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

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Outline of the talk

1. Sparse, spiked Wigner model
2. Extensions
3. Conclusions and remarks
Sparse, Spiked Wigner Model

\[ Y = \frac{\lambda}{\sqrt{n}} v^*(v^*)^T + W \]

- \( \lambda \) is a fixed constant
Sparse, Spiked Wigner Model

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

- \( \lambda \) is a fixed constant
- \( W_{ii} \) i.i.d. \( \sim \mathcal{N}(0, 2) \) and \( W_{ij} = W_{ji} \) i.i.d. \( \sim \mathcal{N}(0, 1) \) for \( i < j \)
Sparse, Spiked Wigner Model

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- \( W_{ii} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 2) \) and \( W_{ij} = W_{ji} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \) for \( i < j \)
- \( v^*_i \overset{\text{i.i.d.}}{\sim} (1 - p) \delta_0 + \frac{p}{2} \delta_1 + \frac{p}{2} \delta_{-1} \) for a fixed \( p \in [0, 1] \)
Sparse, Spiked Wigner Model

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- \( v_i^* \overset{\text{i.i.d.}}{\sim} (1 - p)\delta_0 + \frac{p}{2}\delta_1 + \frac{p}{2}\delta_{-1} \) 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

\[ n = 400, \ p = 0.25, \ \lambda = 10 \]
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] ...

Row sum statistic is informative

Row sum statistic is uninformative
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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:

  $$H_0 : Y = W \quad \text{v.s.} \quad H_1 : Y = \frac{\lambda}{\sqrt{n}} v^*(v^*)^\top + W$$

  Type-I + Type-II error probabilities $\to 0$
Two statistical tasks

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

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

- **Detection**:

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

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

**Main Questions**

- When is estimation or detection **informationally possible**?
- Is IT-limit achievable in **polynomial-time**?
Prior work: Spectral phase transition [Péché 06]

\[
Y = \frac{\lambda}{\sqrt{n}} v^* (v^*)^\top + W
\]
Prior work: Spectral phase transition [Péché 06]

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

\[ \lambda p \leq 1 \]

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

\[ \lambda p > 1 \]

\[ \langle v_1(Y), v^*/\|v^*\|_2 \rangle^2 \rightarrow 1 - (\lambda p)^{-2} \]
Prior work: Approximate message passing

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.
Detection and estimation are information-theoretically possible, if

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

IT-limit is below the spectral limit if \( p \leq 0.054 \).
Proof of upper bound: First moment method

Maximum likelihood estimation (MLE): \[
\hat{v} \in \arg \max_v v^\top Y v \\
\text{s.t. } \|v\|_0 \leq np(1 + \epsilon_n) \\
v \in \{0, \pm 1\}^n
\]
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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

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Detection and estimation are information-theoretically impossible, if

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

When $p \to 0$

- **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]
Proof of lower bound: Second moment method

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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- For estimation, it holds for Gaussian noise model (I-MMSE formula)
- 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)

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

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

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

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

where \( \eta \sim \text{Bern}(p) \) and \( z \sim \mathcal{N}(0, 1) \)
Conjectured IT-limit

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The corner case \( p = 1 \) is proved in [Deshpande-Abbe-Montanari 15]
The IT limit falls below the spectral limit if $p \leq 0.085$. Why?

Jiaming Xu (Purdue)
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]
Proof of conjectured upper bound to mutual information

Theorem (Krzakala-X.-Zdeborová 16)

\[ \frac{1}{n} I(v^*; Y) \leq \min_{\alpha \in [0, p]} i_{RS}(\alpha; \lambda, p) \]
Proof of conjectured upper bound to mutual information

Theorem (Krzakala-X.-Zdeborová 16)

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- Upper bound holds for any finite \( n \)
Proof of conjectured upper bound to mutual information

Theorem (Krzakala-X.-Zdeborová 16)

\[
\frac{1}{n} I(v^*; Y) \leq \min_{\alpha \in [0, p]} i_{RS}(\alpha; \lambda, p)
\]

- 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 \( i_{RS}(\alpha) \) has at most three stationary points
• A simple denoising model: \( y = \sqrt{\alpha} \lambda v^* + w \), where \( w \sim \mathcal{N}(0, I_{n \times n}) \)

\[
\frac{1}{n} I(v^*; y) = I(v_1^*; y_1) = i_{RS}(\alpha; \lambda, p) - \frac{(p - \alpha)^2 \lambda^2}{4}
\]
Proof ideas: Interpolation method [Guerra 03]

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

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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 \( I_1 = I(v^*; Y) \).
A simple denoising model: \( y = \sqrt{\alpha} \lambda v^* + w \), where \( w \sim \mathcal{N}(0, \mathbf{I}_{n \times n}) \)

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Interpolating between the denoising model and the Wigner model

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Y_t = \sqrt{\frac{t}{n}} \lambda v^*(v^*)^\top + W
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y_t = \sqrt{\alpha (1 - t)} \lambda v^* + w
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Let \( I_t = I(v^*; Y_t, y_t) \). Then \( I_0 = I(v^*; y) \) and \( I_1 = I(v^*; Y) \).

Show that

\[
\frac{1}{n} \frac{dI_t}{dt} \leq \frac{(p - \alpha)^2 \lambda^2}{4} \implies \frac{1}{n} I_1 \leq i_{RS}(\alpha; \lambda, p)
\]
Outline of the talk

1. Sparse, spiked Wigner model
2. Extensions
3. Conclusions and remarks
Extension 1: general channel output and prior

\[ X = \frac{\lambda}{\sqrt{n}} v^*(v^*)^\top \quad \rightarrow \quad p_{\text{out}}(y|x) \quad \rightarrow \quad Y \]

- \( v_i \sim p_{\text{prior}} \)
- \( Y_{ij} \sim p_{\text{out}}(\cdot|X_{ij}) \) for \( i \leq j \)
- \( p_{\text{prior}} \) and \( p_{\text{out}} \) are assumed to be independent of \( n \)
Theorem (Krzakala-X.-Zdeborová 16)

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

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

$\Delta$ is the inverse Fisher information

Originally conjectured in [Lesieur-Krzakala-Zdeborová 15]

Equivalence between Bernoulli and Gaussian was established in [Deshpande-Abbe-Montanari 15]

The proof relies on Lindeberg's principle
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$$\frac{1}{\Delta} \triangleq \mathbb{E}_{p_{\text{out}}(y|0)} \left[ \left( \frac{\partial \log p_{\text{out}}(y|x)}{\partial x} \right|_{y,0} \right)^2 \right]$$
Theorem (Krzakala-X.-Zdeborová 16)

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

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- The proof relies on Lindeberg’s principle
Extension 2: High rank and asymmetric case

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

- \( U_i \in \mathbb{R}^k \) i.i.d. \( \sim p_{\text{prior}} \) and \( V_j \in \mathbb{R}^k \) i.i.d. \( \sim q_{\text{prior}} \)
Extension 2: High rank and asymmetric case

\[ X = \frac{\text{snr}}{\sqrt{n}} \begin{bmatrix} U_1^T \\ U_2^T \\ \vdots \\ U_m^T \end{bmatrix} \begin{bmatrix} V_1 & V_2 & \cdots & V_n \end{bmatrix} \rightarrow p_{\text{out}}(y|x) \rightarrow Y \]

- \( U_i \in \mathbb{R}^k \text{ i.i.d.} \sim p_{\text{prior}} \) and \( V_j \in \mathbb{R}^k \text{ i.i.d.} \sim q_{\text{prior}} \)
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- \( Y_{ij} \text{ i.i.d.} \sim p_{\text{out}}(\cdot|X_{ij}) \)
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- \( p_{\text{prior}}, q_{\text{prior}}, \text{and } p_{\text{out}} \) are assumed to be independent of \( n \)
- Proposed in [Lesieur-Krzakala-Zdeborová 15]
Special case 1: Submatrix localization with $k$ blocks

\[ Y = \frac{\mu}{\sqrt{n}} \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ 0 & \cdots & \cdots & 1 \end{bmatrix} + W \]
Special case 1: Submatrix localization with $k$ blocks

\[
Y = \frac{\mu}{\sqrt{n}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + W
\]

\[
= \frac{\mu}{\sqrt{n}} \begin{bmatrix} U_1^T \\ U_2^T \\ \vdots \\ U_n^T \end{bmatrix} \begin{bmatrix} U_1 & U_2 & \cdots & U_n \end{bmatrix} + W
\]

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

$$Y_{m \times n} = \sqrt{\frac{\rho}{n}} v_1 - \bar{v}$$

$$+ W_{m \times n}$$

$$v_2 - \bar{v}$$

$$\vdots$$

$$v_k - \bar{v}$$

- $v_1, \ldots, v_k \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, I_{n \times n})$ and $\bar{v} = (1/k) \sum_s v_s$
Special case 2: Gaussian mixture clustering with $k$ clusters

\[ Y_{m \times n} = \sqrt{\frac{\rho}{n}} v_1 - \bar{v} + W_{m \times n} \]

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

\[ \rho_{\text{up}} = \frac{2k}{k-1} \left( \sqrt{\frac{k \log k}{\alpha}} + \log k \right) \]

\[ \rho_{\text{low}} = k \sqrt{2 \log \frac{k-1}{(k-1)\alpha}} \]

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

• 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?
• 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]
- Channel universality and Interpolation method
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- 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?

Dense regime: $p = 0.1$

Second-order phase transition: discontinuity of 2nd derivative of $i(\alpha^*)$.
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