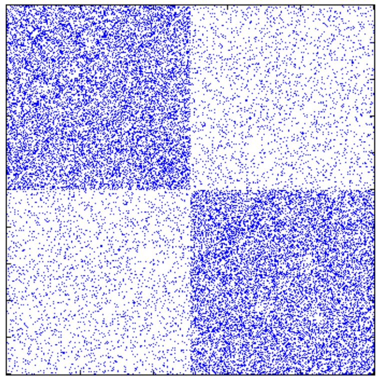


Spectral methods

- Choose a matrix, such as
  - Data matrix A
  - Laplacians $L = D - A$
  - Normalized Laplacian $L_{\mathrm{sym}} = D^{-1/2} L D^{-1/2}$
  - Random walk matrix $P = D^{-1} A$
- Computer first several eigenvectors (or singular vectors) of the matrix.
- Construct clusters or low-rank approximations using the eigenvectors.

Why do they work?

Why do they work?



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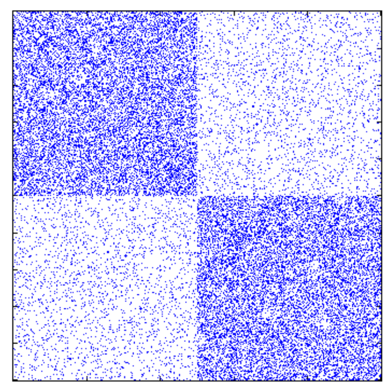

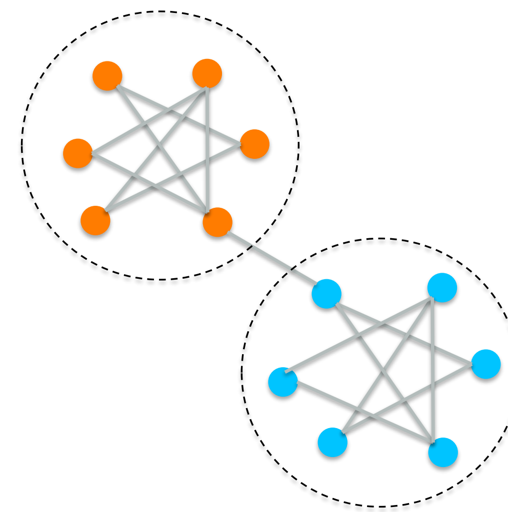

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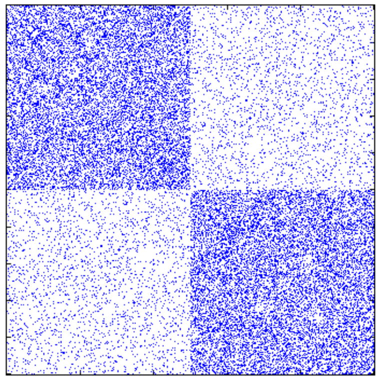

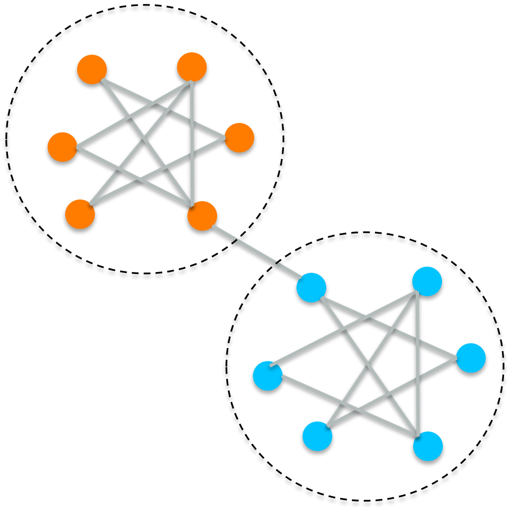

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$$\text{S.T. } x \in \{-1, 1\}^n$$

Original Problem

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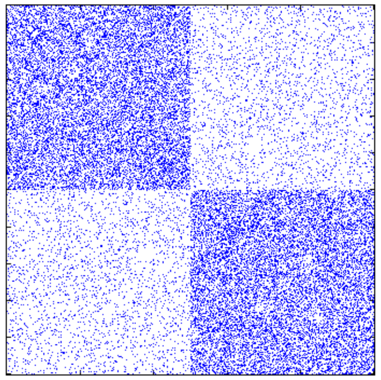

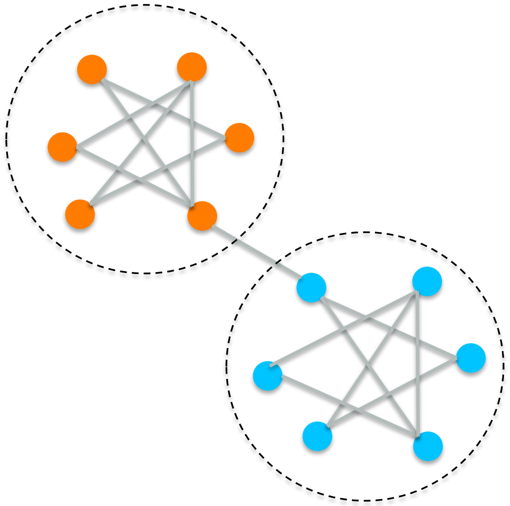

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Original Problem

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Spectral relaxation

When do they work?

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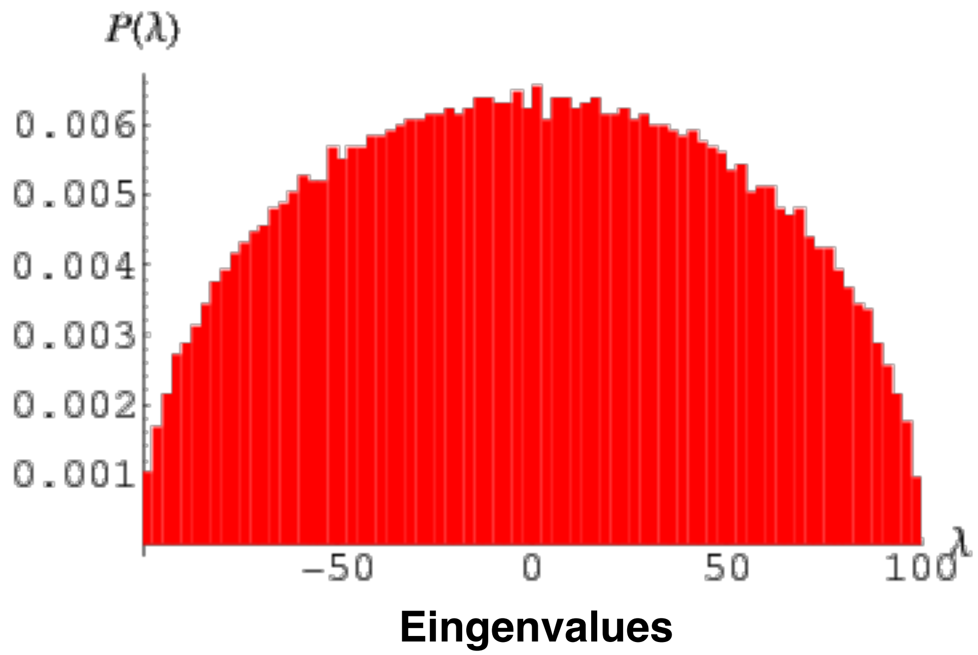

Wigner's semicircle law

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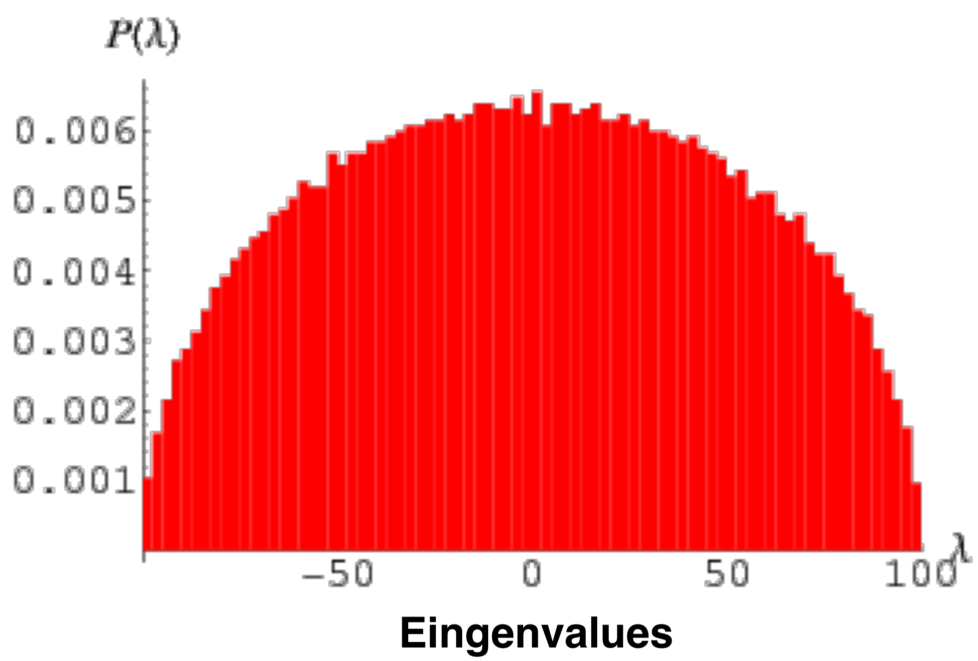

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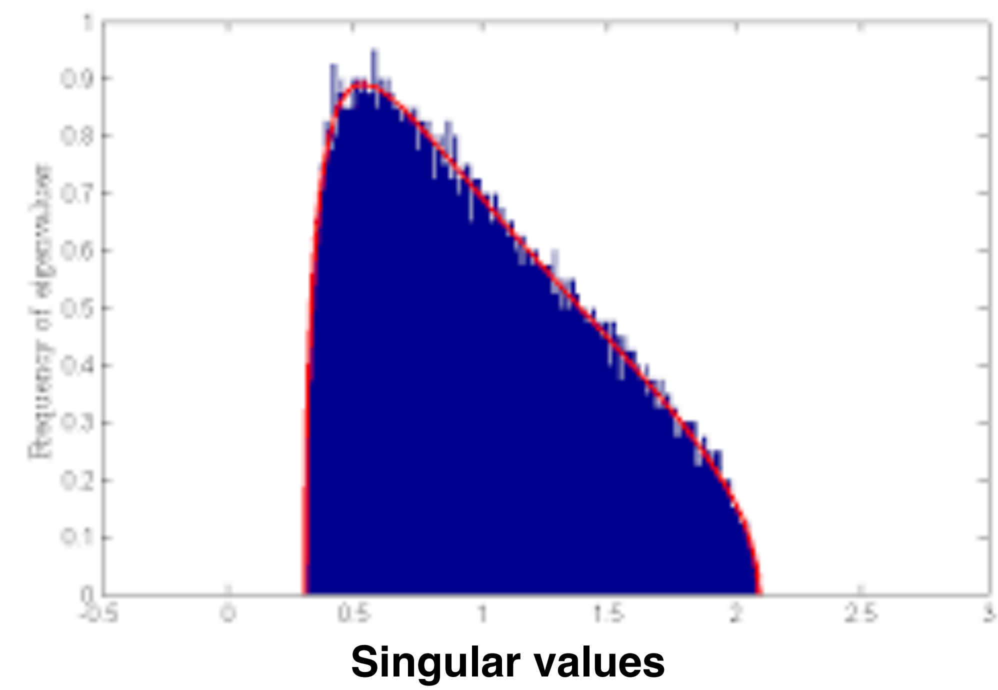
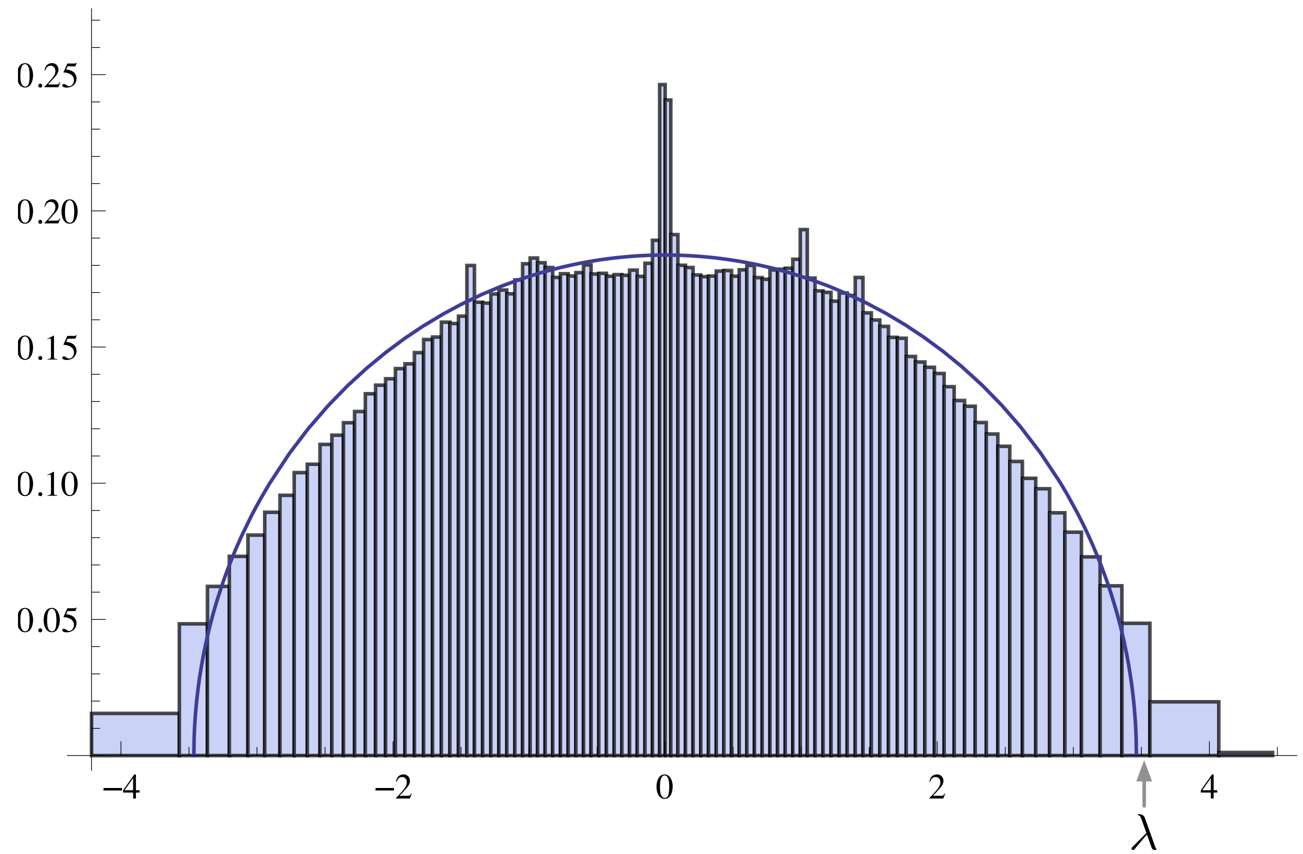


Marchenko Pastur law

However they do not work well in large sparse matrices



- Eigenvalues deviate from the semicircle rule
- Informative eigenvalues get lost in the bulk

Community detection: Krzakala/Moore/Mossel/Neeman/Sly/Zdeborová/Zhang PNAS 13'
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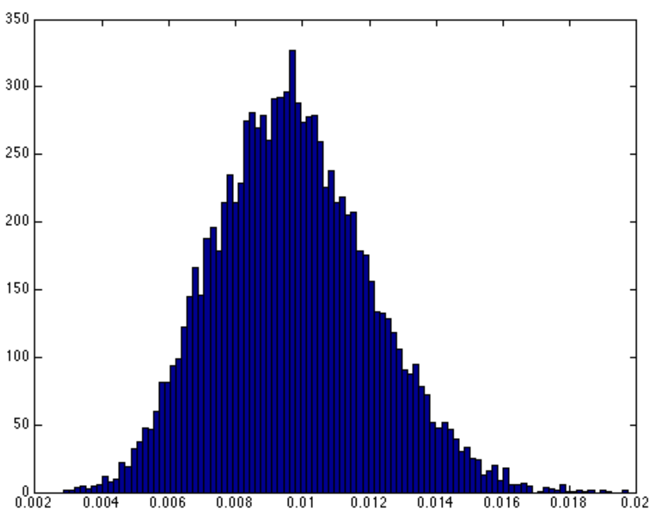

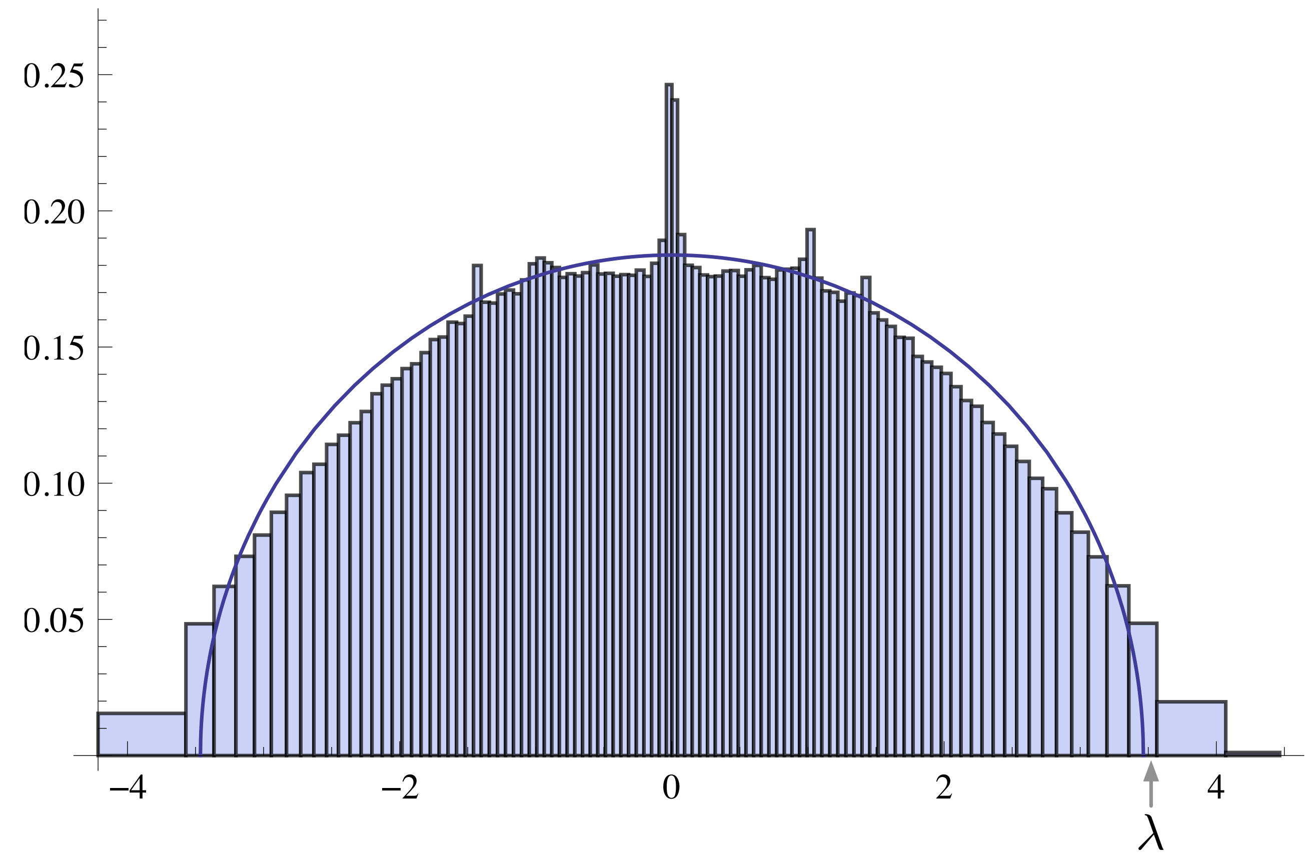

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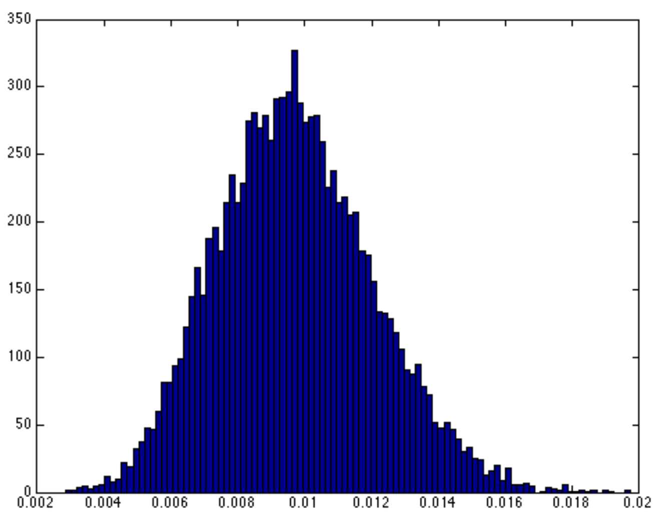

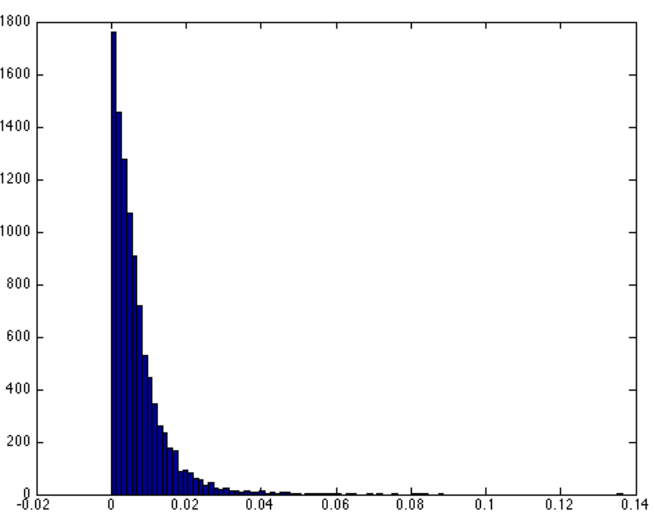

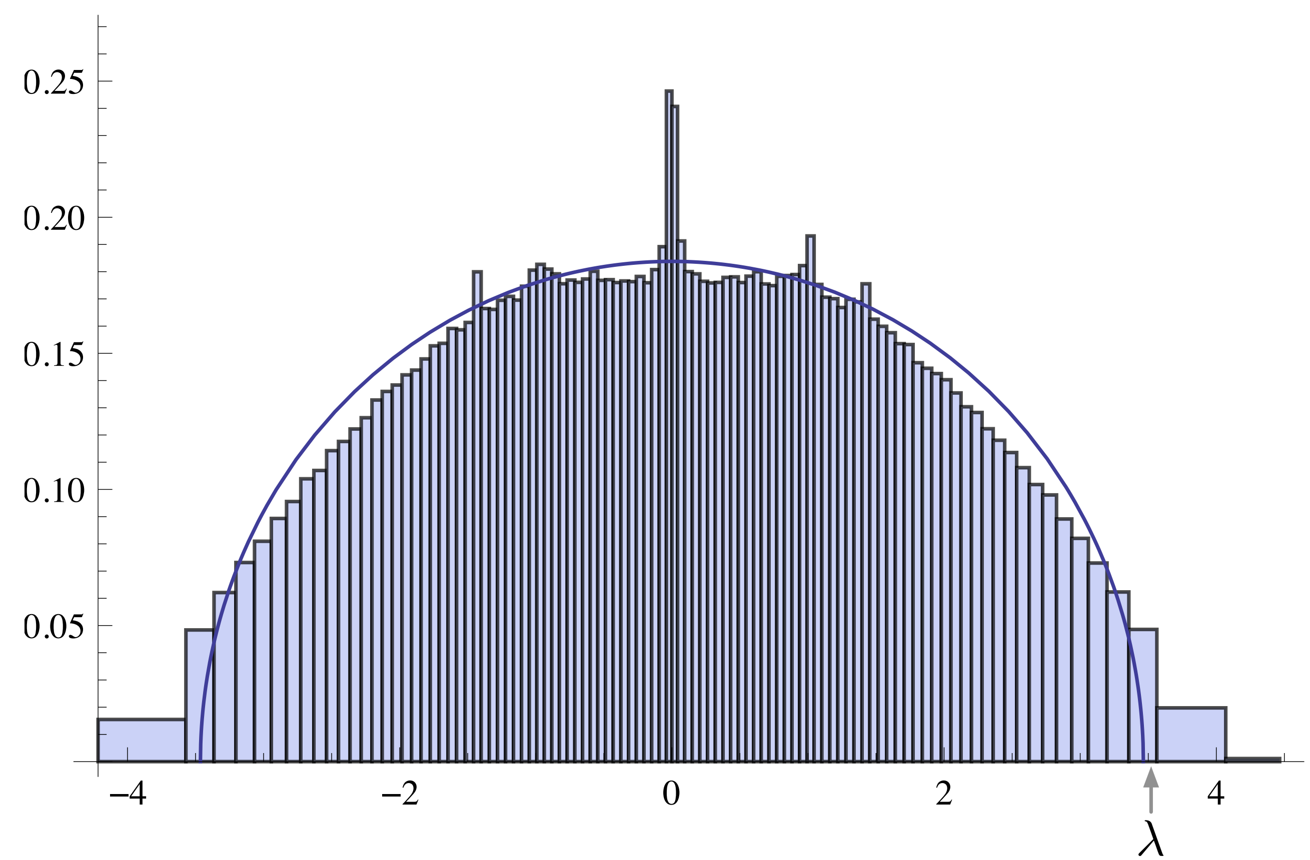

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Reason for the deviation: localization

- For adjacency matrix of Erdős–Rényi random graphs

$$d_{max} \approx \frac{\log n}{\log \log n}$$

$$\lambda_{\max}^2 \geq \frac{x^T A^T A x}{x^T x}$$

$$x = \{0, 0, 0...1...0, 0, 0\}$$

$$\lambda_{max} \geq \sqrt{d_{\max}} \approx \sqrt{\frac{\log n}{\log \log n}}$$

Localization on large-degree nodes

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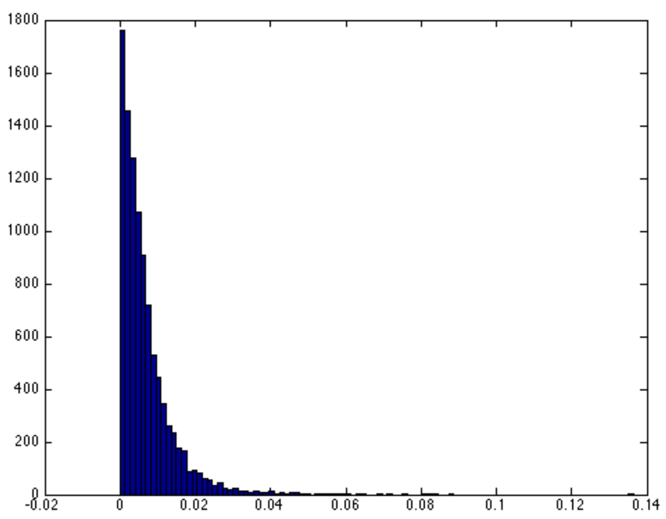

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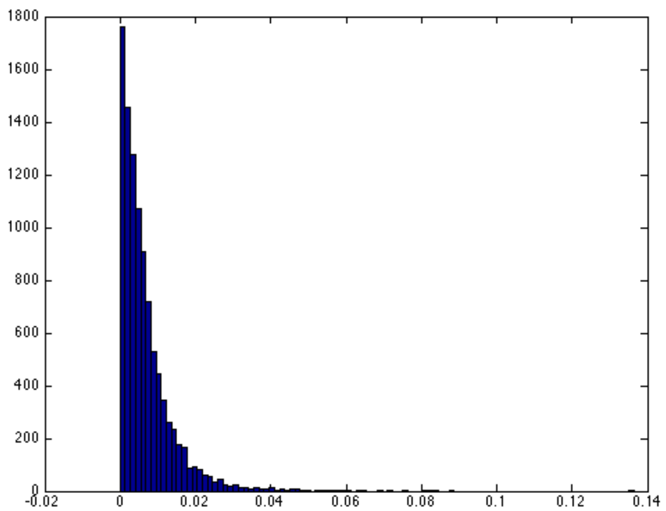

$$\left.\begin{aligned} d_{max} &\approx \frac{\log n}{\log\log n} \\ \lambda^2_{\max} &\geq \frac{x^T A^T A x}{x^T x} \\ x &= \{0,0,0...1...0,0,0\} \end{aligned}\right\} \quad \lambda_{max} \geq \sqrt{d_{\max}} \approx \sqrt{\frac{\log n}{\log\log n}}$$

Localization on large-degree nodes

- For matrices $P = D^{-1/2}A \qquad \tilde{A} = D^{-1/2}AD^{-1/2}$

$$L_{\text{sym}} = D^{-1/2}(D-A)D^{-1/2}$$

Localization on dangling sub-graphs

Localization in physics:

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- Wavefunction amplitudes distribution: Inverse Participation Ratio (**IPR**).

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- Entangle entropy (between two subsystems)

$$S_2 = -\log \mathrm{tr}(\rho^2)$$

  - Low entanglement entropy <-> Localization.

  - Area Law, ground state.

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- Energy-Level Statistic (Eigenvalue statistics)
  Poisson distribution vs. Wigner Dyson distribution

Approaches for localizations in sparse matrices

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- Trimming: Remove rows and columns with large degree/ weights
  [Keshavan/Montanari/Oh 09']
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- Using non-backtracking matrix and Bethe Hessian
  [Krzakala/Moore/Mossel/Neeman/Sly/Zdeborová/Zhang 2013]
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Trimming

- Usually works in practice

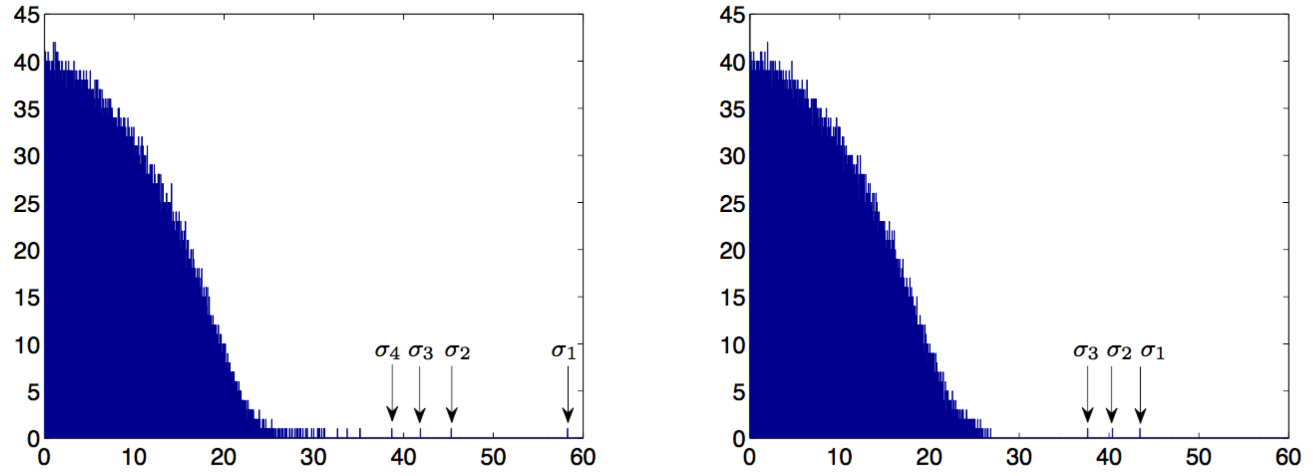

Figure 1: Histogram of the singular values of a partially revealed matrix M^E before trimming (left) and after trimming (right) for $10^4 \times 10^4$ random rank-3 matrix M with $\epsilon = 30$ and $\Sigma = \mathrm{diag}(1, 1.1, 1.2)$. After trimming the underlying rank-3 structure becomes clear. Here the number of revealed entries per row follows a heavy tail distribution with $\mathbb{P}\{N = k\} = \mathrm{const.}/k^3$.

Figure taken from Keshavan/Montanari/Oh 09’

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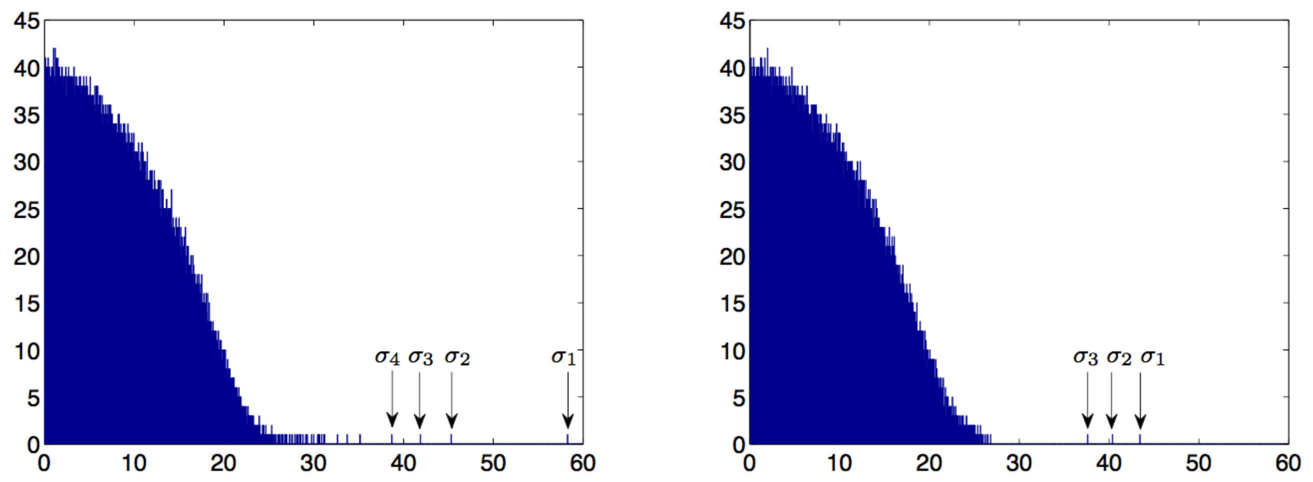

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Figure taken from Keshavan/Montanari/Oh 09'

- However in general suboptimal [Coja-Oghlan 10'], usually performs worse than other methods.

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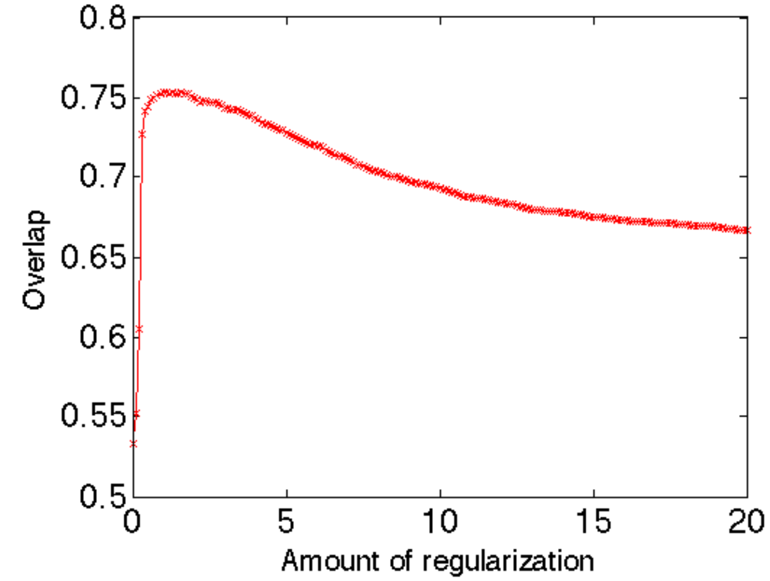

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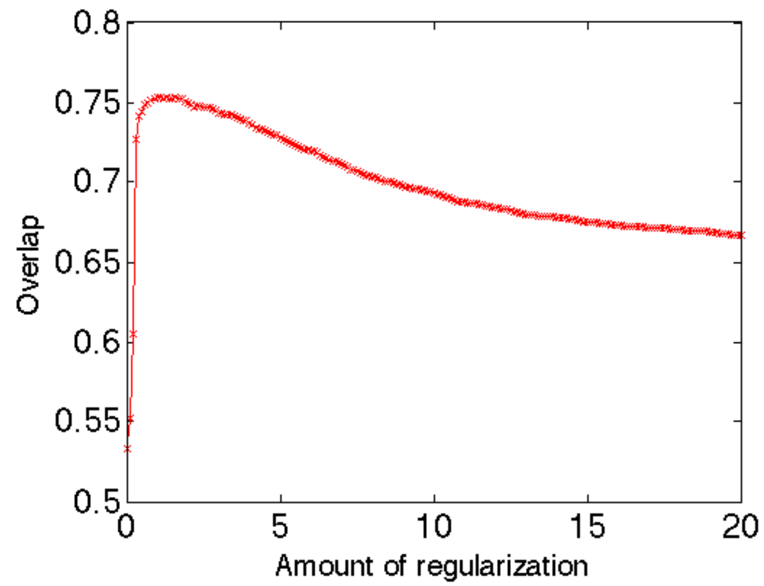

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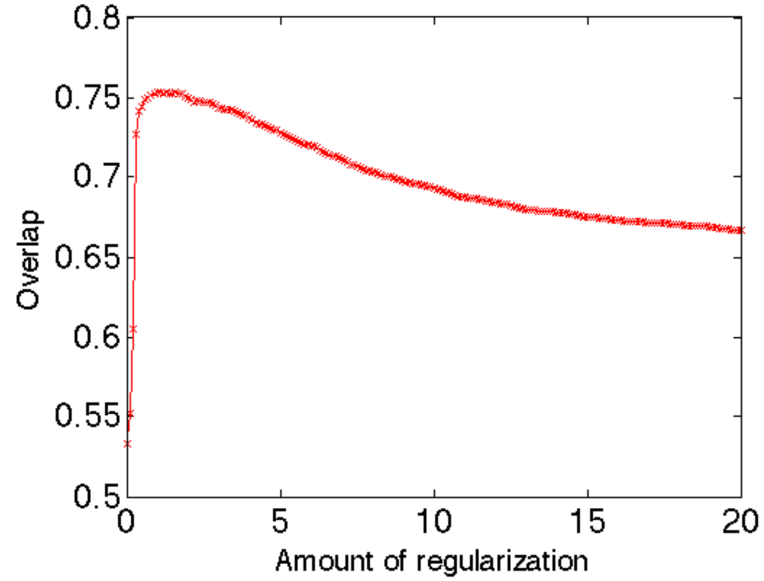

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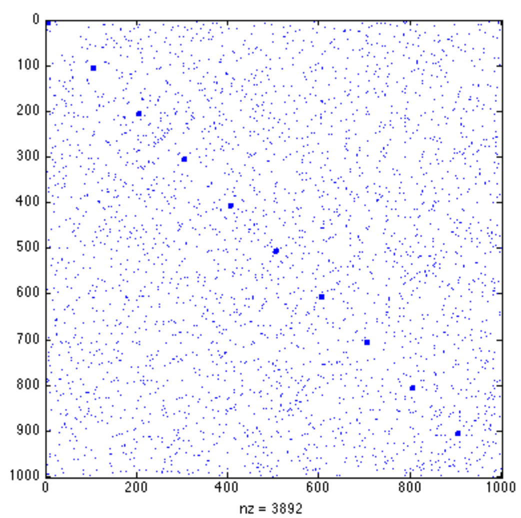

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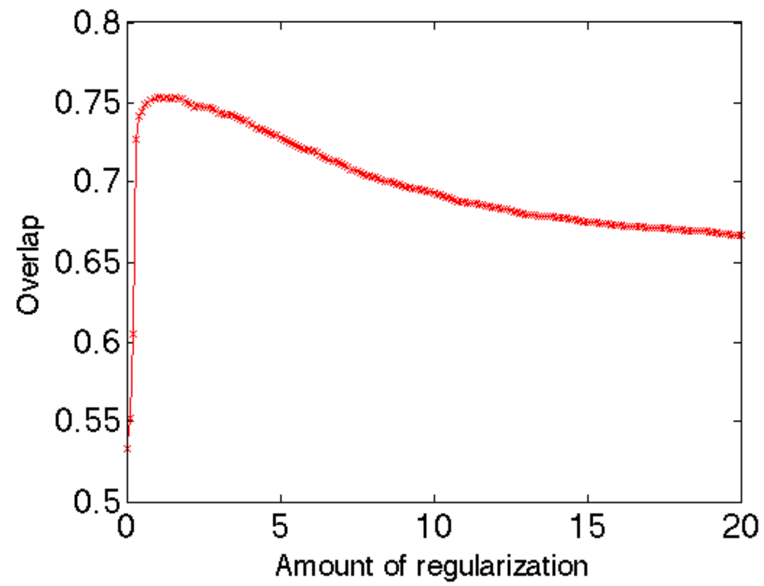

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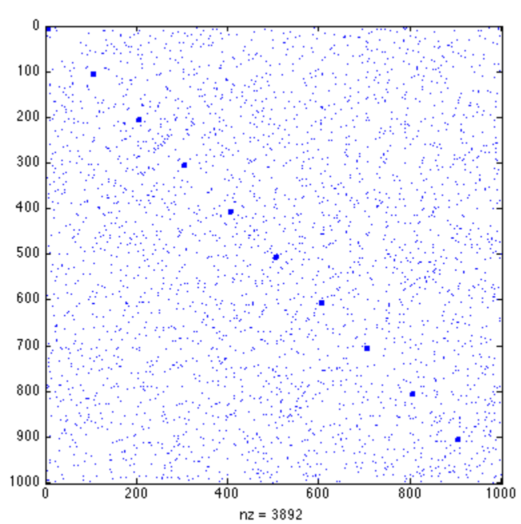

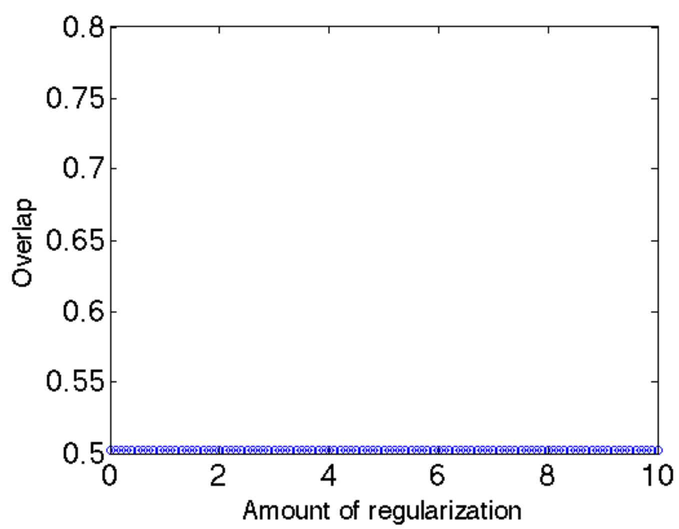

SBM network, c=3 n=10000, epsilon=0.2 with 10 size-10 cliques

Non-backtracking matrix and Bethe-Hessian

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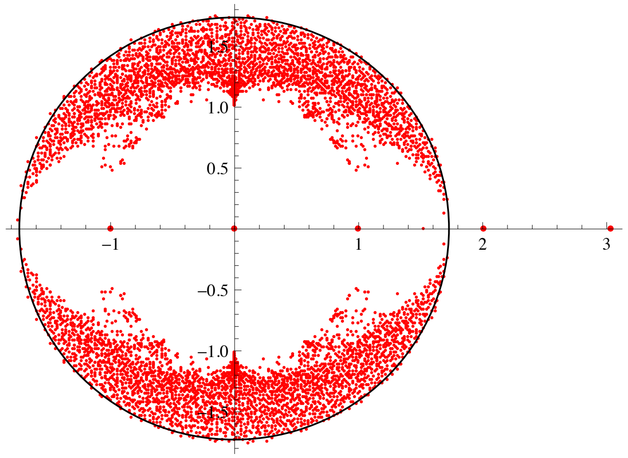

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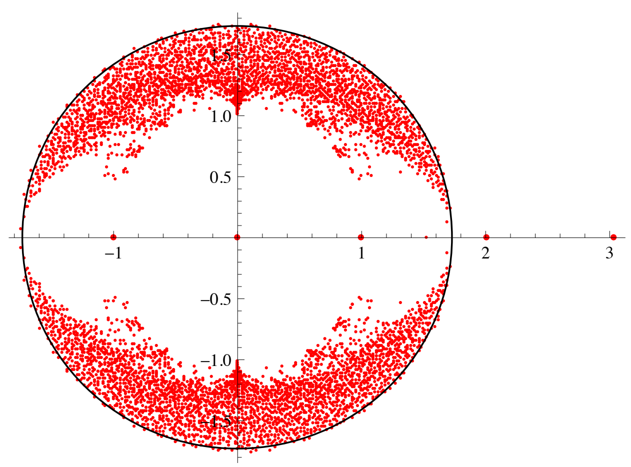

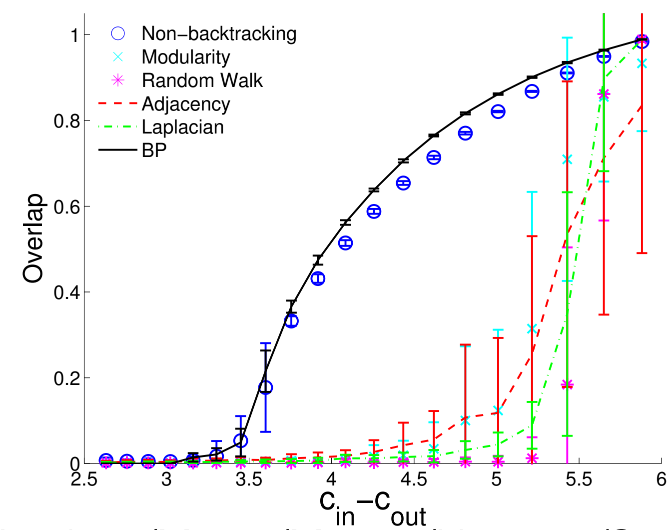

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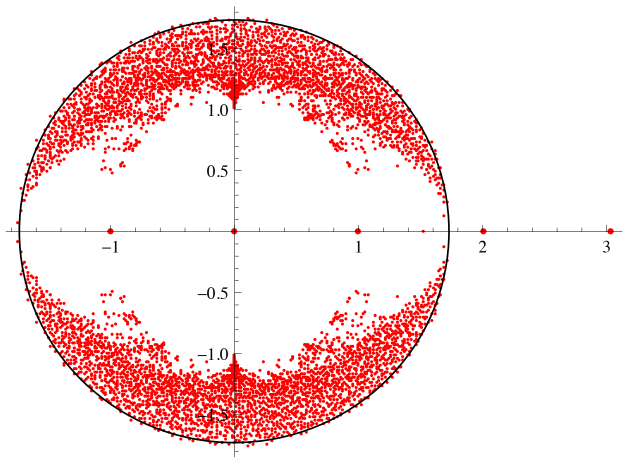

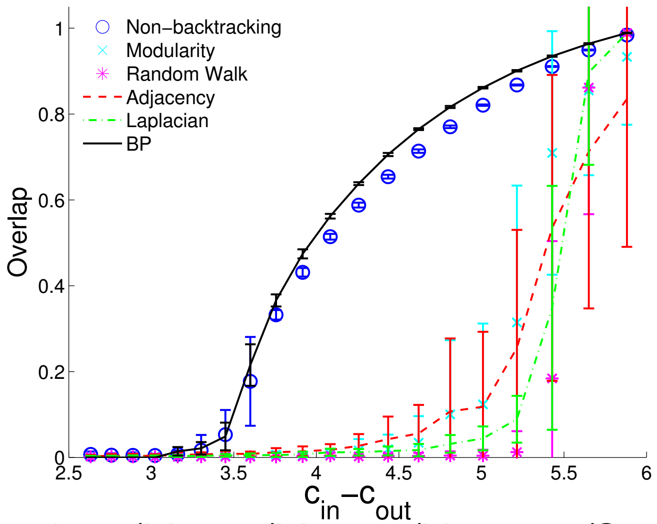

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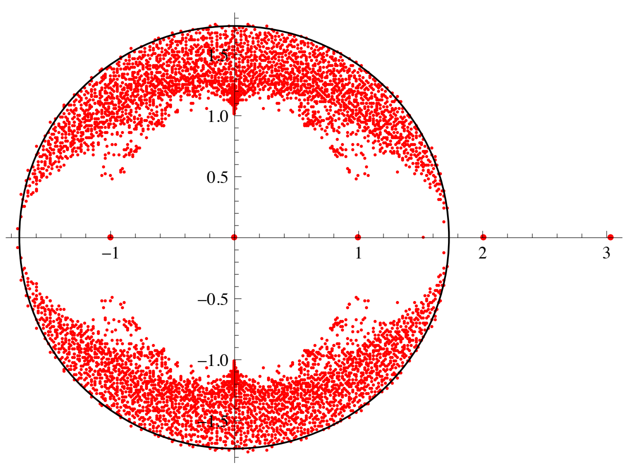

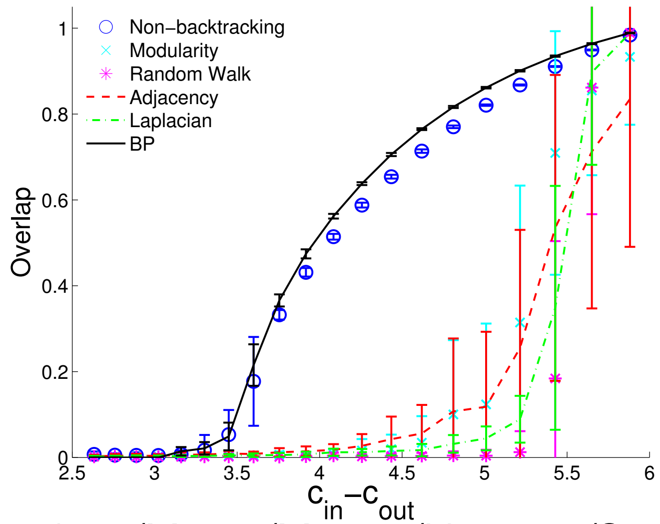

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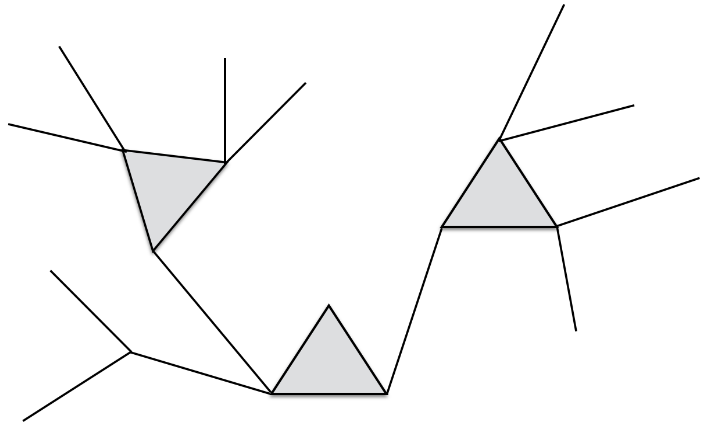

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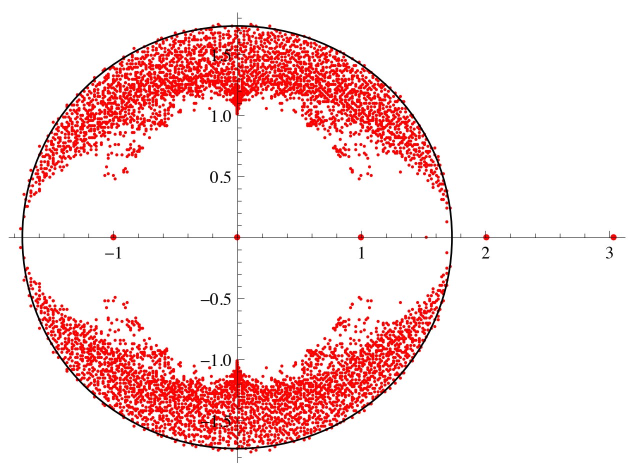

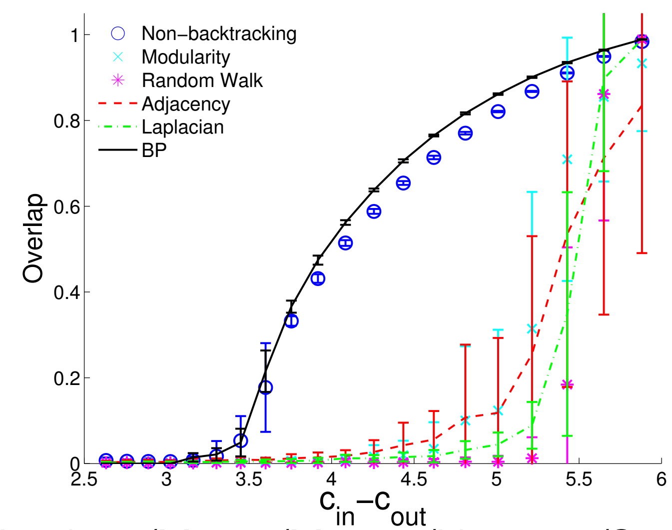

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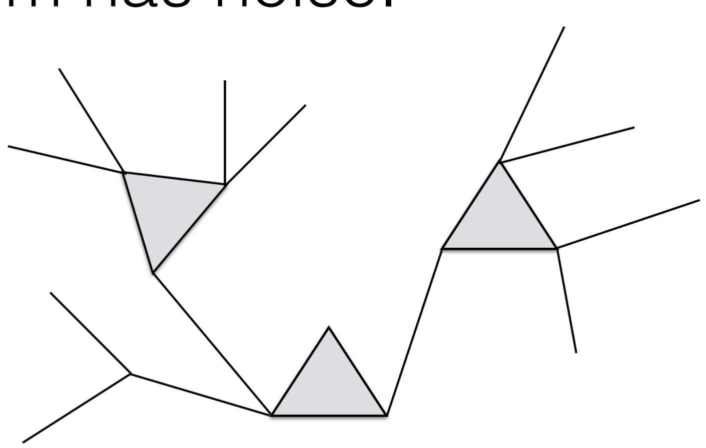

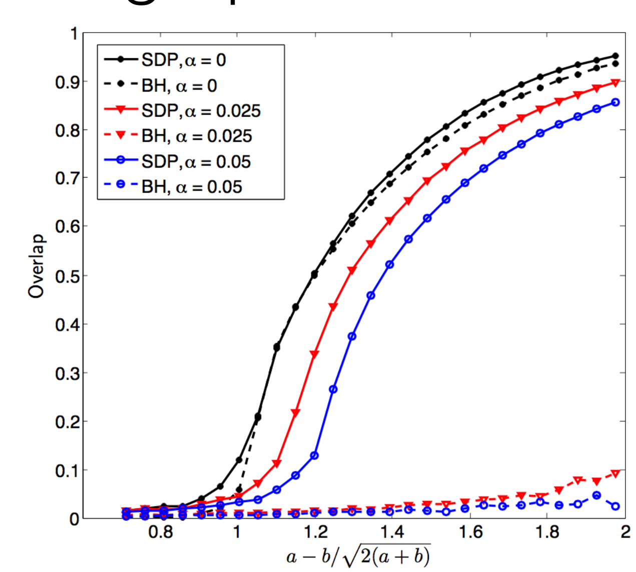

Figure taken from Javanmard/Montanari/Ricci-Tersenghi, PNAS16'

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- However in noisy cases, the source of localization is neither high-degree nor low-degrees!
- What should we do without knowing the source of localization?

My proposal: Learning a regularization

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- Instead, let's learn a regularization from the existing localizations, i.e. localized eigenvectors.

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the X-Laplacian

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4. if $I(v) < \Delta$, return $L_X = A + X$; Otherwise, $\forall i, X_{ii} \leftarrow X_{ii} - \eta v_i^2$, then go to step 2.

Algorithm: Whack-a-mole

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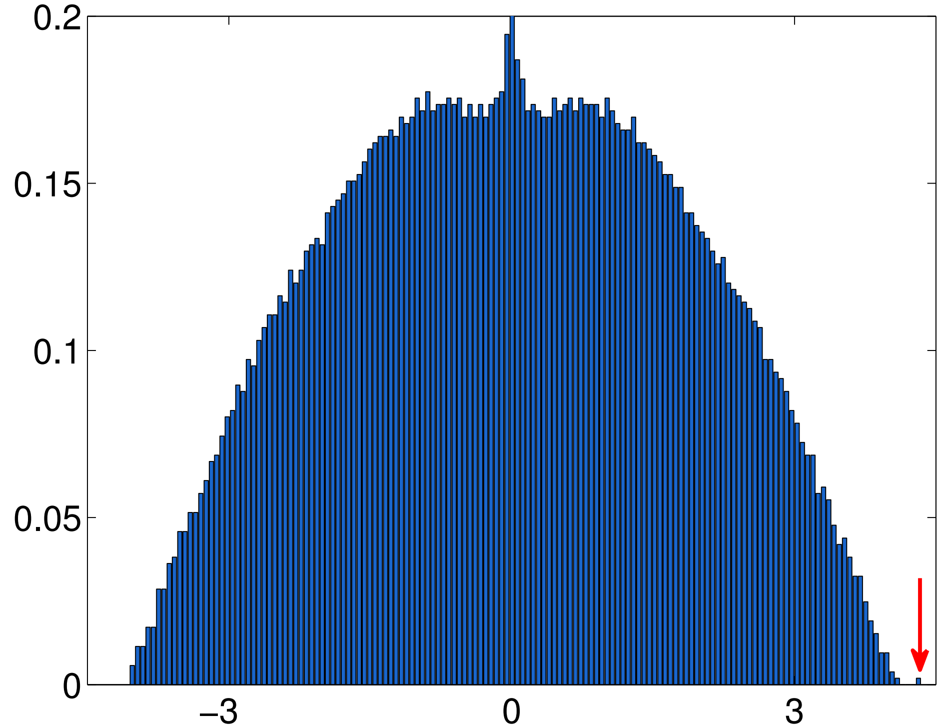
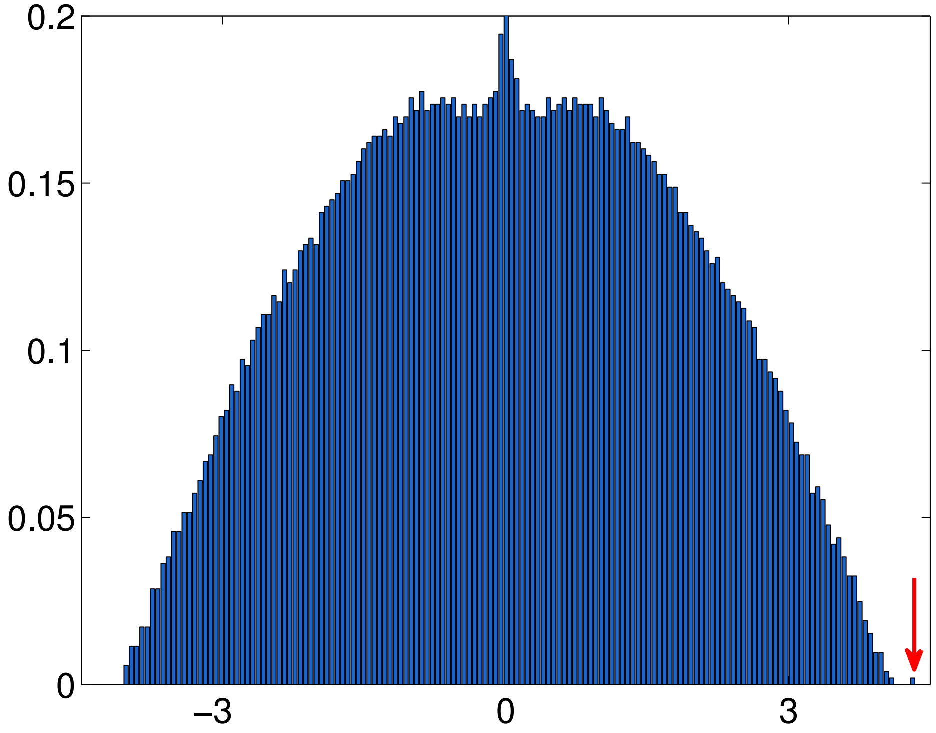


Spectral density of A
Before learning

A is generated by the Stochastic Block Model with n=10000 nodes, average degree c=3, q=2 groups, and c_out/c_in=0.125.

Localized eigenvalues are moles



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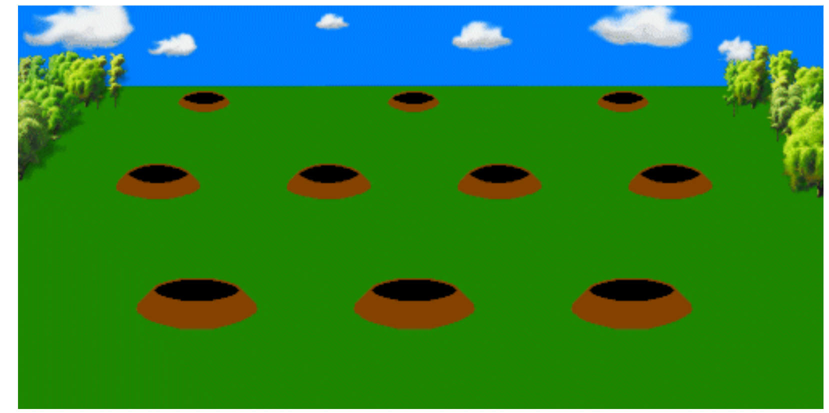

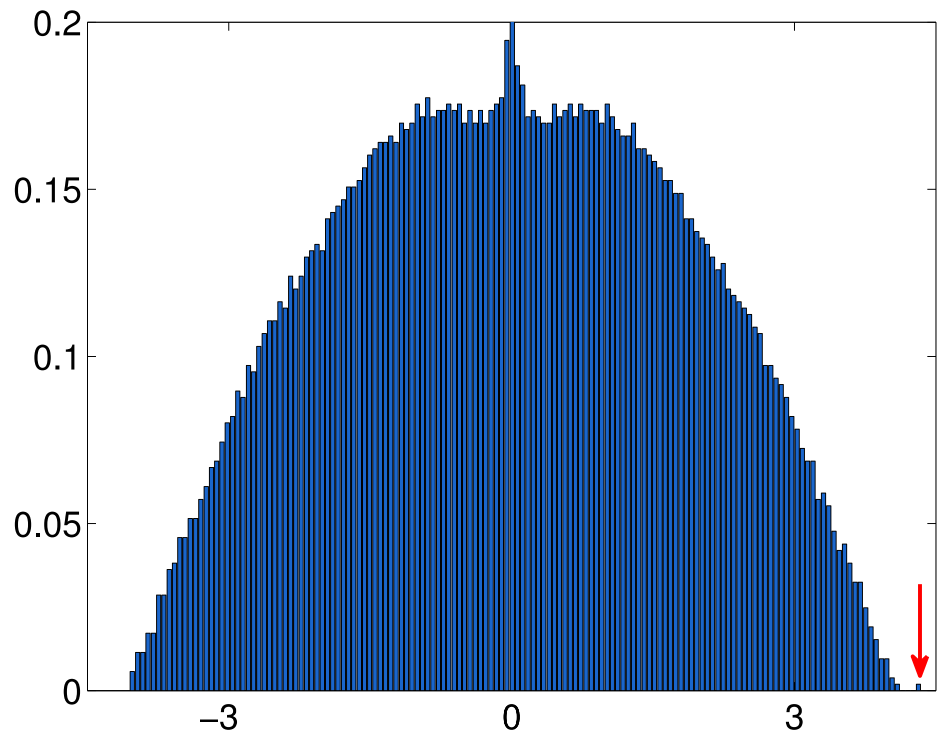

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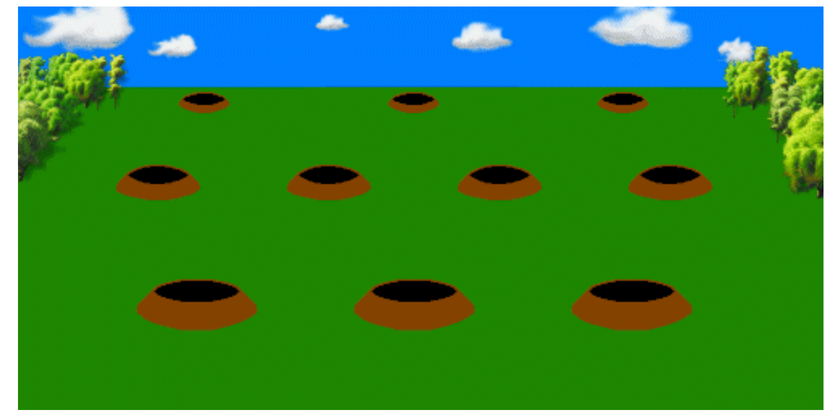

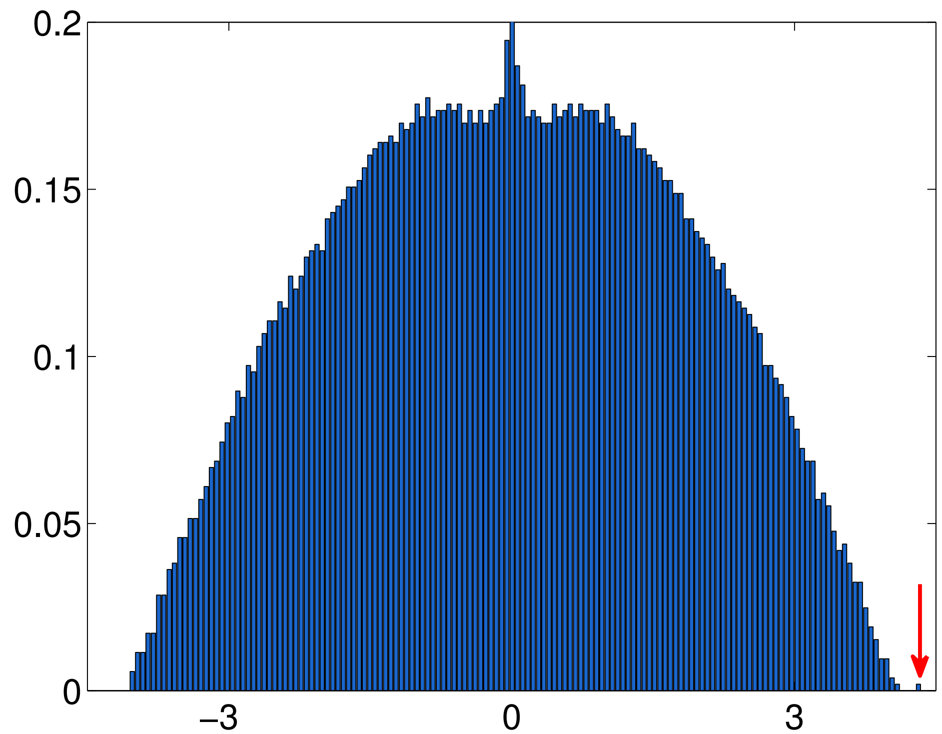

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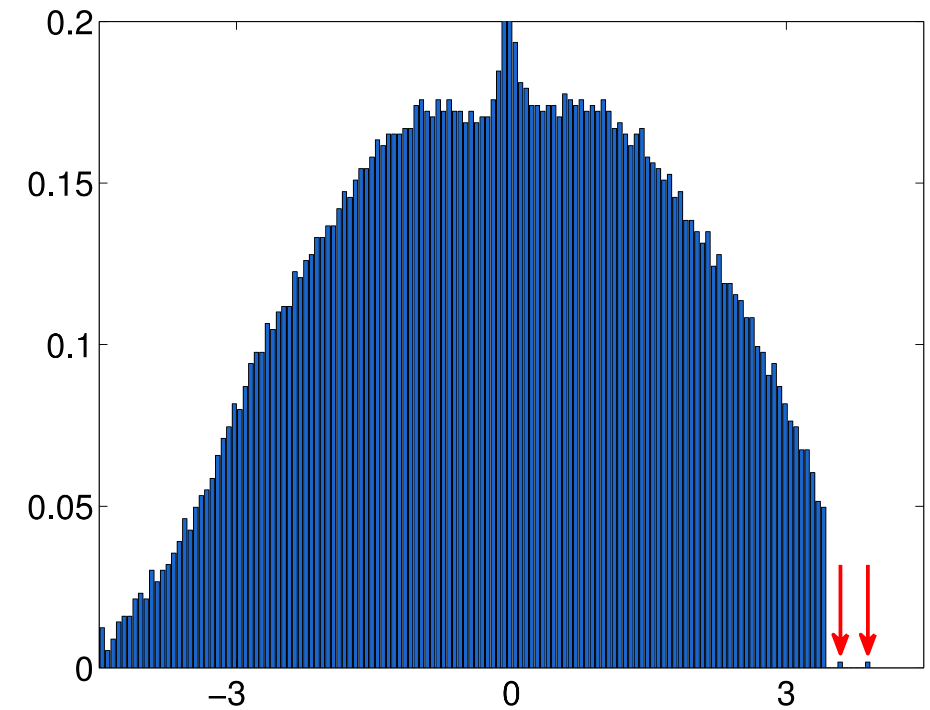

Spectral density of A+X
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Matrix perturbation analysis

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Change of an eigenvalue: $\hat{\lambda}_i = u_i^T \hat{L} u_i$

$$\hat{L} = -\eta v_i^2$$

Matrix perturbation analysis

Learning: $X_{ii} \leftarrow X_{ii} - \eta v_i^2$ $\eta = O(1)$ $v_i^2 = O(1/n)$

Matrix perturbation:

$$L_X u_i = \lambda_i u_i$$

$$(L_X + \hat{L})(u_i + \hat{u}_i) = (\lambda_i + \hat{\lambda}_i)(u_i + \hat{u}_i)$$

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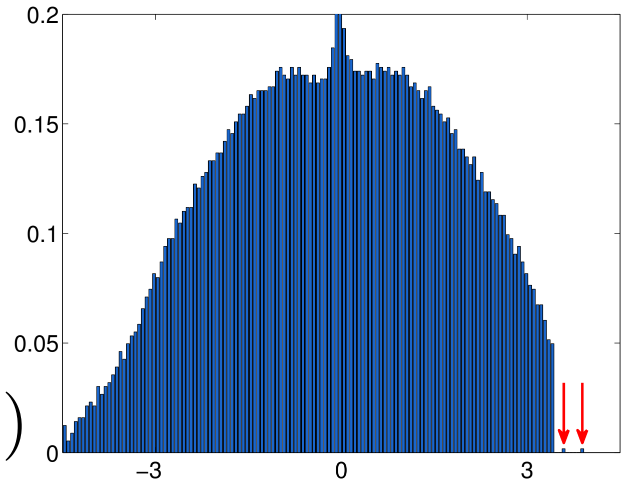

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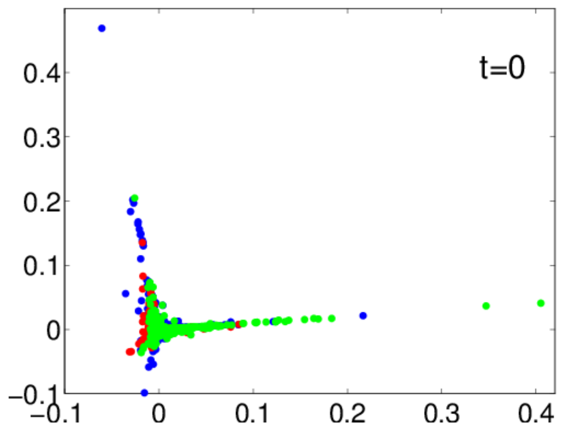

The second eigenvector vs. the third eigenvector, during learning
Network is generated by SBM with n=42000 nodes, average degree c=3, q=3 groups, c_out/c_in=0.08.

Matrix perturbation analysis

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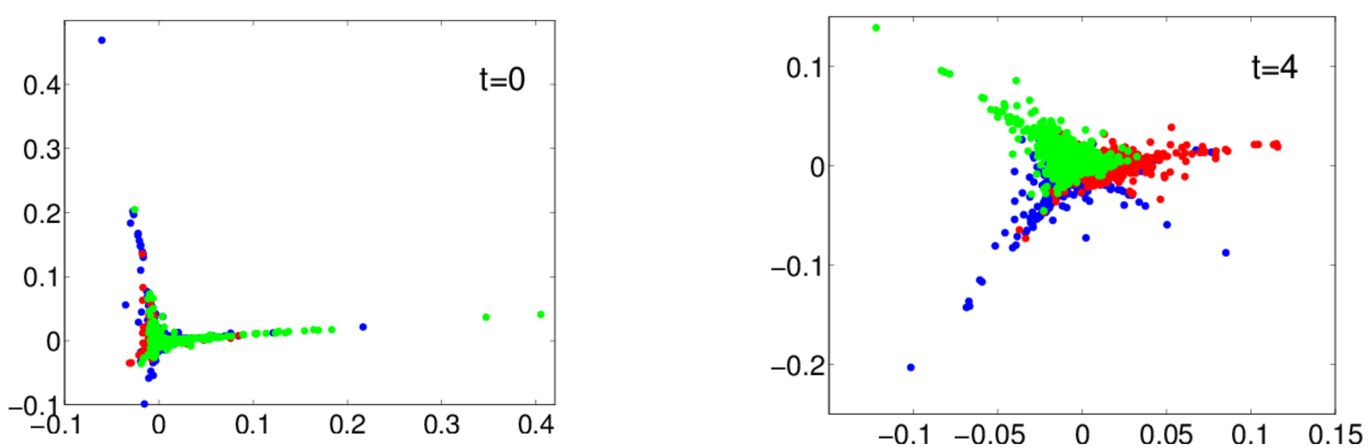

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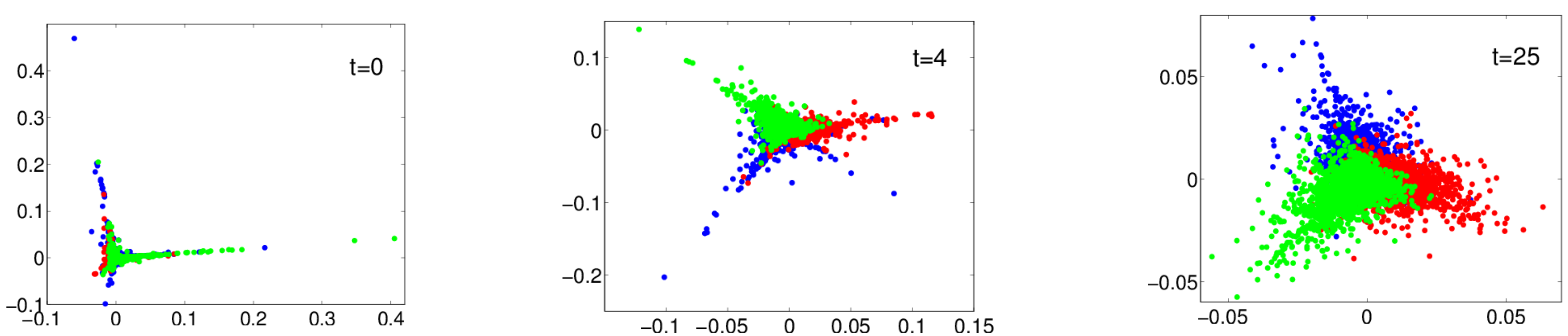

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Experimental evaluations

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- Community detection in sparse graphs with noise.
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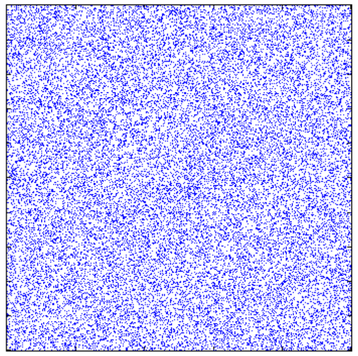
  [Saade/Krzakala/Zdeborová NIPS 14']
  [Javanmard/Montanari/Ricci-Tersenghi PNAS16']



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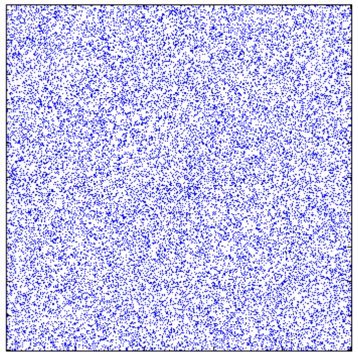

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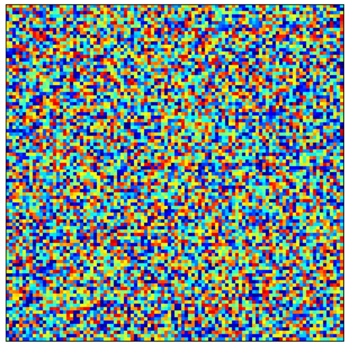

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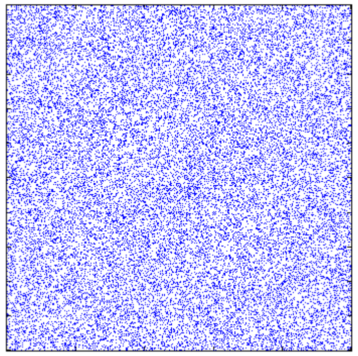

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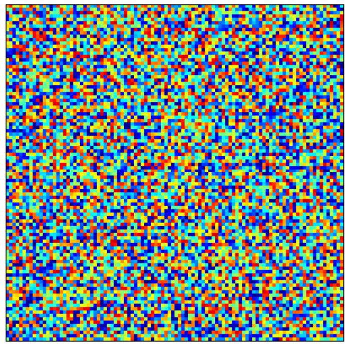

- Rank estimation and matrix completion.
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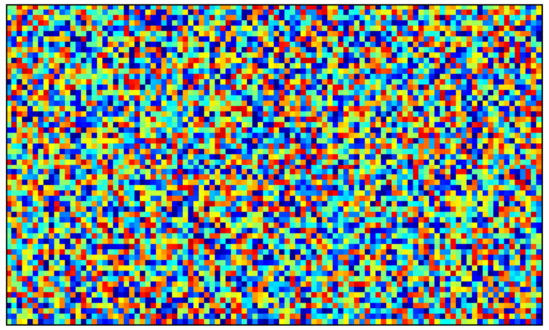

Community detection

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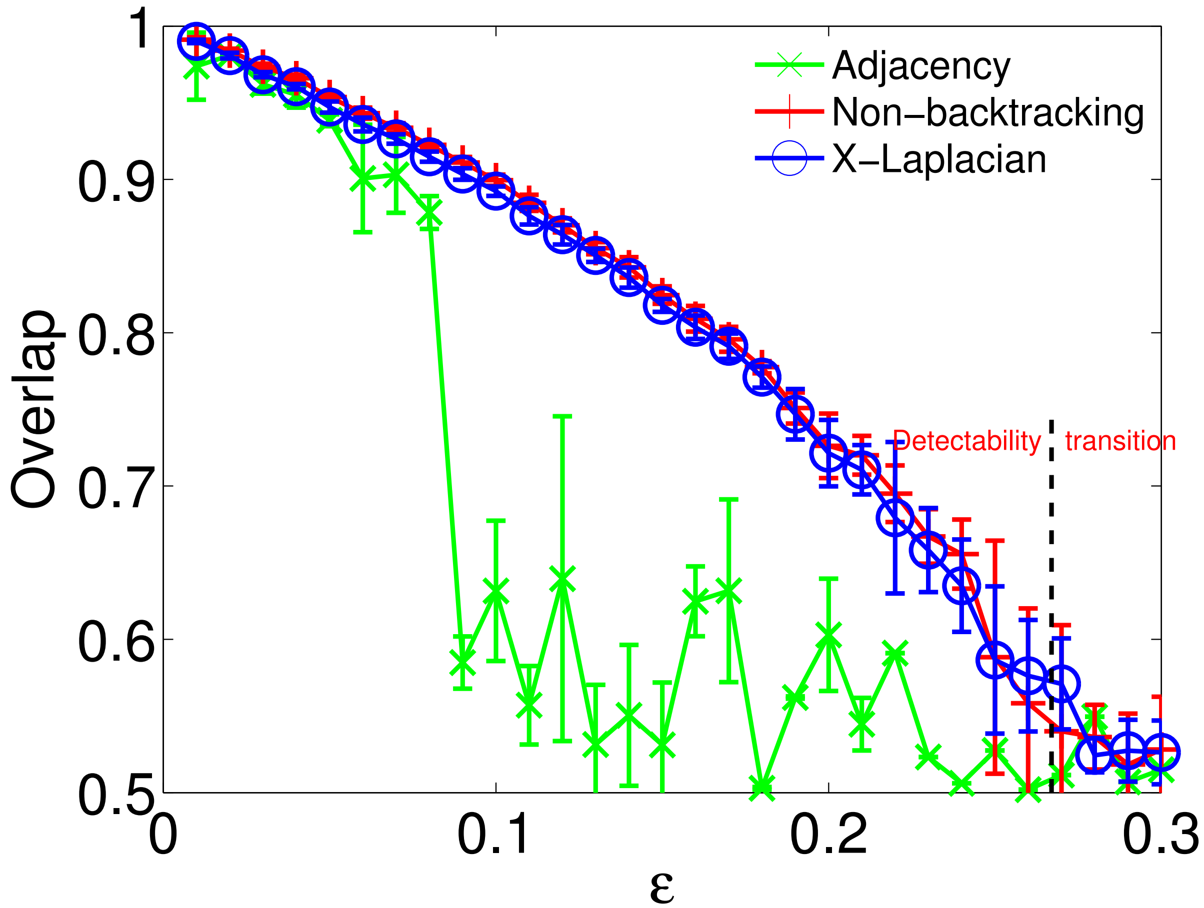
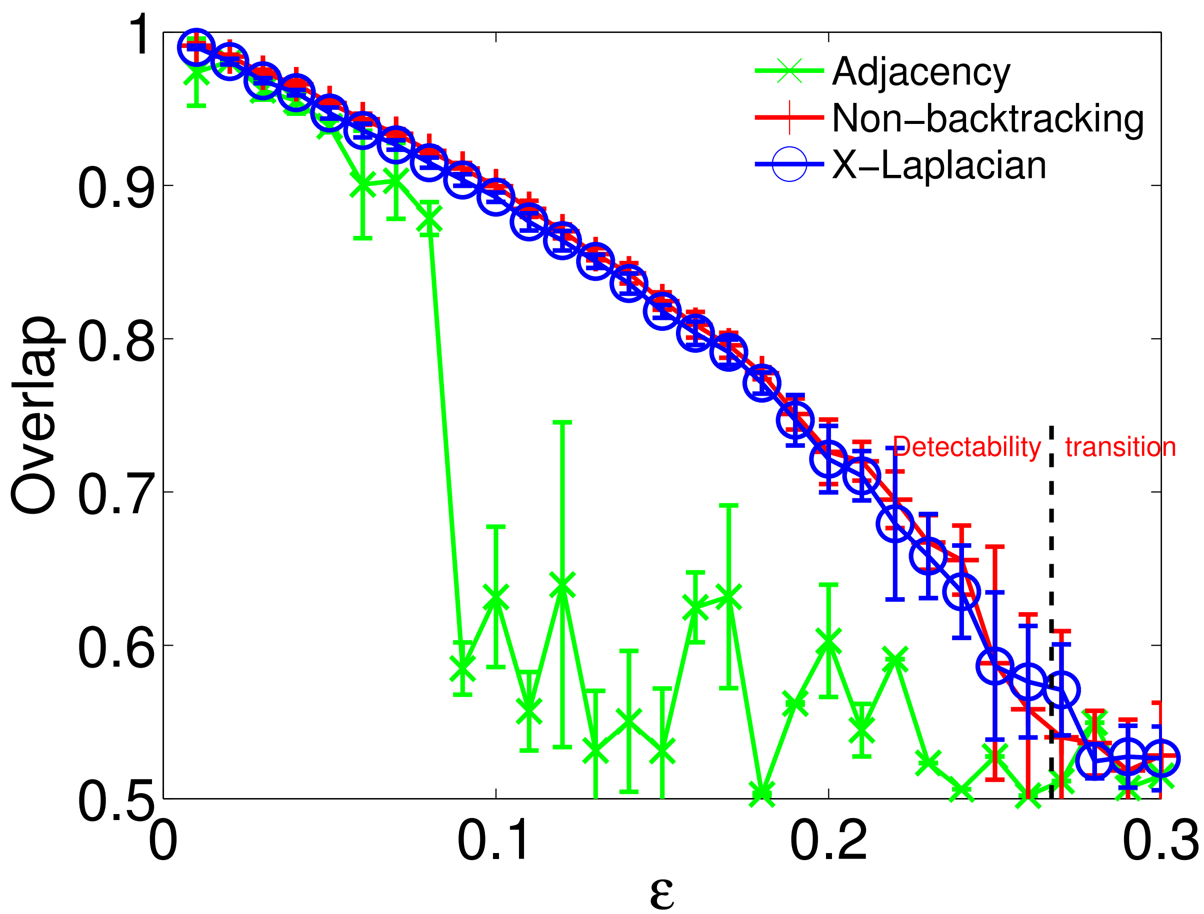


Stochastic Block Model
n=10000, q=2, c=3

Community detection



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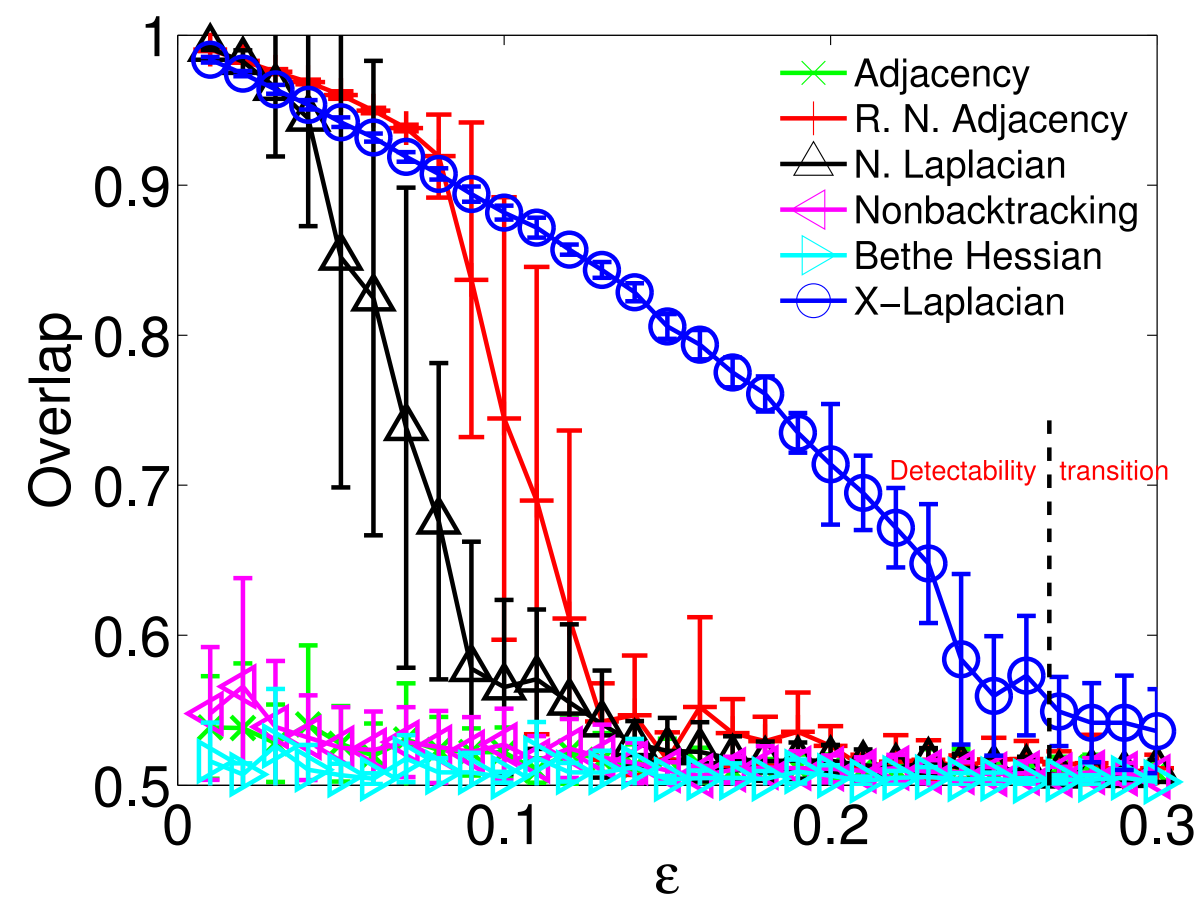


Noisy Stochastic Block Model
n=10000, q=2, c=3

Community detection

Community detection

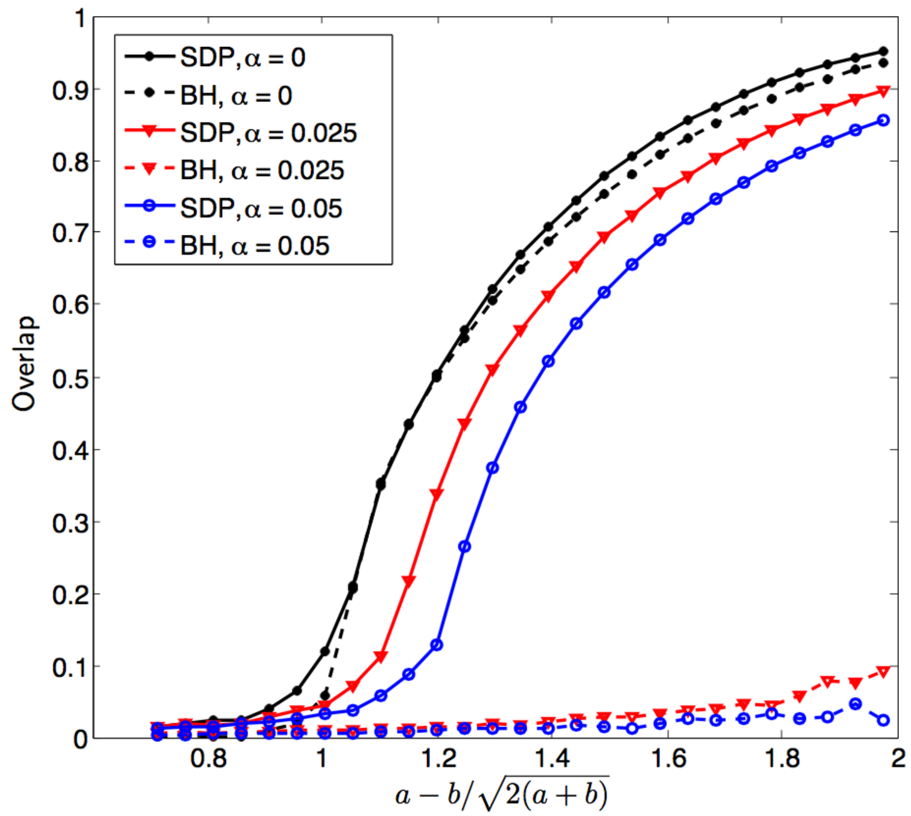
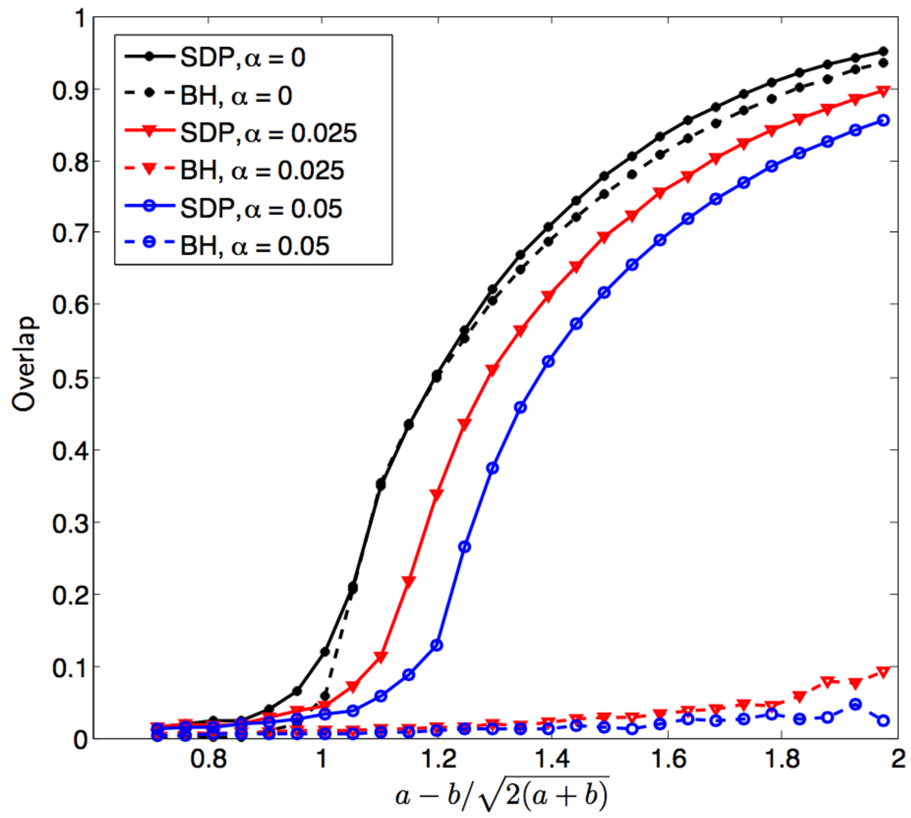


Figure taken from

[Javanmard/Montanari/Ricci-Tersenghi PNAS 16']

Community detection



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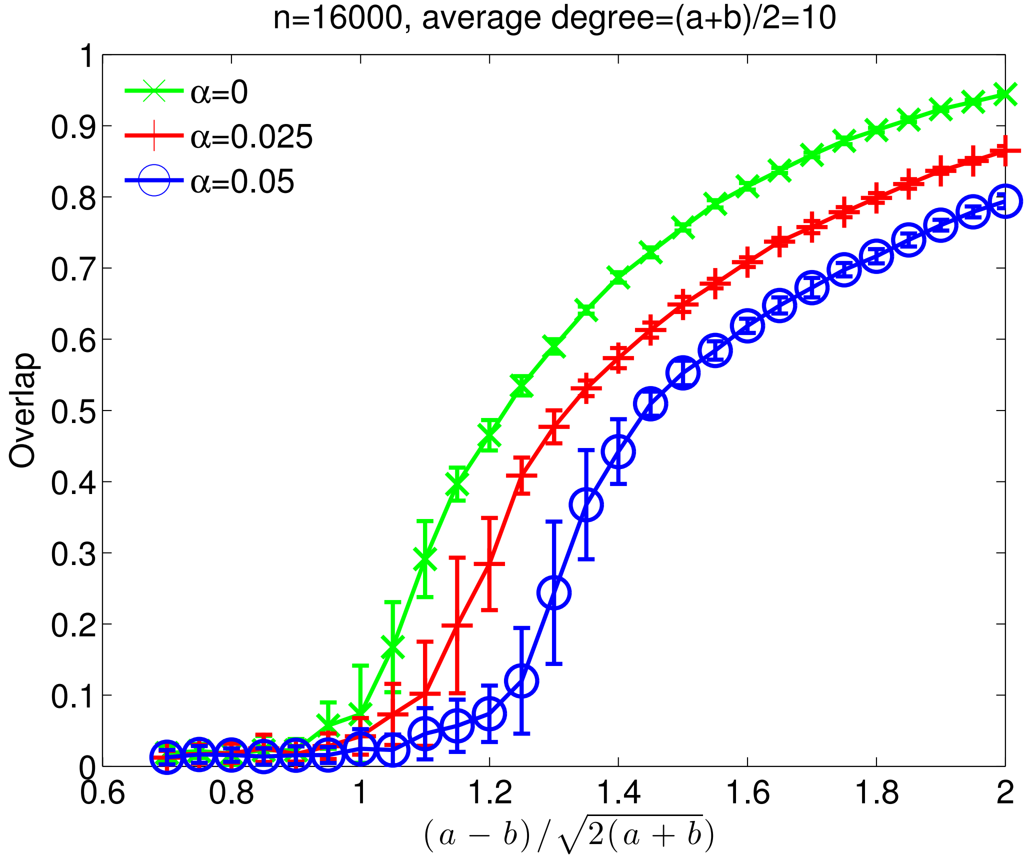


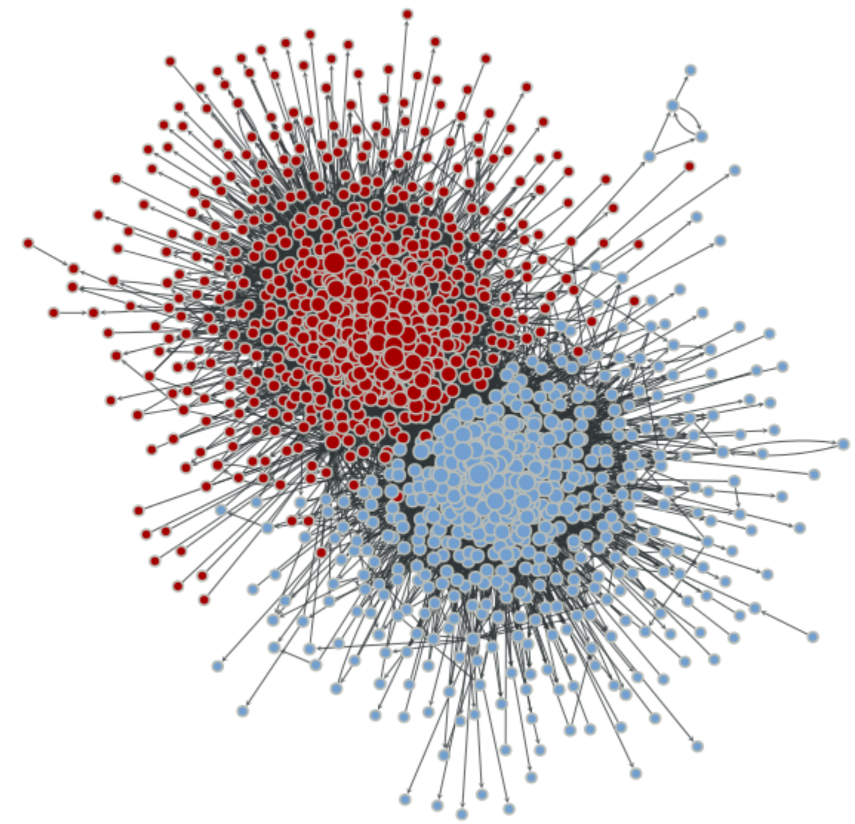
X-Laplacian

Community detection

Community detection

Network of political blogs

[Adamic/Glance 05']
1222 nodes, 16714 edges



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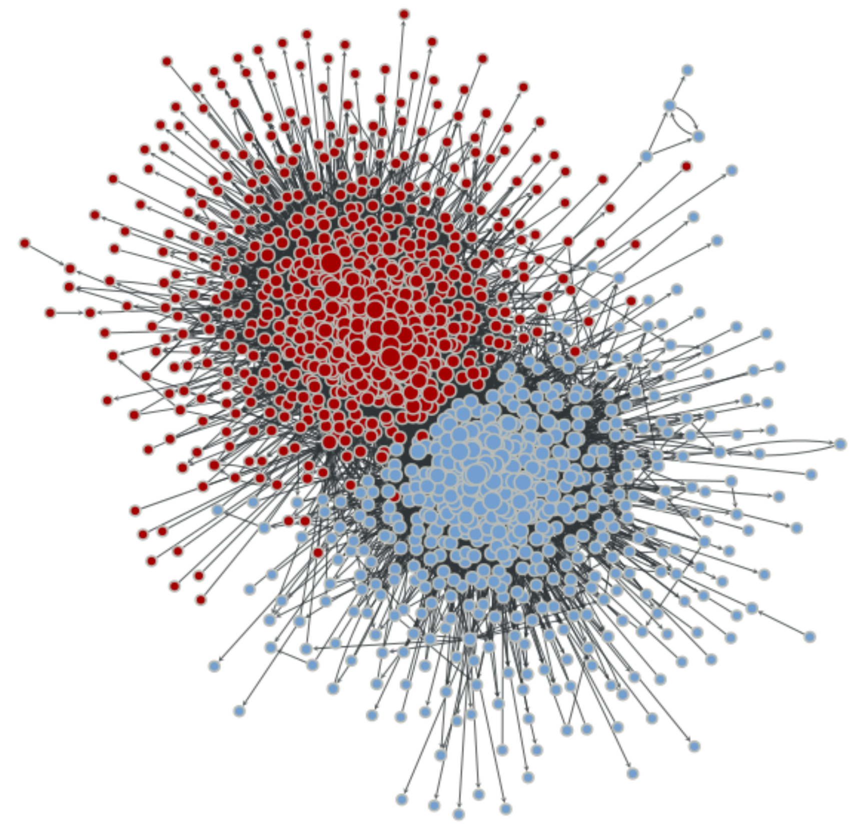

Method	
# Misclassified nodes	

Community detection

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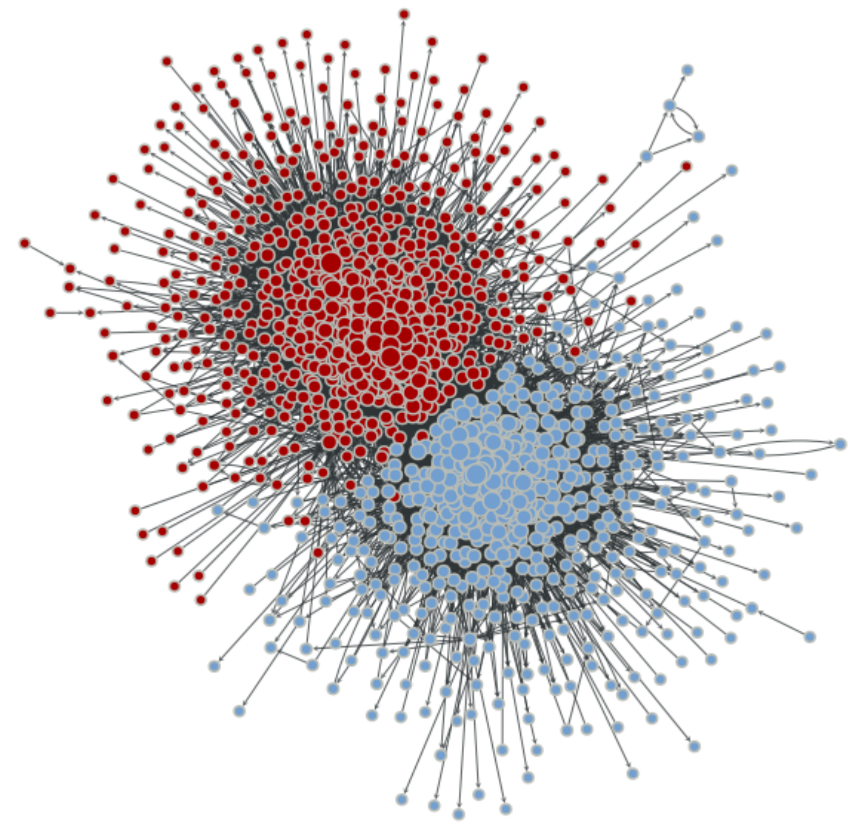

Method	Adjacency matrix
# Misclassified nodes	83

Community detection

Network of political blogs

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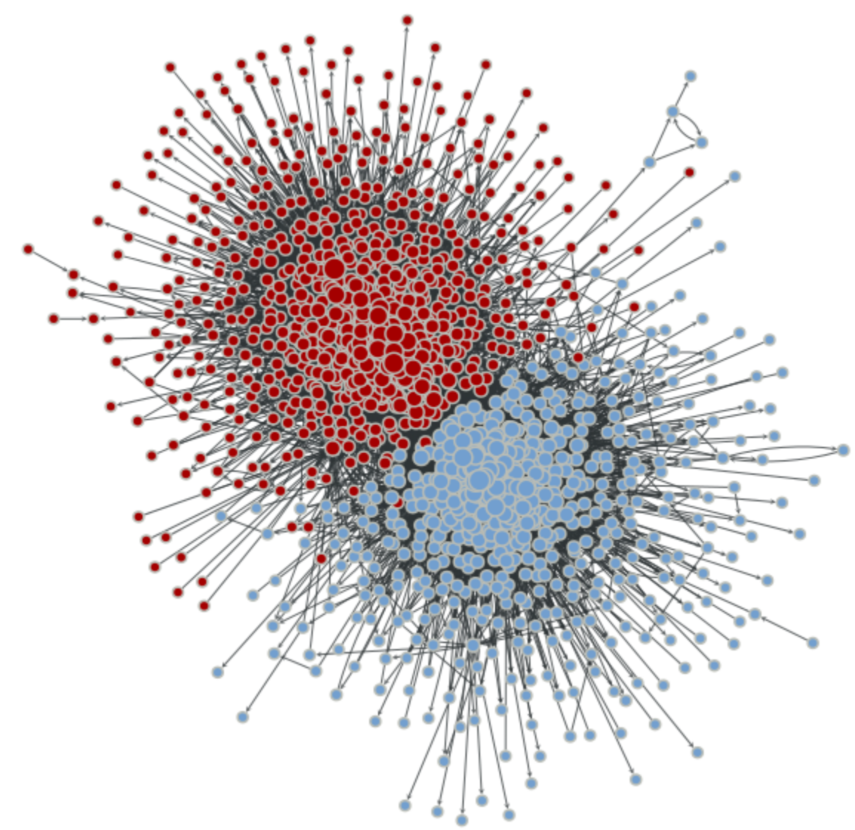

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']
# Misclassified nodes	83	80

Community detection

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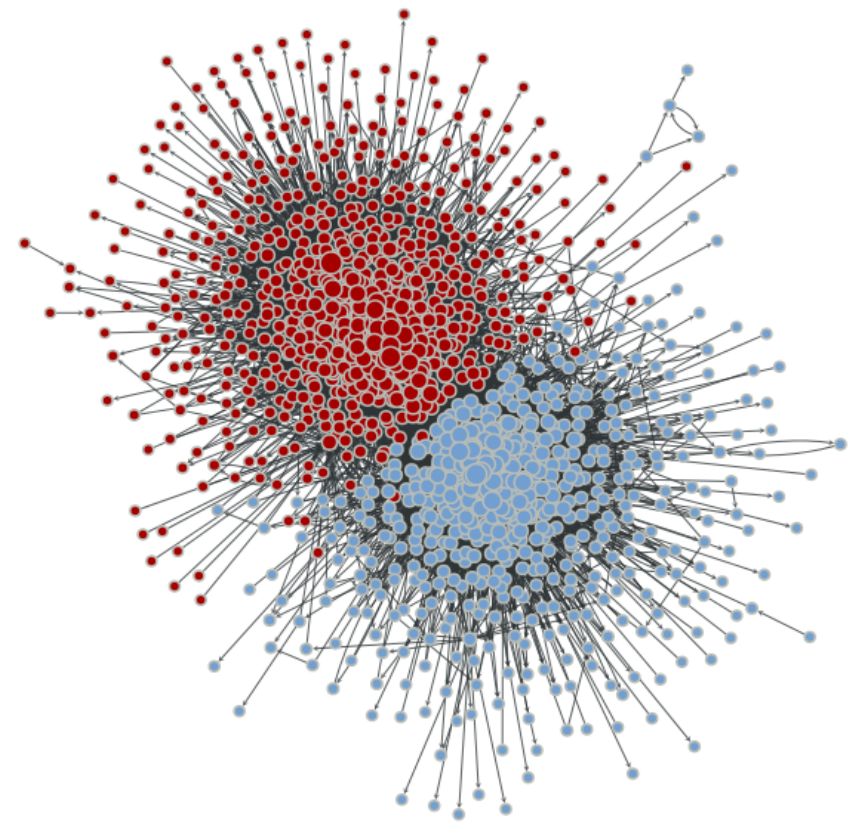

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']
# Misclassified nodes	83	80	63

Community detection

Network of political blogs

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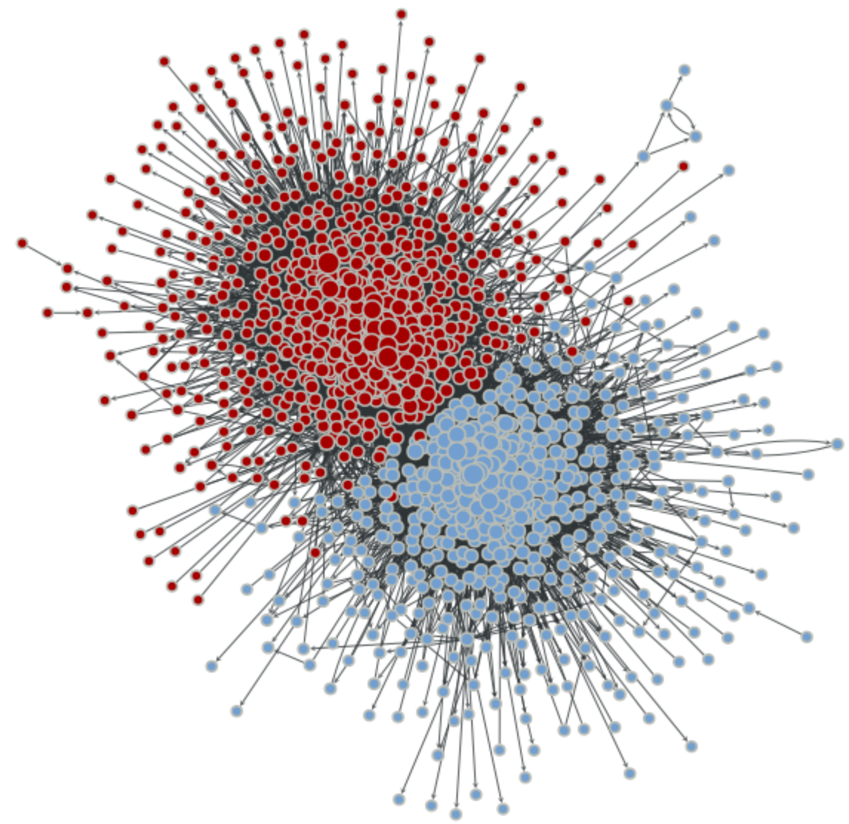

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmming [Cai/Li 13']
# Misclassified nodes	83	80	63	63

Community detection

Network of political blogs

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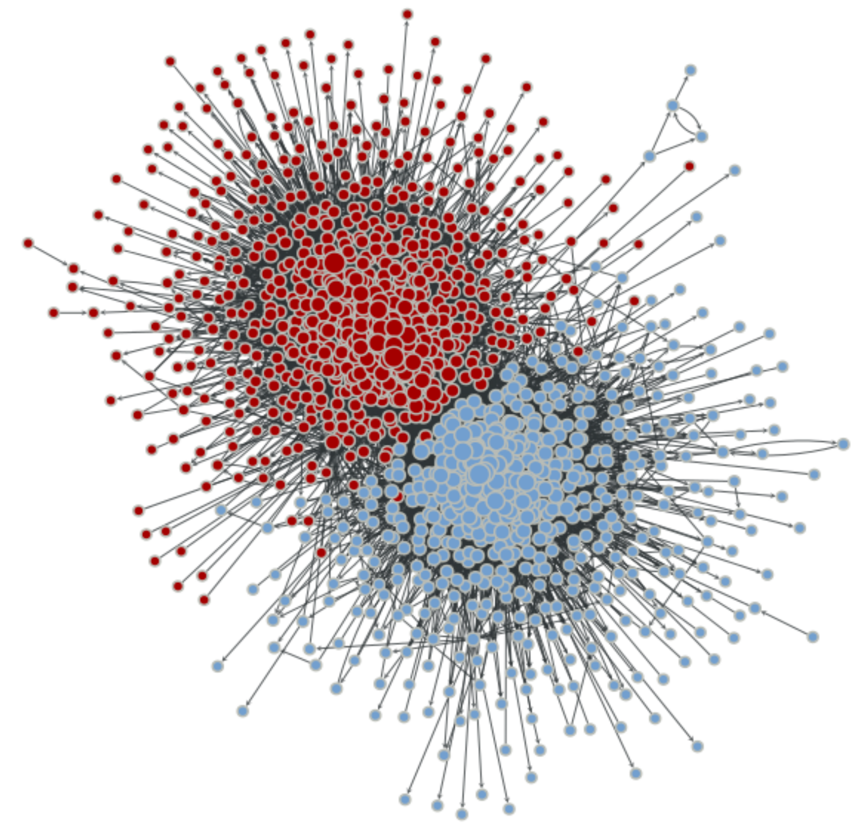

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmmin g [Cai/Li 13']	DCSBM BP
# Misclassified nodes	83	80	63	63	61

Community detection

Network of political blogs

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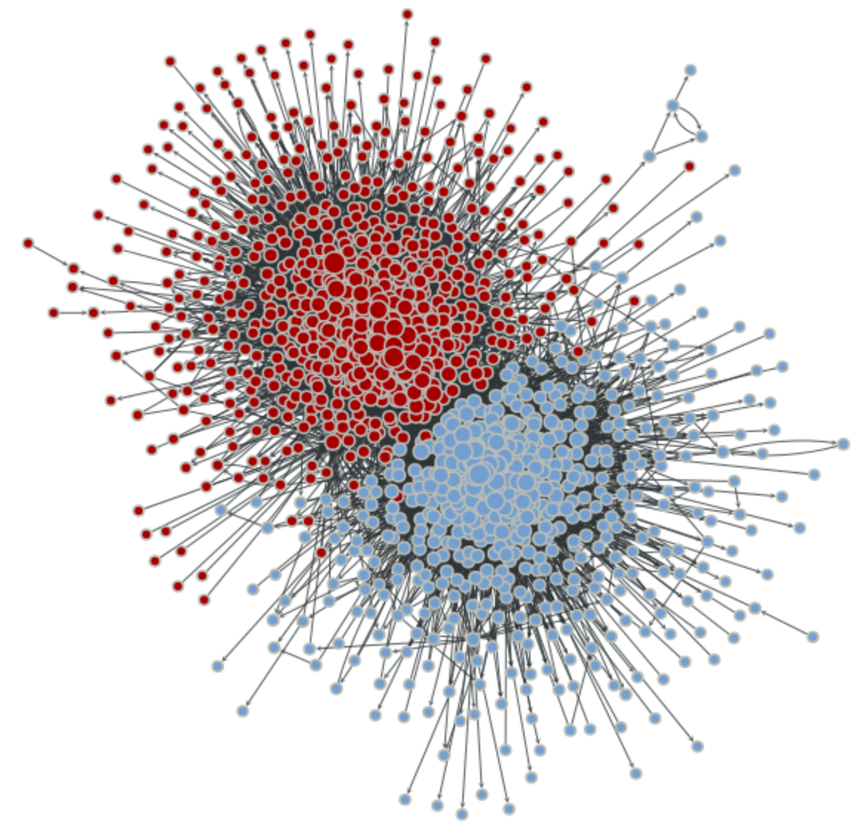

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmmin g [Cai/Li 13']	DCSBM BP	SCORE [Jin 15']
# Misclassified nodes	83	80	63	63	61	58

Community detection

Network of political blogs

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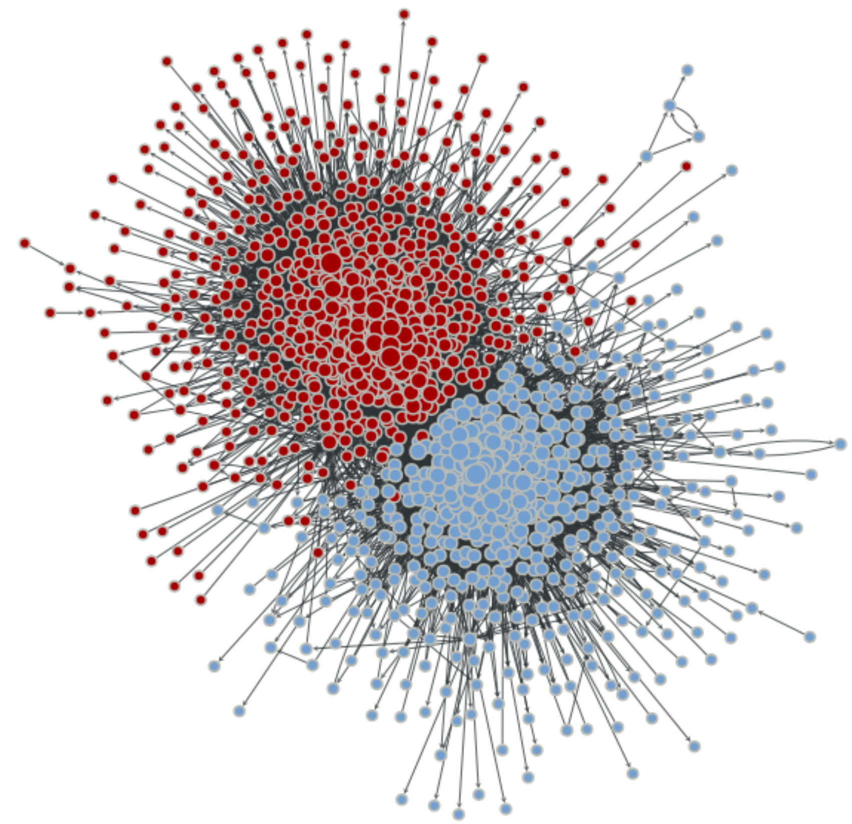

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmmin g [Cai/Li 13']	DCSBM BP	SCORE [Jin 15']
# Misclassified nodes	83	80	63	63	61	58

"Achieving Optimal Misclassification Proportion …"
[Gao et al. 15']

Community detection

Network of political blogs

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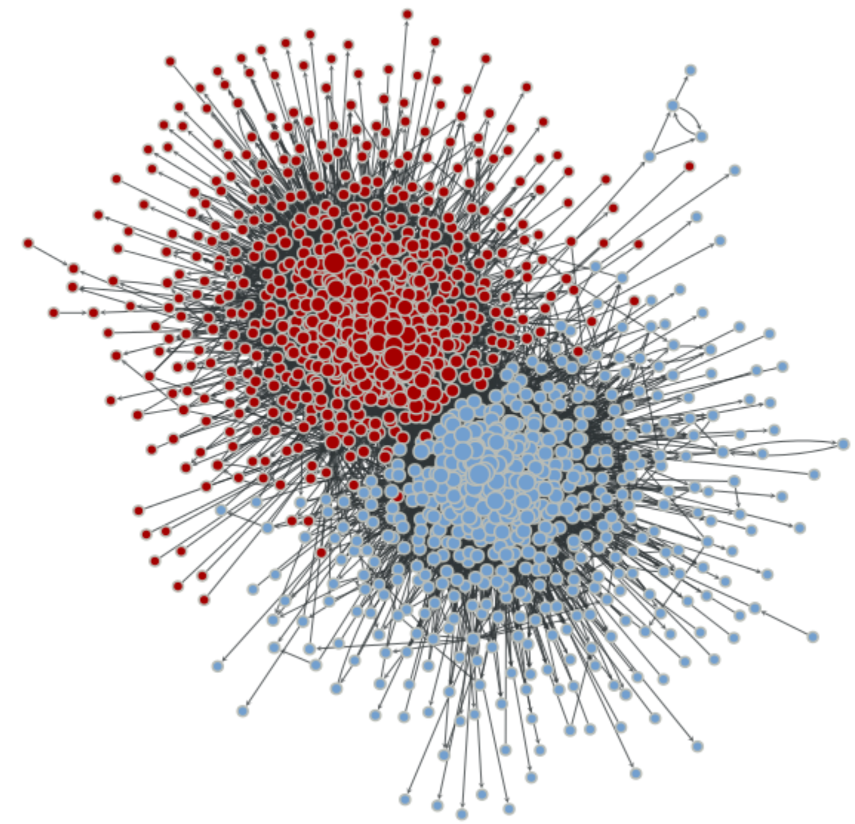

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmmin g [Cai/Li 13']	DCSBM BP	SCORE [Jin 15']	[Gao et al 15']
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Community detection

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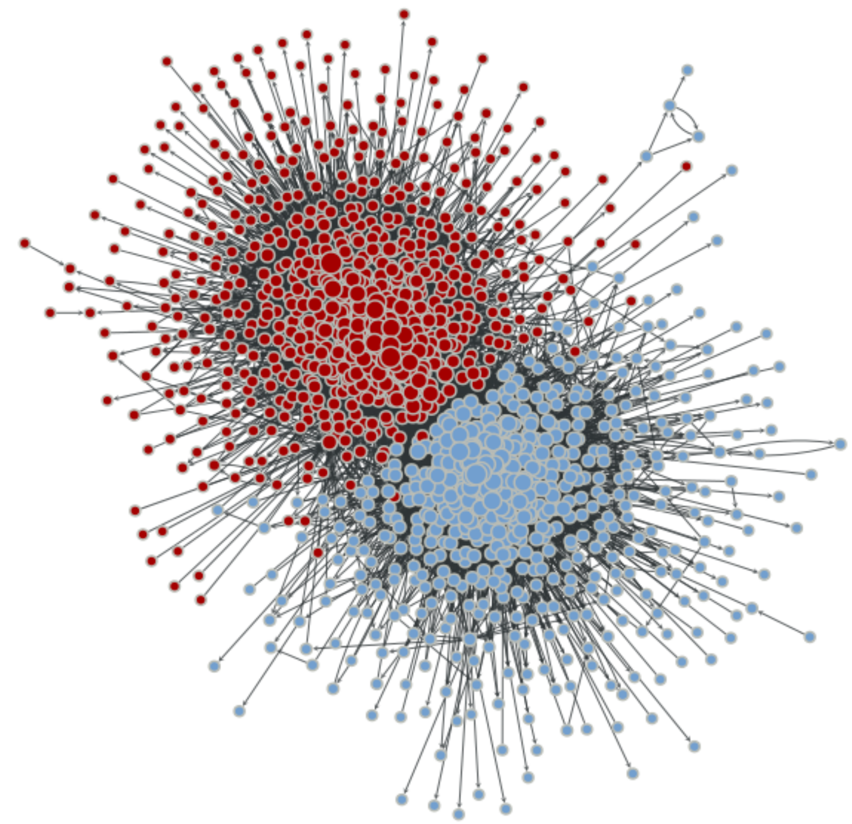

Method	Adjacency matrix	Reg.Spectral Clustering [Qin/Rohe 13']	Modularity BP [Zhang/Moore 14']	Semidefinite Progarmmin g [Cai/Li 13']	DCSBM BP	SCORE [Jin 15']	[Gao et al 15']	X-Laplacian
# Misclassified nodes	83	80	63	63	61	58	58	50

"Achieving Optimal Misclassification Proportion …"
[Gao et al. 15']

Community detection

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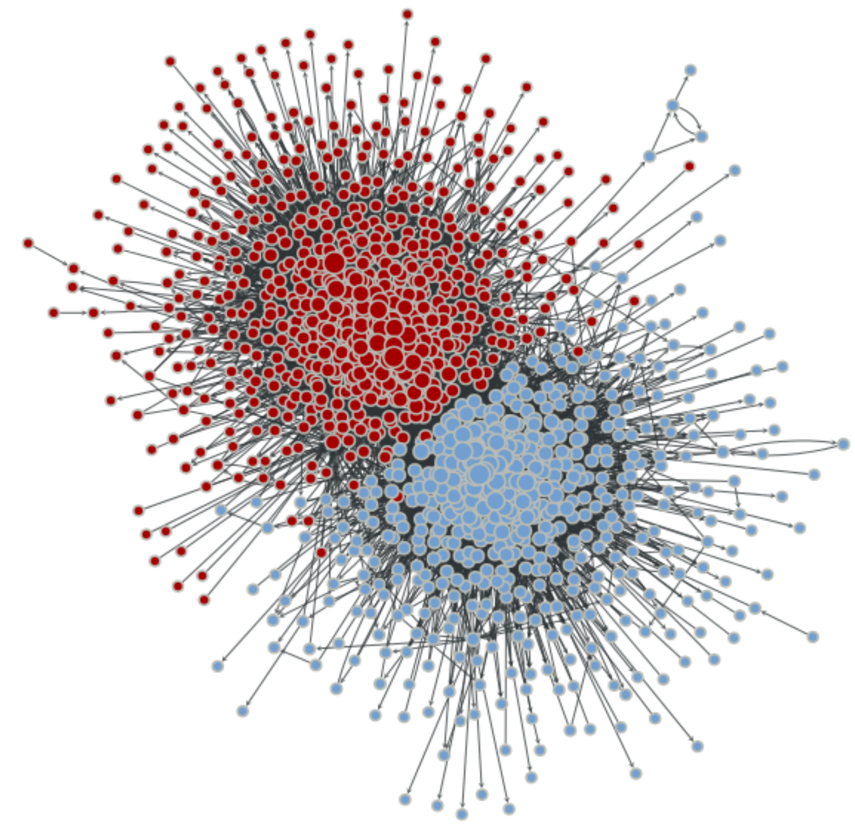

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Clustering from sparse similarities

Model from [Saade/Lelarge/Krzakala/Zdeborová ISIT 16']

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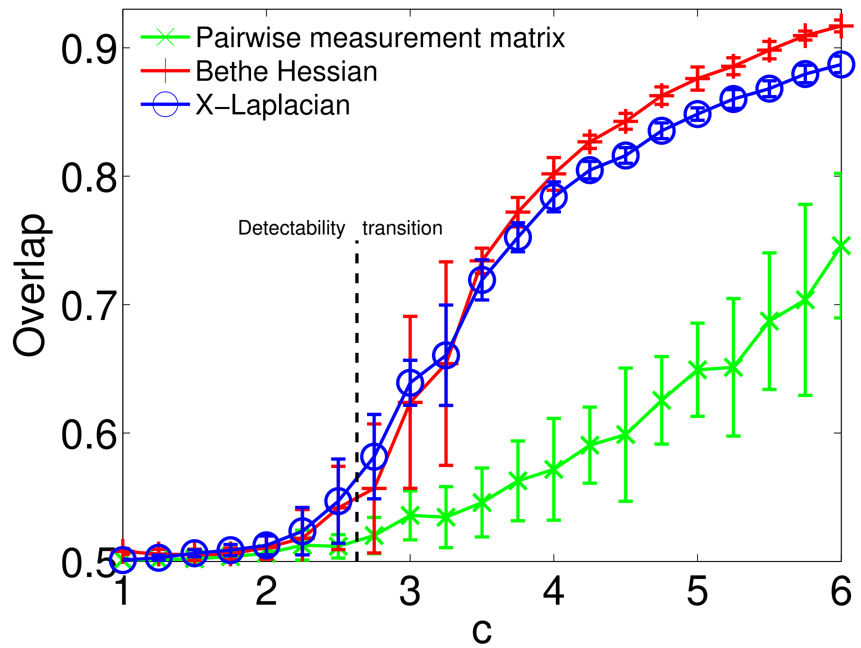
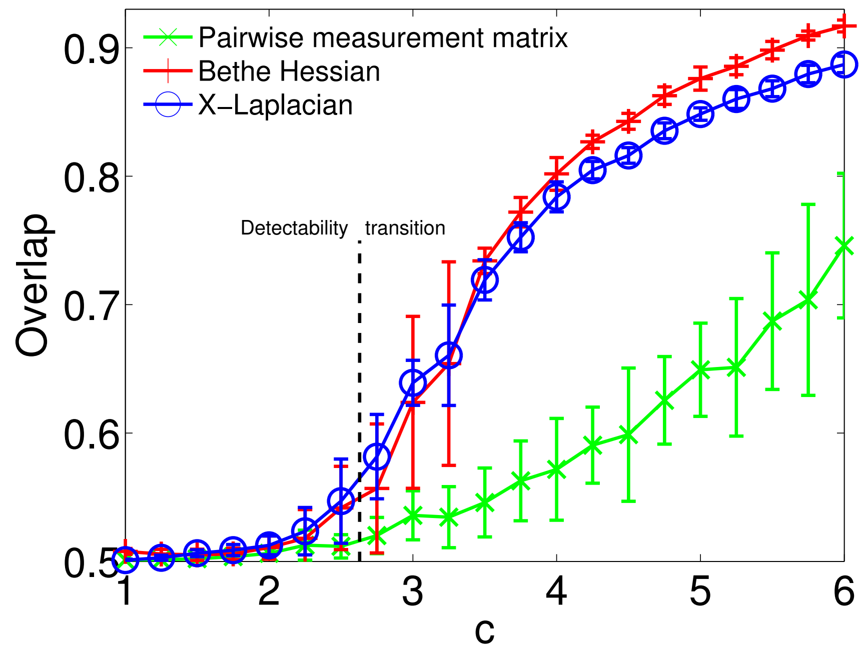


n=10000, q=2, Gaussian variance: 0.75, -0.75

Clustering from sparse similarities

Model from [Saade/Lelarge/Krzakala/Zdeborová ISIT 16']



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Bethe Hessian uses correct parameters, X-Laplacian does not.

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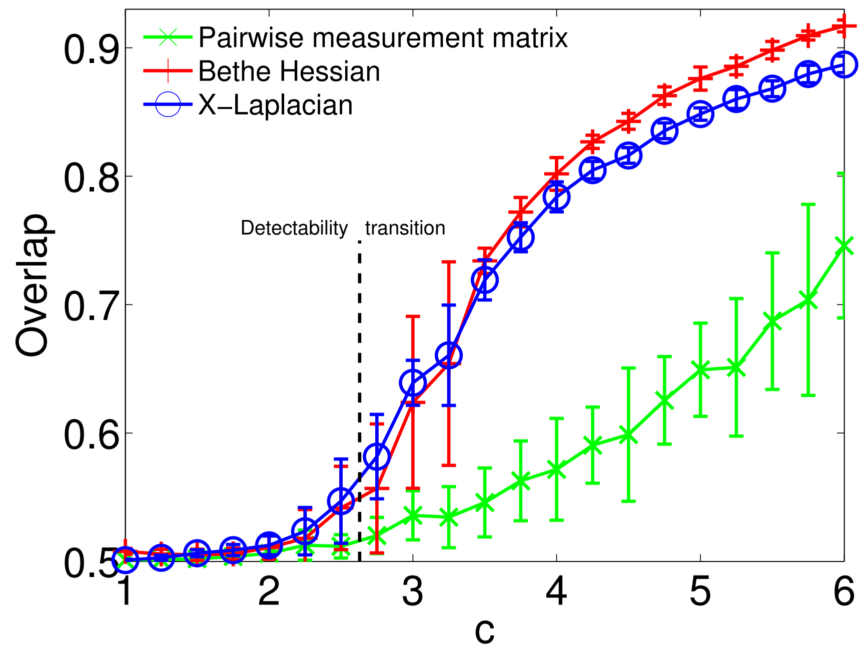

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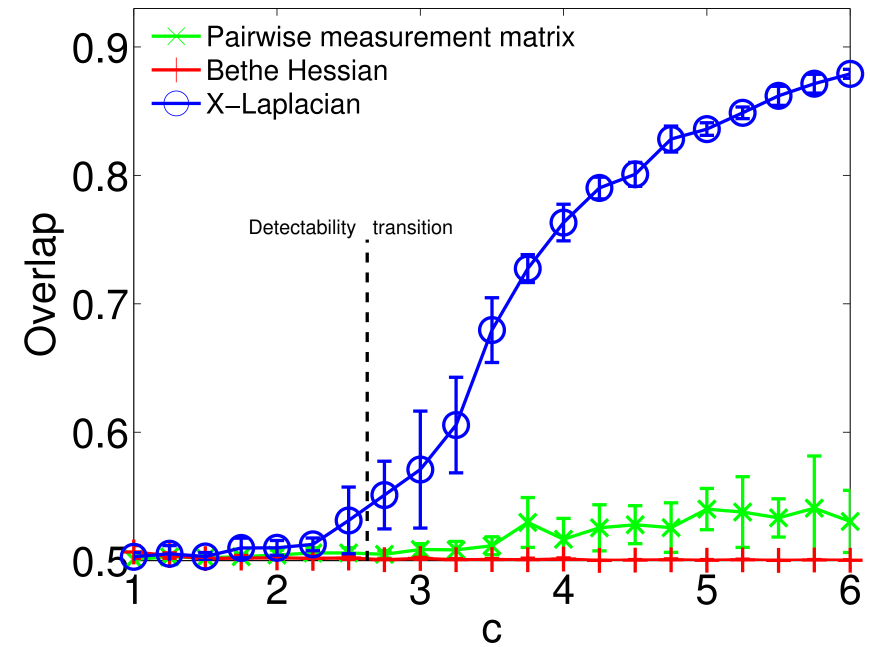
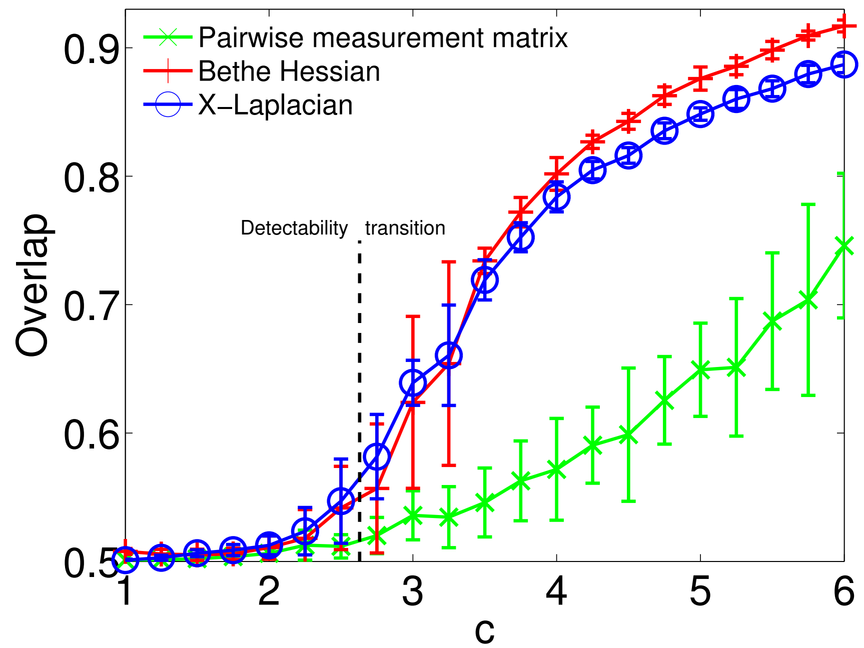


The same as left, but with cliques

Clustering from sparse similarities

Model from [Saade/Lelarge/Krzakala/Zdeborová ISIT 16']



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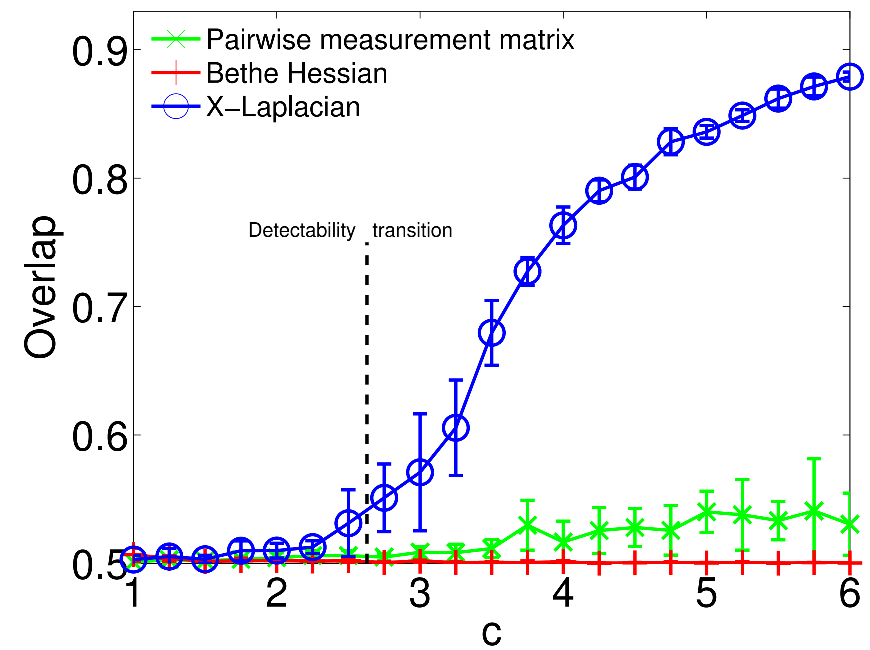
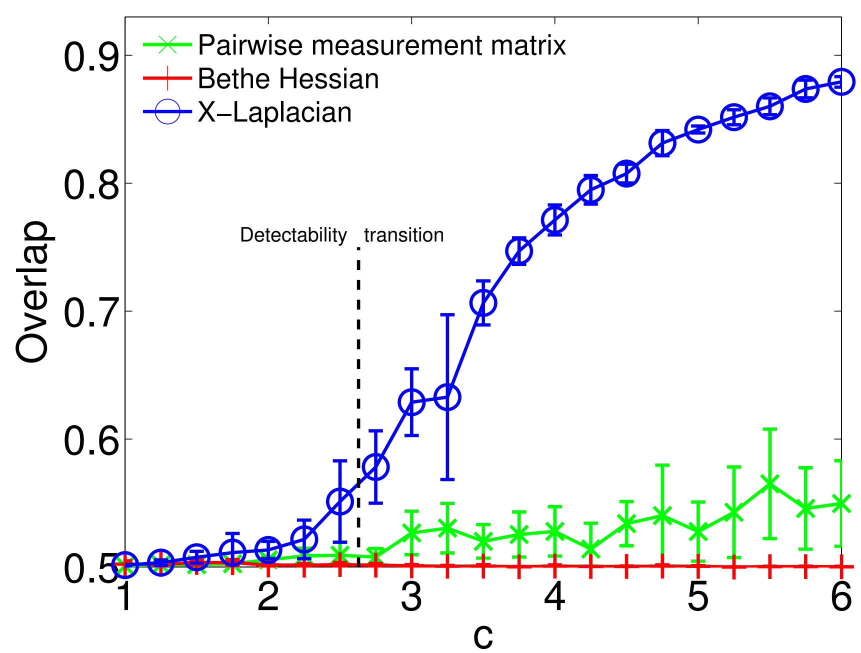


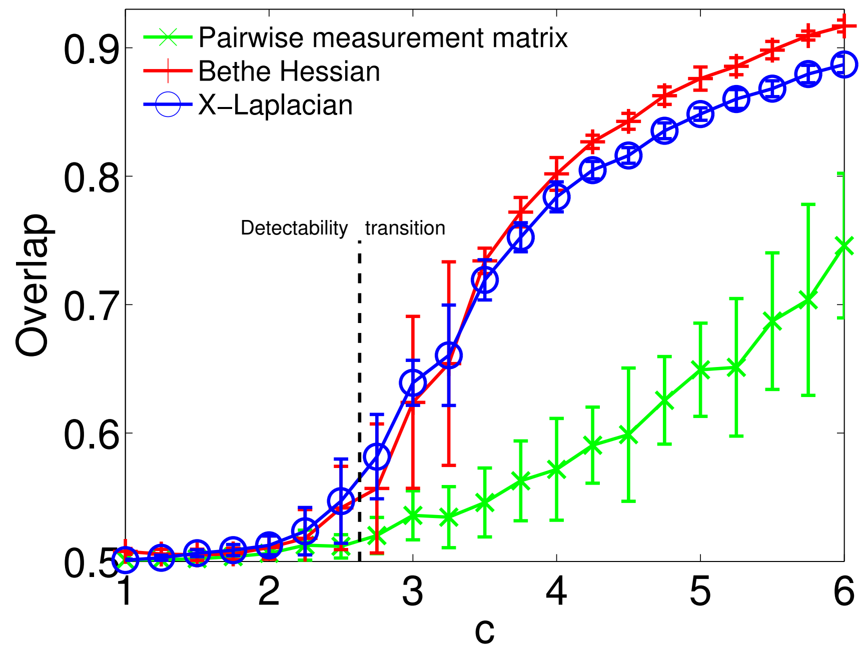
The same as left, but with cliques



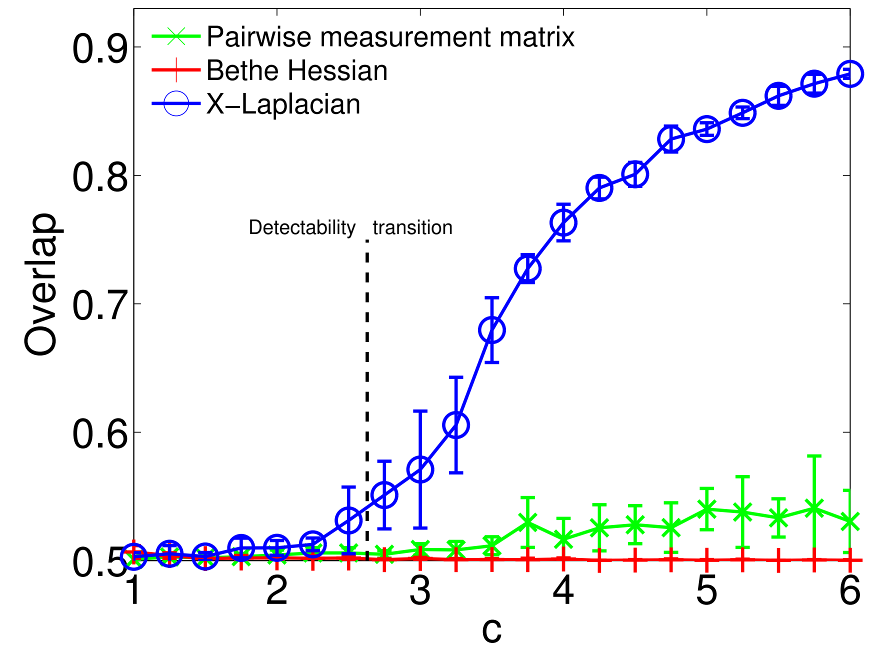
The same as top, but with hubs

Clustering from sparse similarities

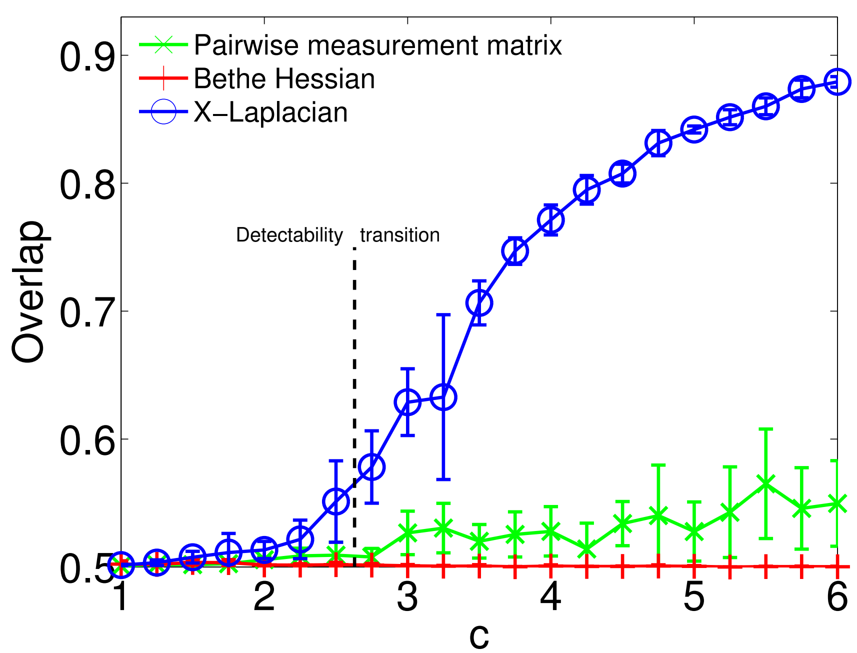
Model from [Saade/Lelarge/Krzakala/Zdeborová ISIT 16']



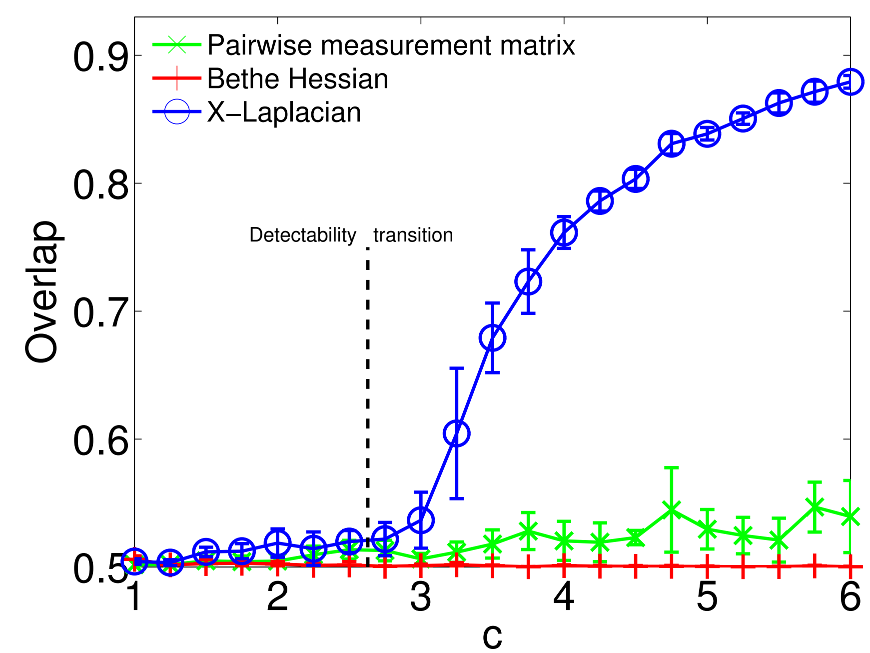
n=10000, q=2, Gaussian variance: 0.75, -0.75
Bethe Hessian uses correct parameters, X-Laplacian does not.



The same as left, but with cliques



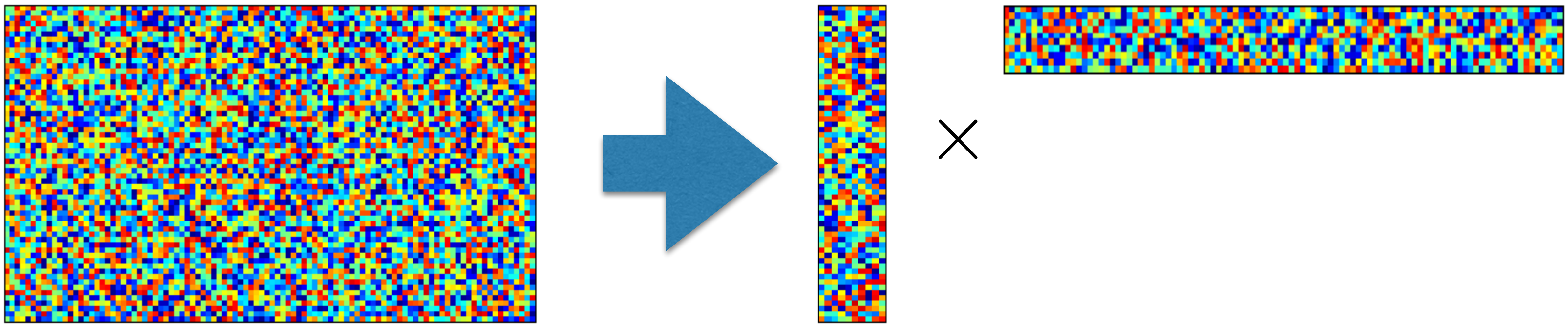
The same as top, but with hubs



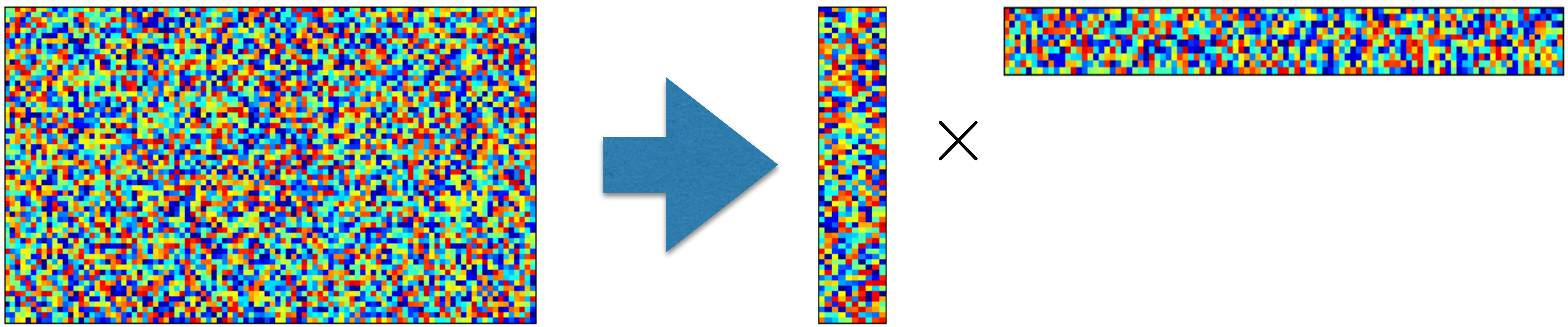
The same as top left, but with neighbors connected, as in [Javanmard/Montanari/Ricci-Tersenghi 16']

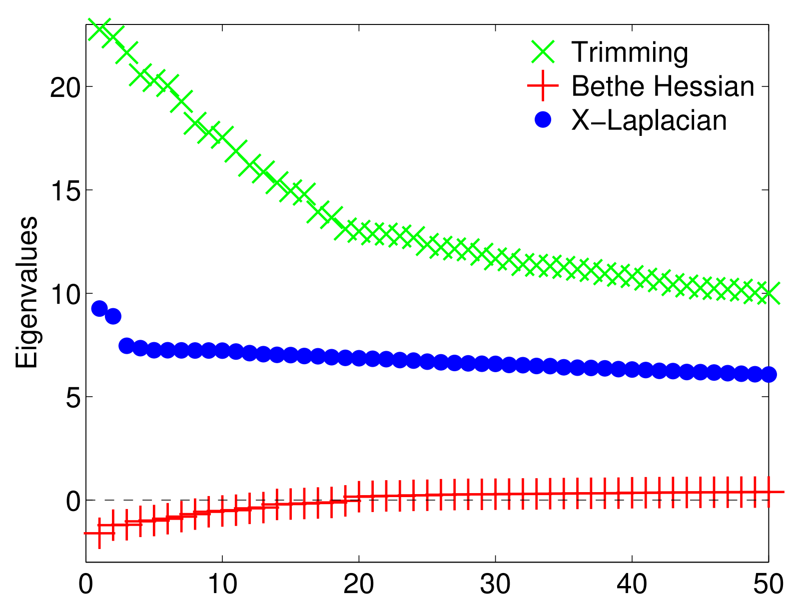
Rank estimation and matrix completion

Rank estimation and matrix completion



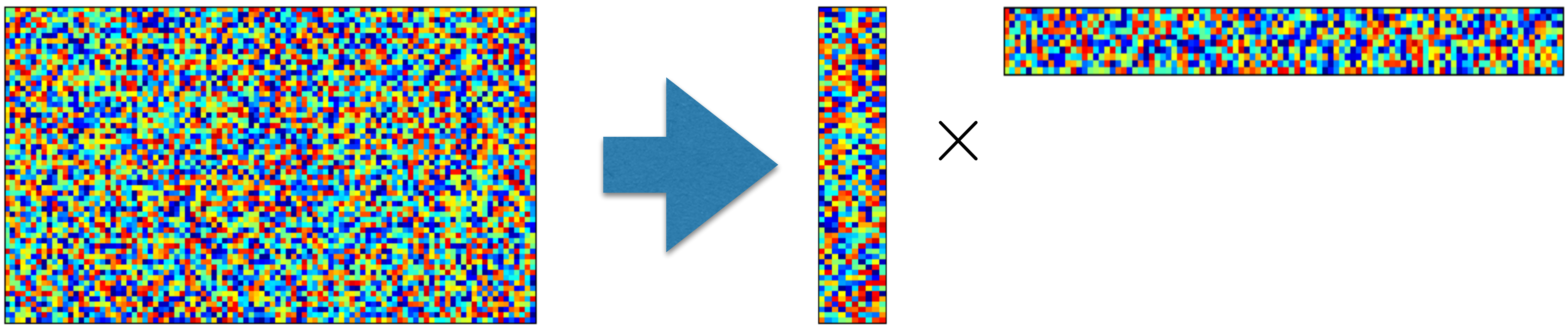
Rank estimation and matrix completion

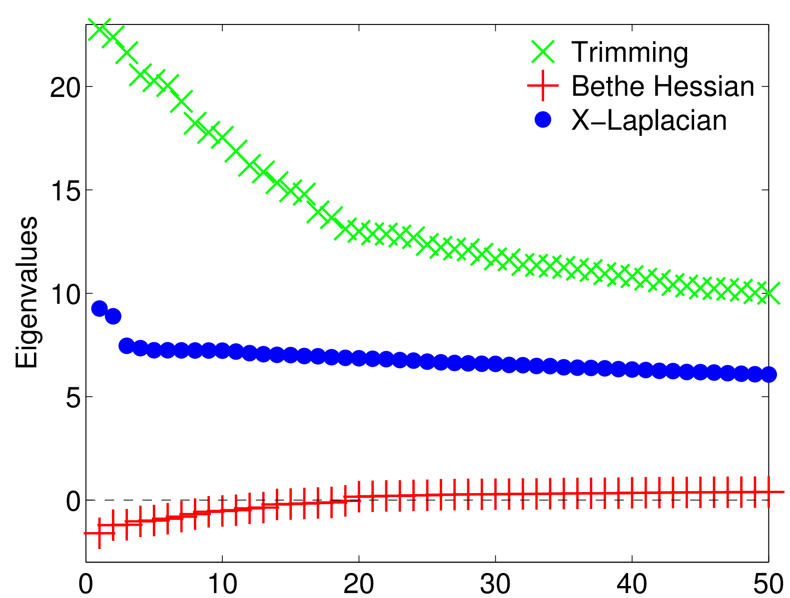




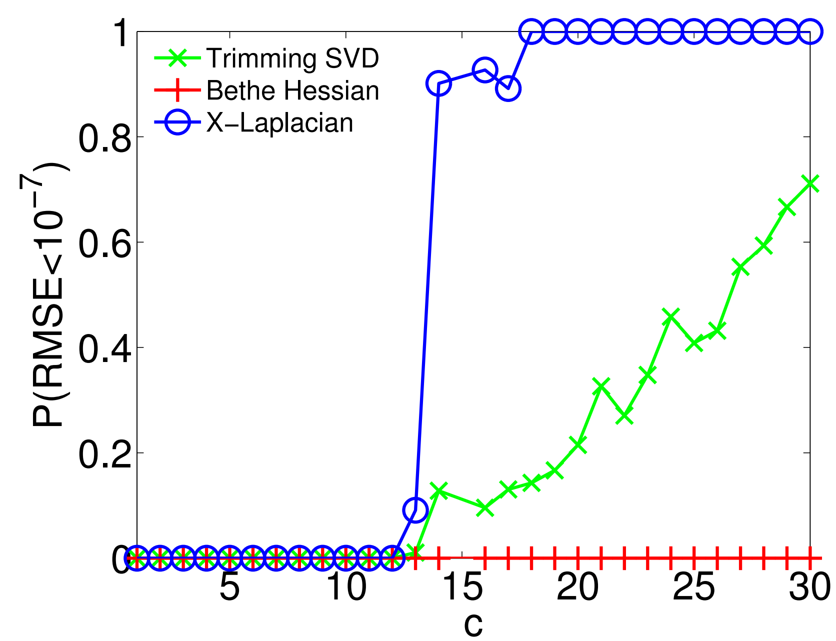
Original rank = 2
1000x10000 matrix, c=8, with 10 size-20 cliques

Rank estimation and matrix completion





Original rank = 2
1000x10000 matrix, c=8, with 10 size-20 cliques



Original rank = 3
1000x10000 matrix, with 10 size-20 cliques

Conclusions

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Conclusions

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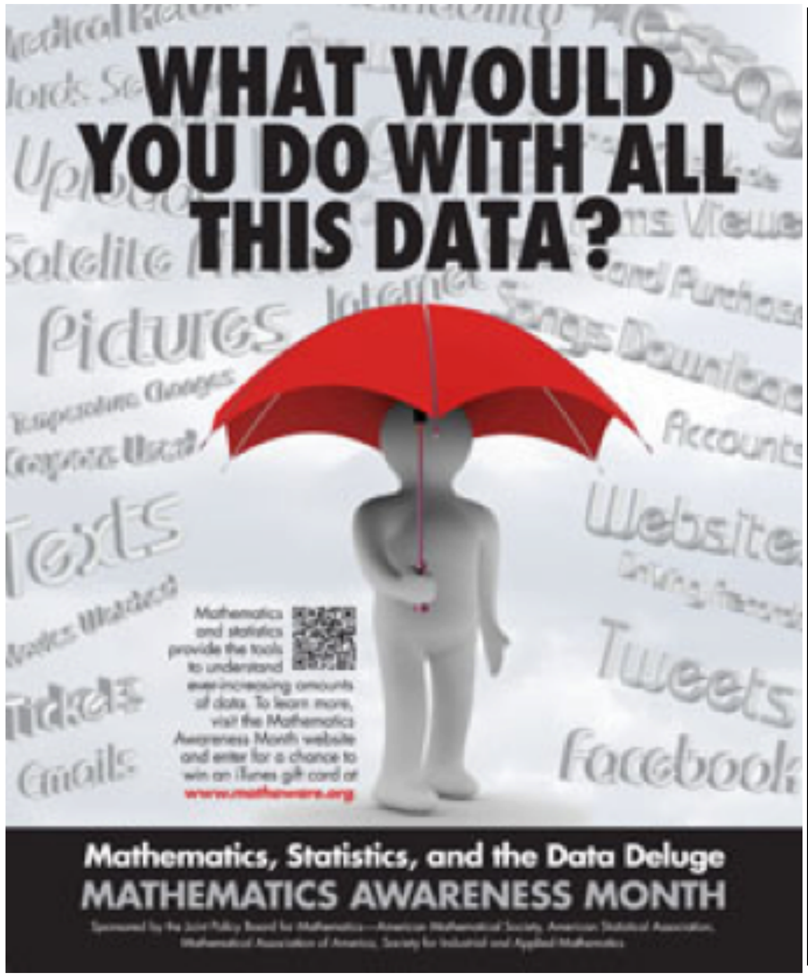
- Many methods for solving localization problem, e.g. trimming, non-backtracking, Bethe Hessian,… can be seen as doing regularizations.
- Fixed-form regularization works only when the source of localization is known.
- Good regularizations can be learnt from the localized eigenvectors.
  (Demo of the X-Laplacian can be found at http://panzhang.net)

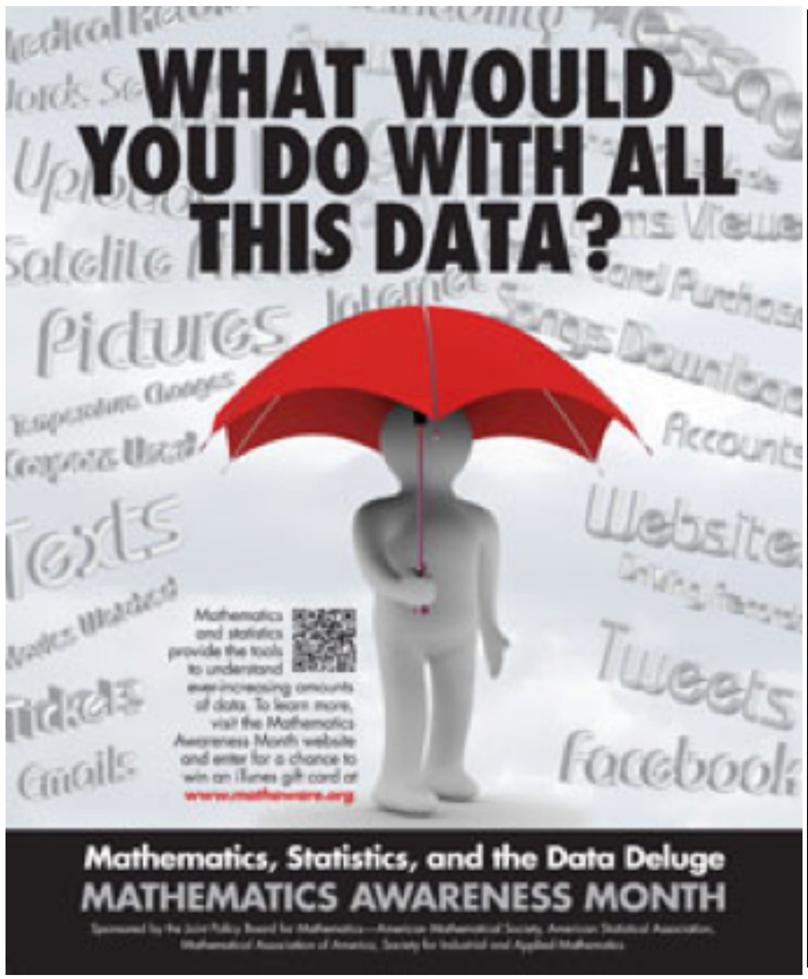
Thank you for your attention



We do it by Regularization!

Reference:
Pan Zhang, "Robust Spectral Detection of Global Structures in the Data by Learning a Regularization", *Advances In Neural Information Processing Systems 29*, 541 (2016)

Thank you for your attention



X-Laplacian

We do it by Regularization!

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