

Information-theoretic bounds and phase transitions in clustering, sparse PCA, and submatrix localization

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Joint work with Florent Krzakala (ENS) and Lenka Zdeborová (IPhT)
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Outline of the talk

- ① Sparse, spiked Wigner model
- ② Extensions
- ③ Conclusions and remarks

$$Y = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top + W$$

- λ is a fixed constant

Sparse, Spiked Wigner Model

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Sparse, Spiked Wigner Model

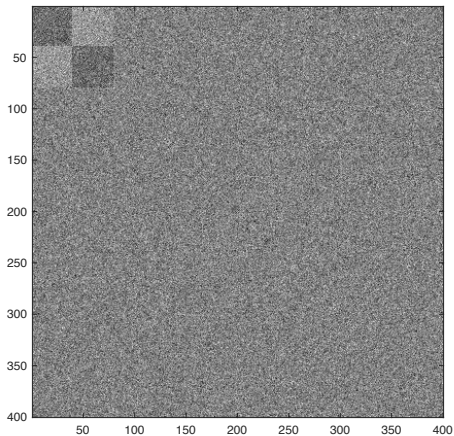
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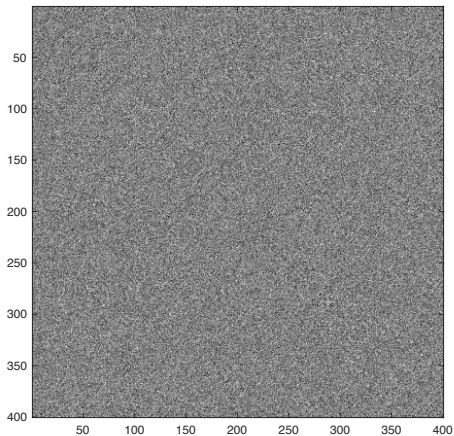
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- $v_i^* \stackrel{\text{i.i.d.}}{\sim} (1-p)\delta_0 + \frac{p}{2}\delta_1 + \frac{p}{2}\delta_{-1}$ for a fixed $p \in [0, 1]$
- $\|v^*\|_0 \approx np$: sparse level p



$$n = 400, p = 0.25, \lambda = 10$$

Of course not ordered



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Motivation 1: Sparse PCA

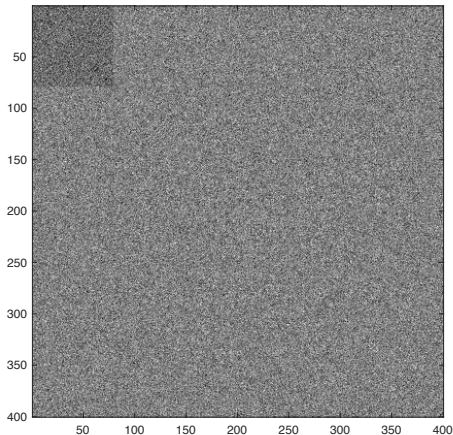
Sparse principal component analysis: [Johnstone-Lu 09], [Amini-Wainwright 09]...

$$Y = \frac{\lambda}{\sqrt{n}} u(v^*)^\top + W,$$

- $v^* \in \mathbb{R}^d$: **sparse principal component**
- W : Gaussian random matrix with i.i.d. entres

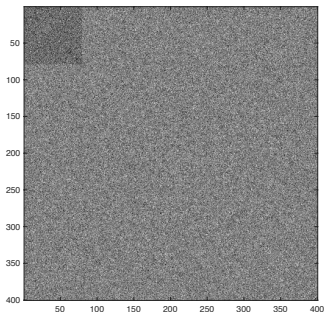
Motivation 2: Submatrix localization

Submatrix localization [Kolar-Balakrishnan-Rinaldo-Singh 11]
[Butucea-Ingster 13] ...

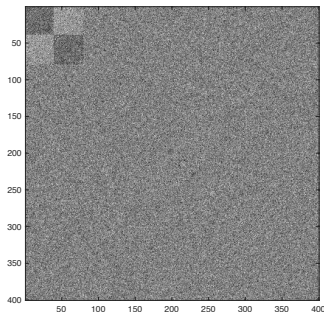


Motivation 2: Submatrix localization

Submatrix localization [Kolar-Balakrishnan-Rinaldo-Singh 11]
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Row sum statistic is informative



Row sum statistic is uninformative

Two statistical tasks

Focus on $\lambda = \Theta(1)$ and $p = \Theta(1)$

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- Estimation: $\mathbb{E} \left[\left(\frac{1}{n} \langle \hat{v}, v^* \rangle \right)^2 \right] \geq \epsilon$
- Detection:

$$\mathcal{H}_0 : Y = W \quad \text{v.s.} \quad \mathcal{H}_1 : Y = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top + W$$

Type-I + Type-II error probabilities $\rightarrow 0$

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Main Questions

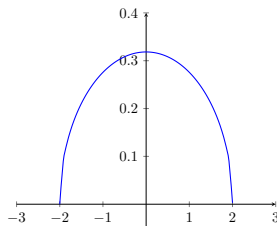
- When is estimation or detection **informationally possible**?
- Is IT-limit achievable in **polynomial-time**?

$$Y = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top + W$$

Prior work: Spectral phase transition [Péché 06]

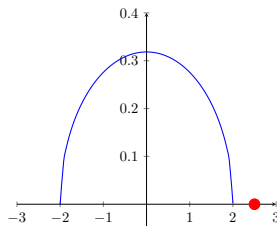
$$Y = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top + W$$

$$\lambda p \leq 1$$



$$\langle v_1(Y), v^* / \|v^*\|_2 \rangle^2 \rightarrow 0$$

$$\lambda p > 1$$



$$\langle v_1(Y), v^* / \|v^*\|_2 \rangle^2 \rightarrow 1 - (\lambda p)^{-2}$$

Approximate message passing algorithm: [Thouless-Anderson-Palmer 77]
[Rangan-Fletcher 12], [Deshpande-Montanari 14],
[Lesieur-Krzakala-Zdeborová 15]

Conjecture (Lesieur-Krzakala-Zdeborová 15)

There exists $p^ \in (0, 1)$ such that*

- ① *If $p \geq p^*$, then the IT limit is $\lambda p = 1$.*
- ② *If $p < p^*$, then the computational limit is $\lambda p = 1$, but the IT-limit is strictly lower.*

Upper bound to the IT-limit

Theorem (Banks-Moore-Vershynin-X. 16)

Detection and estimation are information-theoretically possible, if

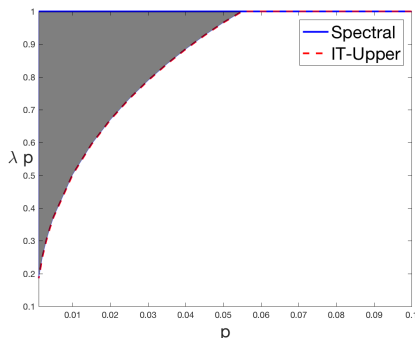
$$\lambda p > 2\sqrt{h(p) + p \log 2}$$

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IT-limit is below the spectral limit if $p \leq 0.054$.

Proof of upper bound: First moment method

Maximum likelihood estimation (MLE):

$$\begin{aligned}\hat{v} &\in \arg \max_v v^\top Y v \\ \text{s.t. } &\|v\|_0 \leq np(1 + \epsilon_n) \\ &v \in \{0, \pm 1\}^n\end{aligned}$$

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- Estimation: show $\frac{1}{n} |\langle \hat{v}, v^* \rangle| \geq \delta$; it suffices to show

$$\max_{v: |\langle v, v^* \rangle| \leq n\delta} v^\top Y v < (v^*)^\top Y v^*$$

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- Detection: show

$$\max_v v^\top Y v \text{ under } \mathcal{H}_0 < (v^*)^\top Y v^* \text{ under } \mathcal{H}_1$$

Theorem (Banks-Moore-Vershynin-X. 16)

Detection and estimation are information-theoretically impossible, if

$$\lambda p < \sqrt{2p \mathcal{W}\left(\frac{1-p}{2\sqrt{ep}}\right)}$$

where $\mathcal{W}(y)$ is the root x of $xe^x = y$.

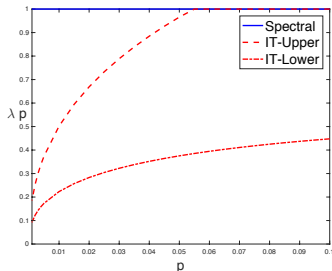
Lower bound to the IT-limit

Theorem (Banks-Moore-Vershynin-X. 16)

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When $p \rightarrow 0$

- **IT-upper limit:**

$$\lambda p > 2\sqrt{-p \log p} + O_p(p)$$

- **IT-lower limit:**

$$\lambda p < \sqrt{-2p \log p} - O_p(p)$$

- Closed the gap of $\sqrt{2}$ [Verzelen 16]

Theorem (Banks-Moore-Vershynin-X. 16)

Detection and estimation are information-theoretically impossible, if

$$\mathbb{E}_{Y \sim Q} \left[\left(\frac{P(Y)}{Q(Y)} \right)^2 \right] = O(1).$$

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- In sparse, spiked Wigner model,

$$\mathbb{E}_{Y \sim Q} \left[\left(\frac{P(Y)}{Q(Y)} \right)^2 \right] \approx \mathbb{E} \left[\exp \left(\frac{\lambda^2 R^2}{2n} \right) \right]$$

where R is a T -step, symmetric random walk, where $T \sim \text{Hyp}(n, np, p)$ [Cai-Ma-Wu 15].

Conjecture (Lesieur-Krzakala-Zdeborová 15)

$$\lim_{n \rightarrow \infty} \frac{1}{n} I(v^*; Y) = \min_{\alpha \in [0, p]} i_{\text{RS}}(\alpha; \lambda, p)$$

Moreover, let $\alpha^*(\lambda, p)$ denote the smallest minimizer. Then the IT-limit for estimation is $\lambda^*(p) = \inf\{\lambda : \alpha^*(\lambda, p) > 0\}$.

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Bethe mutual information i_{RS} (replica methods [Sherrington-Kirkpatrick 75] or cavity methods [Mezard-Parisi-Virasoro 86])

$$i_{\text{RS}}(\alpha) = \frac{\lambda^2(p^2 + \alpha^2)}{4} - \mathbb{E} \log \left(1 - p + p e^{-\alpha \lambda^2 / 2} \cosh(\alpha \lambda^2 \eta + \sqrt{\alpha} \lambda z) \right)$$

where $\eta \sim \text{Bern}(p)$ and $z \sim \mathcal{N}(0, 1)$

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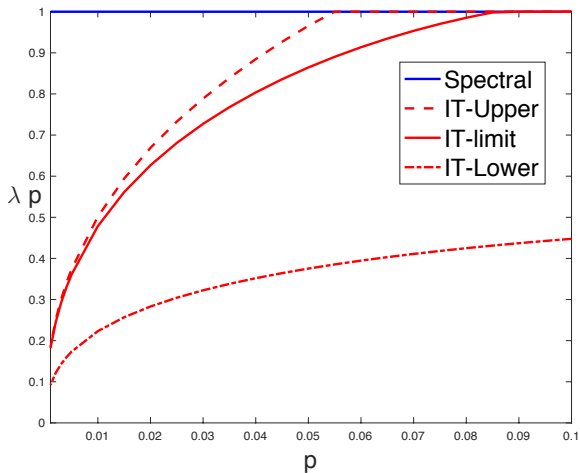
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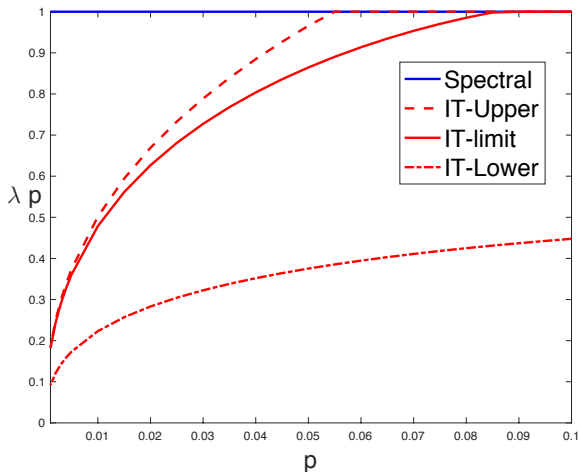
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The corner case $p = 1$ is proved in [Deshpande-Abbe-Montanari 15]

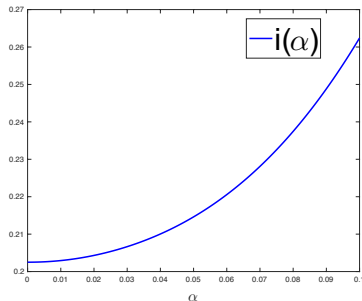




IT limit falls below spectral limit if $p \leq 0.085$. Why?

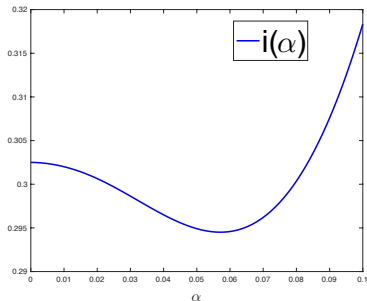
Statistical physics picture: dense regime ($p = 0.1$)

$\lambda p = 0.9$ (Below spectral limit)



$$\alpha^* = 0$$

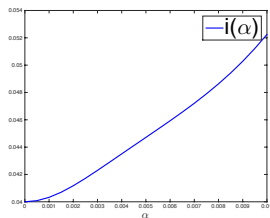
$\lambda p = 1.1$ (Above spectral limit)



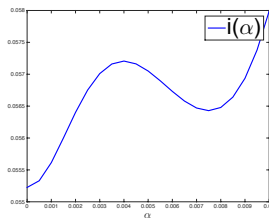
$$\alpha^* > 0$$

Statistical physics picture: sparse regime ($p = 0.01$)

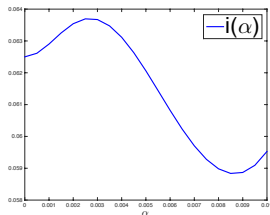
$\lambda p = 0.4$ (Uninformative)



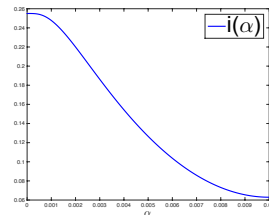
$\lambda p = 0.47$ (Uninformative: spinodal)



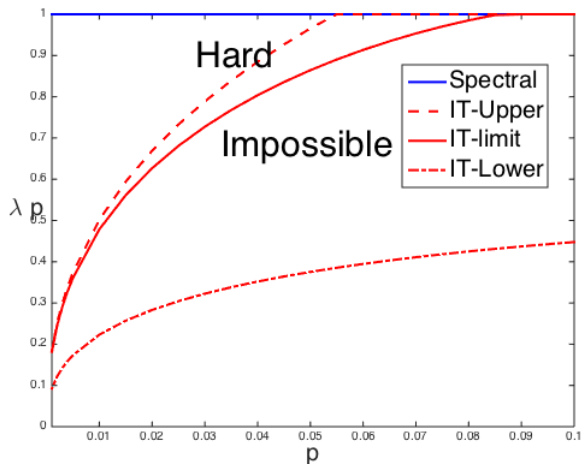
$\lambda p = 0.5$ (Informative: spinodal)



$\lambda p = 1.01$ (Above spectral limit)



Conjectured “possible but hard” regime [Lesieur-Krzakala-Zdeborová 15]



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- Upper bound holds for any finite n
- Asymptotic, matching lower bound is proved in [\[Barbier-Dia-Macris-Krzakala-Lesieur-Zdeborová 16\]](#) under the assumption that $i_{\text{RS}}(\alpha)$ has at most three stationary points

- A simple denoising model: $y = \sqrt{\alpha}\lambda v^* + w$, where $w \sim \mathcal{N}(0, \mathbf{I}_{n \times n})$

$$\frac{1}{n}I(v^*; y) = I(v_1^*; y_1) = i_{\text{RS}}(\alpha; \lambda, p) - \frac{(p - \alpha)^2 \lambda^2}{4}$$

Proof ideas: Interpolation method [Guerra 03]

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- Interpolating between the denoising model and the Wigner model

$$Y_t = \frac{\sqrt{t}\lambda}{\sqrt{n}}v^*(v^*)^\top + W$$
$$y_t = \sqrt{\alpha(1-t)}\lambda v^* + w$$

Let $I_t = I(v^*; Y_t, y_t)$. Then $I_0 = I(v^*; y)$ and $I_1 = I(v^*; Y)$.

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- Show that

$$\frac{1}{n} \frac{dI_t}{dt} \leq \frac{(p - \alpha)^2 \lambda^2}{4} \implies \frac{1}{n} I_1 \leq i_{\text{RS}}(\alpha; \lambda, p)$$

Outline of the talk

- ① Sparse, spiked Wigner model
- ② Extensions
- ③ Conclusions and remarks

Extension 1: general channel output and prior

$$X = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top \longrightarrow \boxed{p_{\text{out}}(y|x)} \longrightarrow Y$$

- $v_i \stackrel{\text{i.i.d.}}{\sim} p_{\text{prior}}$
- $Y_{ij} \stackrel{\text{i.i.d.}}{\sim} p_{\text{out}}(\cdot | X_{ij})$ for $i \leq j$
- p_{prior} and p_{out} are assumed to be independent of n

Theorem (Krzakala-X.-Zdeborová 16)

Suppose p_{prior} has a finite support and $\log p_{\text{out}}(y|x)$ satisfies some mild regularity conditions. Then

$$I(X; Y) = I(X; X + \sqrt{\Delta}W) + O(\sqrt{n})$$

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- The proof relies on Lindeberg's principle

Extension 2: High rank and asymmetric case

$$X = \frac{\text{snr}}{\sqrt{n}} \begin{bmatrix} U_1^\top \\ U_2^\top \\ \vdots \\ U_m^\top \end{bmatrix} \begin{bmatrix} V_1 & V_2 & \cdots & V_n \end{bmatrix} \longrightarrow \boxed{p_{\text{out}}(y|x)} \longrightarrow Y$$

- $U_i \in \mathbb{R}^k \stackrel{\text{i.i.d.}}{\sim} p_{\text{prior}}$ and $V_j \in \mathbb{R}^k \stackrel{\text{i.i.d.}}{\sim} q_{\text{prior}}$

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- Proposed in [\[Lesieur-Krzakala-Zdeborová 15\]](#)

Special case 1: Submatrix localization with k blocks

$$Y = \frac{\mu}{\sqrt{n}} \begin{array}{|c|c|c|} \hline 1 & & \\ \hline & 1 & 0 \\ \hline & 0 & 1 \\ \hline \end{array} + W$$

Special case 1: Submatrix localization with k blocks

$$Y = \frac{\mu}{\sqrt{n}} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 0 & \\ & 0 & & 1 \end{bmatrix} + W$$
$$= \frac{\mu}{\sqrt{n}} \begin{bmatrix} U_1^\top \\ U_2^\top \\ \vdots \\ U_n^\top \end{bmatrix} [U_1 \ U_2 \ \cdots \ U_n] + W$$

U_i is i.i.d. uniformly drawn from $\{e_1, \dots, e_k\}$

Upper and lower bounds for submatrix localization

Theorem

Let

$$\mu^{\text{up}} = 2k\sqrt{\frac{\log k}{k-1}}$$
$$\mu^{\text{low}} = k\sqrt{\frac{2\log(k-1)}{k-1}}$$

Then detection and reconstruction are information-theoretically possible when $\mu > \mu^{\text{up}}$ and impossible when $\mu < \mu^{\text{low}}$.

Upper and lower bounds for submatrix localization

Theorem

Let

$$\mu^{\text{up}} = 2k\sqrt{\frac{\log k}{k-1}}$$
$$\mu^{\text{low}} = k\sqrt{\frac{2\log(k-1)}{k-1}}$$

Then detection and reconstruction are information-theoretically possible when $\mu > \mu^{\text{up}}$ and impossible when $\mu < \mu^{\text{low}}$.

- When k is large, upper and lower bounds differ by a factor of $\sqrt{2}$
- When $k \geq 11$, IT limit is below the **spectral limit** $\mu^{\text{spectral}} = k$
- When $k = 2$, $\mu^{\text{low}} = \mu^{\text{spectral}} = \mu^{\text{IT}} = 2$

Special case 2: Gaussian mixture clustering with k clusters

$$Y_{m \times n} = \sqrt{\frac{\rho}{n}} \begin{array}{|c|} \hline v_1 - \bar{v} \\ \hline v_2 - \bar{v} \\ \hline \vdots \\ \hline v_k - \bar{v} \\ \hline \end{array} + W_{m \times n}$$

- $v_1, \dots, v_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \mathbf{I}_{n \times n})$ and $\bar{v} = (1/k) \sum_s v_s$

Special case 2: Gaussian mixture clustering with k clusters

$$Y_{m \times n} = \sqrt{\frac{\rho}{n}} \begin{array}{|c|} \hline v_1 - \bar{v} \\ \hline v_2 - \bar{v} \\ \hline \vdots \\ \hline v_k - \bar{v} \\ \hline \end{array} + W_{m \times n}$$

- $v_1, \dots, v_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \mathbf{I}_{n \times n})$ and $\bar{v} = (1/k) \sum_s v_s$
- Cluster center separation $\approx \sqrt{2n\rho}$
- Let $m = \alpha n$ for a fixed $\alpha > 0$

Upper and lower bounds for Gaussian mixture clustering

Theorem

Let

$$\rho^{\text{up}} = \frac{2k}{k-1} \left(\sqrt{\frac{k \log k}{\alpha}} + \log k \right)$$
$$\rho^{\text{low}} = k \sqrt{\frac{2 \log(k-1)}{(k-1)\alpha}}$$

Then detection and reconstruction are possible when $\rho > \rho^{\text{up}}$ and impossible when $\rho < \rho^{\text{low}}$.

Upper and lower bounds for Gaussian mixture clustering

Theorem

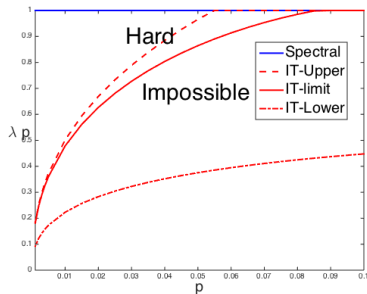
Let

$$\rho^{\text{up}} = \frac{2k}{k-1} \left(\sqrt{\frac{k \log k}{\alpha}} + \log k \right)$$
$$\rho^{\text{low}} = k \sqrt{\frac{2 \log(k-1)}{(k-1)\alpha}}$$

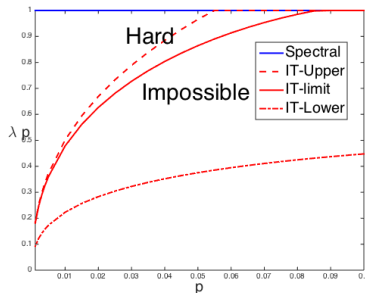
Then detection and reconstruction are possible when $\rho > \rho^{\text{up}}$ and impossible when $\rho < \rho^{\text{low}}$.

- When k is large, upper and lower bounds differ by a factor of $\sqrt{2}$
- When $k \geq 26$, IT limit is below the **spectral limit** $\rho^{\text{spectral}} = \frac{k}{\sqrt{\alpha}}$
- When $k = 2$, $\rho^{\text{low}} = \rho^{\text{spectral}} = \rho^{\text{IT}} = \frac{2}{\sqrt{\alpha}}$

Conclusion and remarks

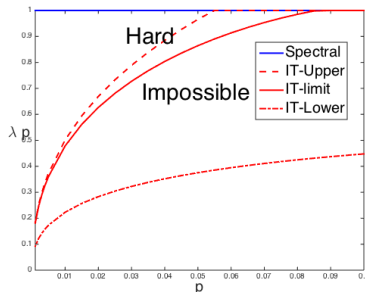


Conclusion and remarks



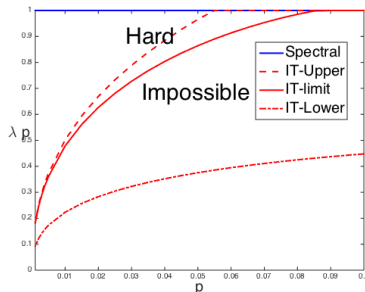
- First and second moment method: powerful tools to locate IT-limit [Abbe-Sandon 15] [Banks-Moore-Neeman-Netrapalli 16]

Conclusion and remarks



- First and second moment method: powerful tools to locate IT-limit [Abbe-Sandon 15] [Banks-Moore-Neeman-Netrapalli 16]
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Conclusion and remarks

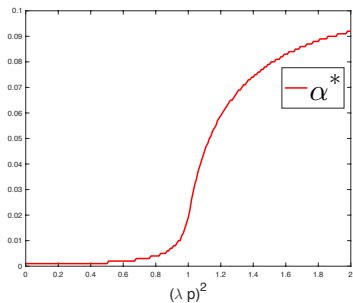
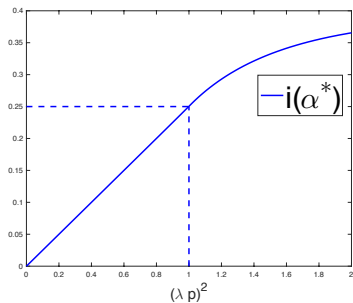


- First and second moment method: powerful tools to locate IT-limit [Abbe-Sandon 15] [Banks-Moore-Neeman-Netrapalli 16]
- Channel universality and Interpolation method
- Open question: computational limit?

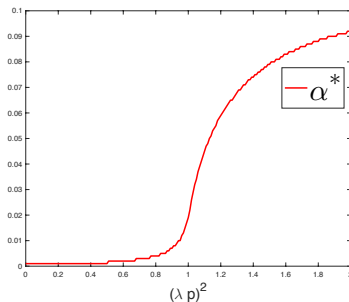
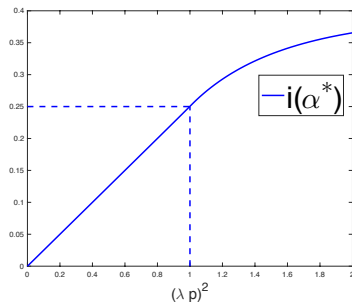
References

- J. Banks & C. Moore & R. Vershynin & J. X. (2016). *Information-theoretic bounds and phase transitions in clustering, sparse PCA, and submatrix localization*. [arXiv:1607.05222](#)
- F. Krzakala & J. X. & L. Zdeborová (2016). *Mutual Information in Rank-One Matrix Estimation*. [arXiv:1603.08447](#) (ITW '16)

Dense regime: $p = 0.1$



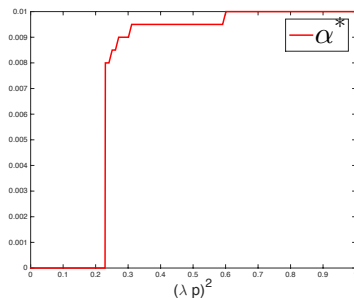
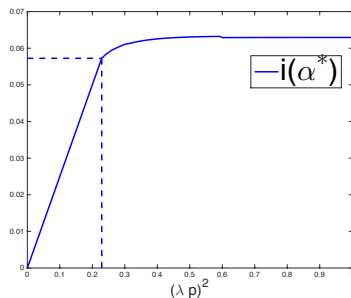
Dense regime: $p = 0.1$



Second-order phase transition: discontinuity of 2nd derivative of $i_{RS}(\alpha^*)$

IT limit coincides with spectral limit; similar to binary symmetric SBM

Sparse regime: $p = 0.01$



First-order phase transition: discontinuity of 1st derivative of $i_{RS}(\alpha^*)$

IT limit falls below spectral limit; similar to SBM with $k > 4$ communities