Phase Transitions in Semidefinite Relaxations

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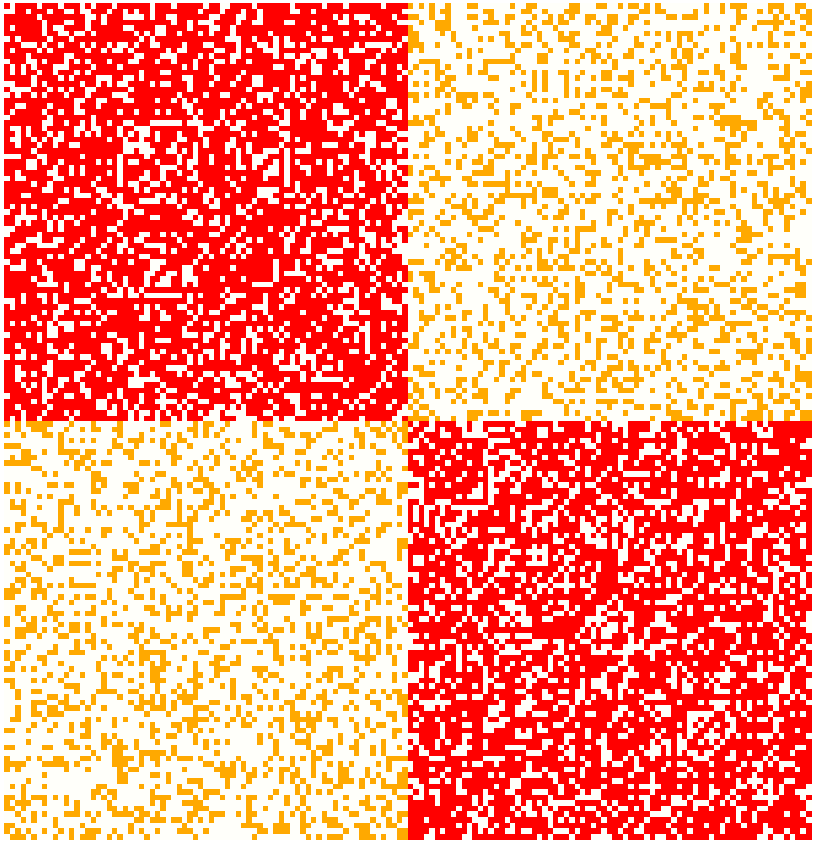
What is this talk about?

SDP for Matrix/Graph estimation

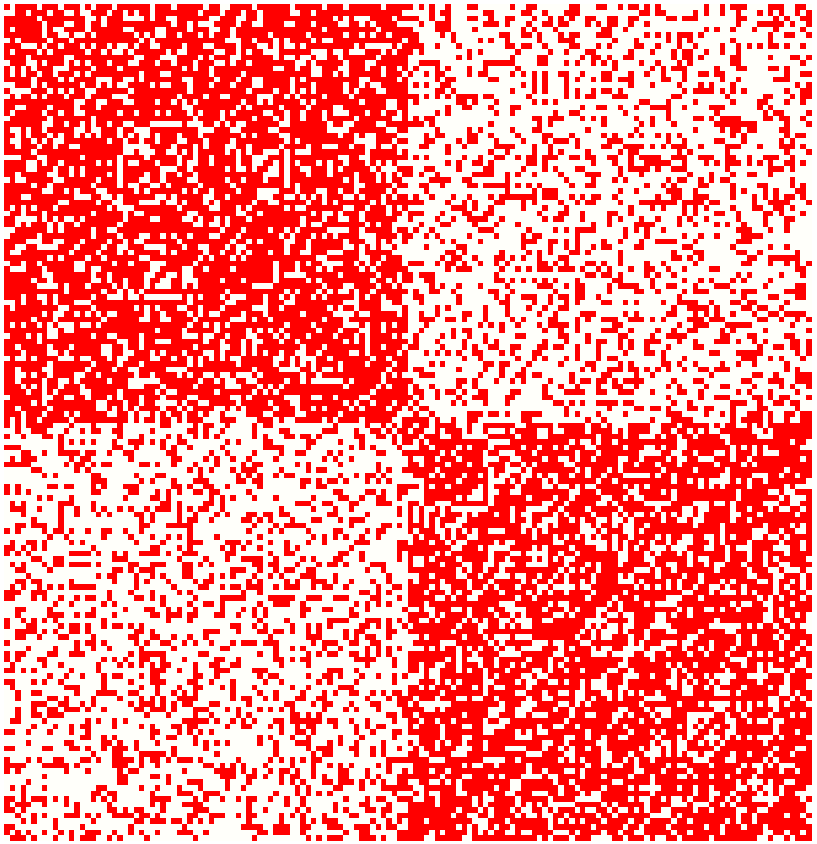
The hidden partition model



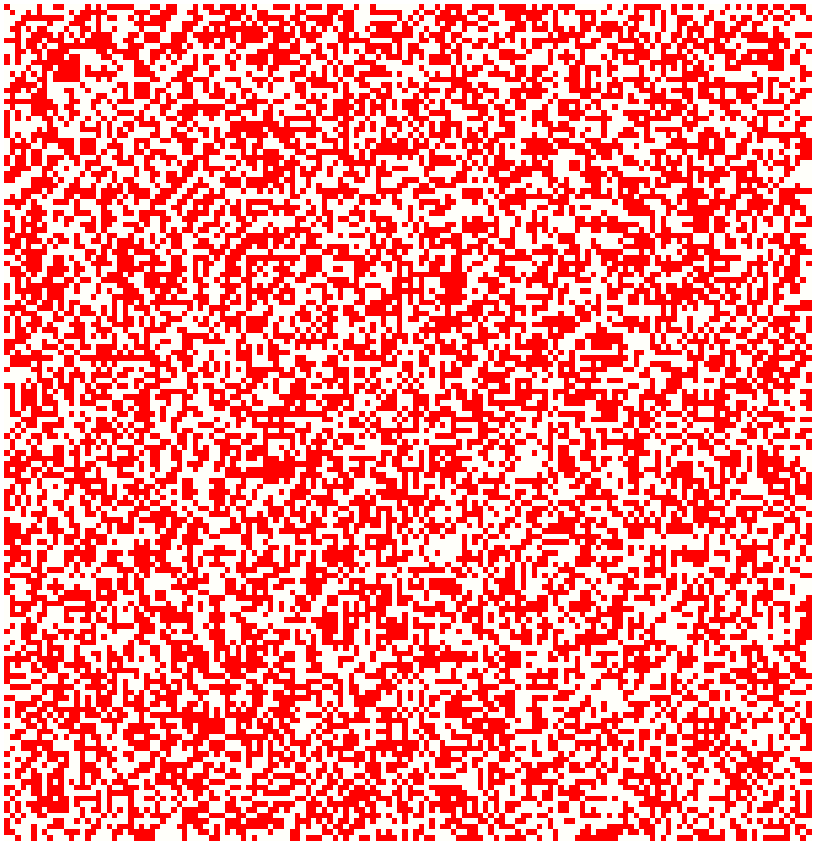
Vertices V, $|V| = n$, $V = V_+ \cup V_-$, $|V_+| = |V_-| = n/2$

$$\mathbb{P}\{(i,j) \in E\} = \begin{cases} p & \text{if } \{i,j\} \subseteq V_+ \text{ or } \{i,j\} \subseteq V_-, \\ q < p & \text{otherwise.} \end{cases}$$

Of course entries are not colored...



...and rows/columns are not ordered



Problem: Detect/estimate the partition

What is this talk about?

SDP for Matrix/Graph estimation

Exact phase transition(?)

Outline

Background

Hypothesis testing

Hypothesis H_0:

$$\mathbb{P}\{(i,j) \in E\} = \frac{p+q}{2}$$

Hypothesis H_1: $V = V_+ \cup V_-$, $|V_+| = |V_-| = n/2$

$$\mathbb{P}\{(i,j) \in E\} = \begin{cases} p & \text{if } \{i,j\} \subseteq V_+ \text{ or } \{i,j\} \subseteq V_-, \\ q < p & \text{otherwise.} \end{cases}$$

Hypothesis testing ($p = a/n$, $q = b/n$)

Hypothesis H_0:

$$\mathbb{P}\{(i,j) \in E\} = \frac{a+b}{2n}$$

Hypothesis H_1: $V = V_+ \cup V_-$, $|V_+| = |V_-| = n/2$

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Information theory threshold

Theorem (Mossel, Neeman, Sly, 2012)

There is a test that succeed with high probability if and only if $a + b > 2$ *and*

$$\frac{a-b}{\sqrt{2(a+b)}} > 1\,.$$

[Proves conjecture by Decelle, Krzakala, Moore, Zdeborova, 2011]

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Computational threshold

- Dyer, Frieze 1989 $\qquad p = na > q = nb$ fixed.
- Condon, Karp 2001 $\qquad a - b \gg n^{1/2}$
- McSherry 2001 $\qquad a - b \gg \sqrt{b \log n}$
- Coja-Oghlan 2010 $\qquad a - b \gg \sqrt{b}$
- Massoulie 2013 and Mossel, Neeman, Sly, 2013

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Very ingenious spectral methods!

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Very ingenious spectral methods!

What if I am not ingenious?

Maximum Likelihood

Adjacency matrix

$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

$$\boldsymbol{A} = (A_{ij})_{1 \le i,j \le n}$$

Maximum likelihood

$$\sigma_i = \begin{cases} +1 & \text{if } i \in V_+, \\ -1 & \text{if } i \in V_-. \end{cases}$$

$$\begin{aligned} \text{maximize} \quad & \sum_{i,j=1}^{n} A_{ij}\, \sigma_i \sigma_j \,, \\ \text{subject to} \quad & \sum_{i=1}^{n} \sigma_i = 0 \,, \\ & \sigma_i \in \{+1, -1\} \,. \end{aligned}$$

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Lagrangian

$$\begin{aligned} \text{maximize} \quad & \sum_{i,j=1}^{n} A_{ij}\,\sigma_i\sigma_j - \gamma\Big(\sum_{i=1}^{n}\sigma_i\Big)^2 . \\ \text{subject to} \quad & \sigma_i \in \{+1,-1\} . \end{aligned}$$

A good choice:

$$\gamma = \frac{a+b}{2n} \equiv \frac{d}{n}$$

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A good choice:

$$\gamma = \frac{a+b}{2n} \equiv \frac{d}{n}$$

Centered adjacency matrix

$$A_{ij}^{\mathrm{cen}} = \begin{cases} 1 - (d/n) & \text{if } (i,j) \in E, \\ -(d/n) & \text{otherwise.} \end{cases}$$

$$\boldsymbol{A}^{\mathrm{cen}} = \boldsymbol{A} - \frac{d}{n} \mathbf{1}\,\mathbf{1}^{\mathsf{T}}$$

Lagrangian

$$\begin{aligned} \text{maximize} \quad & \langle \boldsymbol{A}^{\text{cen}}, \boldsymbol{\sigma}\boldsymbol{\sigma}^{\mathsf{T}} \rangle \,, \\ \text{subject to} \quad & \boldsymbol{\sigma} \in \{+1, -1\}^n \,. \end{aligned}$$

- NP-hard
- SDP($\boldsymbol{A}^{\text{cen}}$) is a very natural convex relaxation

Lagrangian

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Relaxation

$$\begin{aligned} \text{maximize} \quad & \langle \boldsymbol{A}^{\text{cen}}, \boldsymbol{\sigma}\boldsymbol{\sigma}^{\mathsf{T}} \rangle \,, \\ \text{subject to} \quad & \boldsymbol{\sigma} \in \{+1, -1\}^n \,. \end{aligned}$$

SDP($\boldsymbol{A}^{\text{cen}}$):

$$\begin{aligned} \text{maximize} \quad & \langle \boldsymbol{A}^{\text{cen}}, \boldsymbol{X} \rangle \,, \\ \text{subject to} \quad & \boldsymbol{X} \in \mathbb{R}^{n \times n}, \ \boldsymbol{X} \succeq 0 \,, \\ & X_{ii} = 1 \,. \end{aligned}$$

$$T_{\mathsf{SDP}}(G) = \begin{cases} 1 & \text{if } \mathsf{SDP}(\boldsymbol{A}_G^{\mathrm{cen}}) \geq \theta_*, \\ 0 & \text{otherwise.} \end{cases}$$

- This is really **off-the-shelf**
- How well does it work?

Near-optimality of SDP

Before we pass to SDP

- What's the problem with sparse graphs?
- What's the problem vanilla PCA?

Why PCA?

Ground truth

$$x_{0,i} = \begin{cases} +1 & \text{if } i \in V_+, \\ -1 & \text{if } i \in V_-. \end{cases}$$

Data = RankOne + Wigner

$$\frac{1}{\sqrt{d}} \boldsymbol{A}^{\text{cen}} = \frac{\lambda}{n} \boldsymbol{x_0} \boldsymbol{x_0}^{\mathsf{T}} + \boldsymbol{W}\,, \qquad \lambda \equiv \frac{a-b}{\sqrt{2(a+b)}}$$

$$E\{W_{ij}\} = 0\,, \qquad \mathbb{E}\{W_{ij}^2\} \in \left\{ \frac{a}{dn}\,,\, \frac{b}{dn} \right\} \approx \frac{1}{n}\,.$$

Why PCA?

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The *right* parametrization

$$d = \frac{a+b}{2}\,, \qquad \lambda = \frac{a-b}{\sqrt{2(a+b)}}$$

Naive PCA

$$\widehat{\mathbf{x}}^{\mathrm{PCA}}(\boldsymbol{A}^{\mathrm{cen}}) = \sqrt{n}\, \boldsymbol{v}_1(\boldsymbol{A}^{\mathrm{cen}})\,.$$

Does it work?

$$\frac{1}{\sqrt{d}}\boldsymbol{A}^{\mathsf{cen}} = \frac{\lambda}{n}\,\boldsymbol{x_0}\boldsymbol{x_0}^{\mathsf{T}} + \boldsymbol{W}$$

Naive idea:

$$\|\boldsymbol{W}\|_2 \le \text{const.}, \quad \left\|\frac{\lambda}{n}\boldsymbol{x_0}\boldsymbol{x_0}^{\mathsf{T}}\right\|_2 = \lambda \quad \Rightarrow \text{Works for } \lambda = O(1)$$

Wrong!

Does it work?

$$\frac{1}{\sqrt{d}}\boldsymbol{A}^{\mathrm{cen}} = \frac{\lambda}{n}\,\boldsymbol{x_0}\boldsymbol{x_0}^{\mathsf{T}} + \boldsymbol{W}$$

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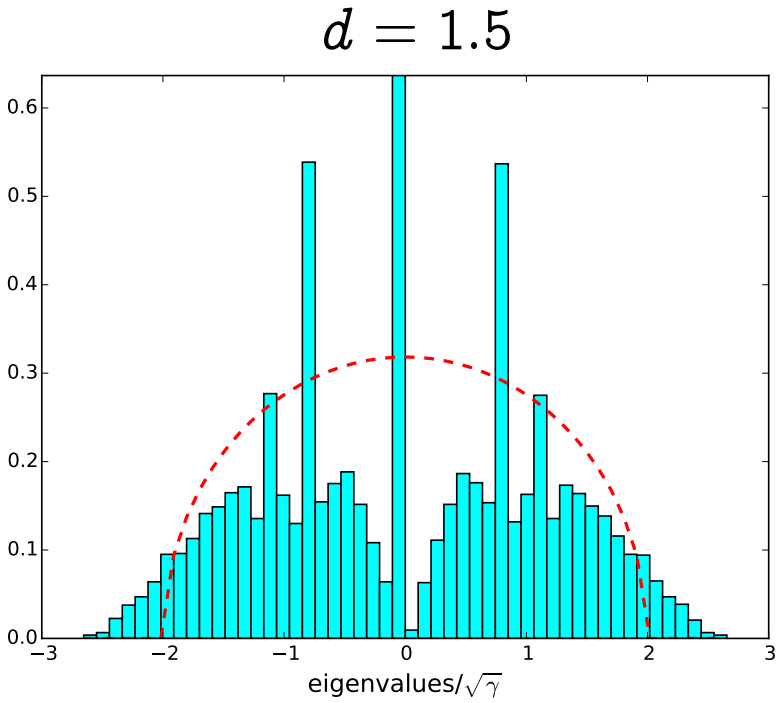
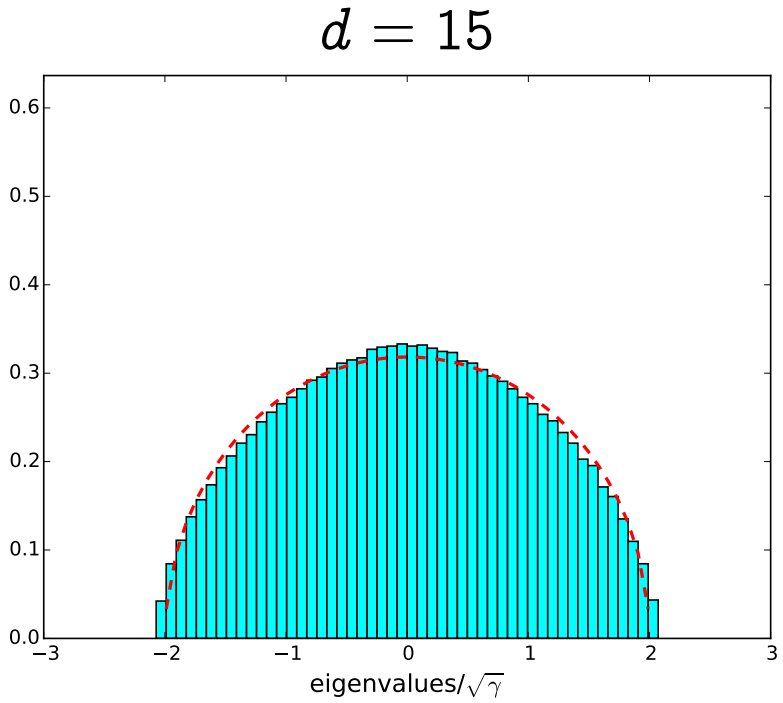
Wrong!

Spectral relaxation bad in the sparse regime!



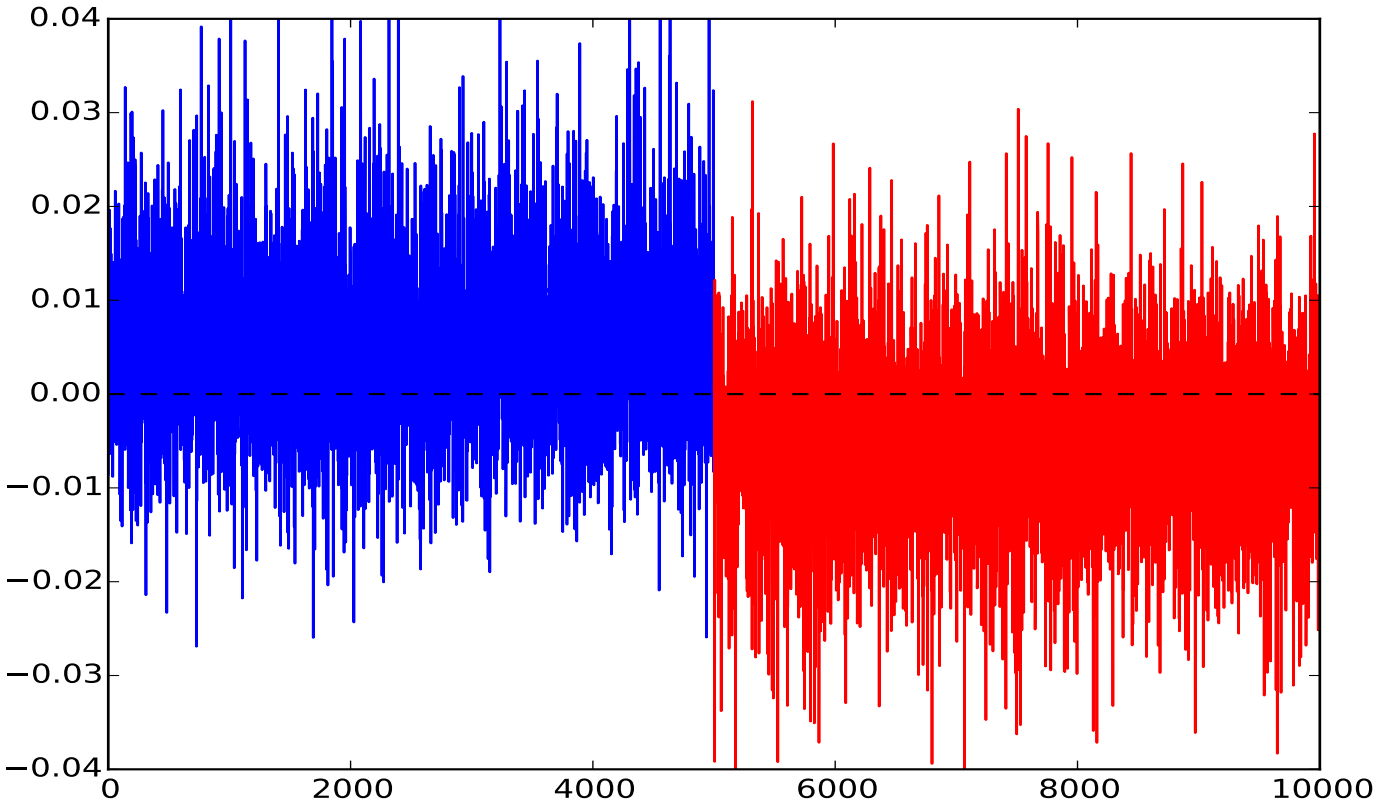


Theorem (Krivelevich, Sudakov 2003+Vu 2005)

With high probability,

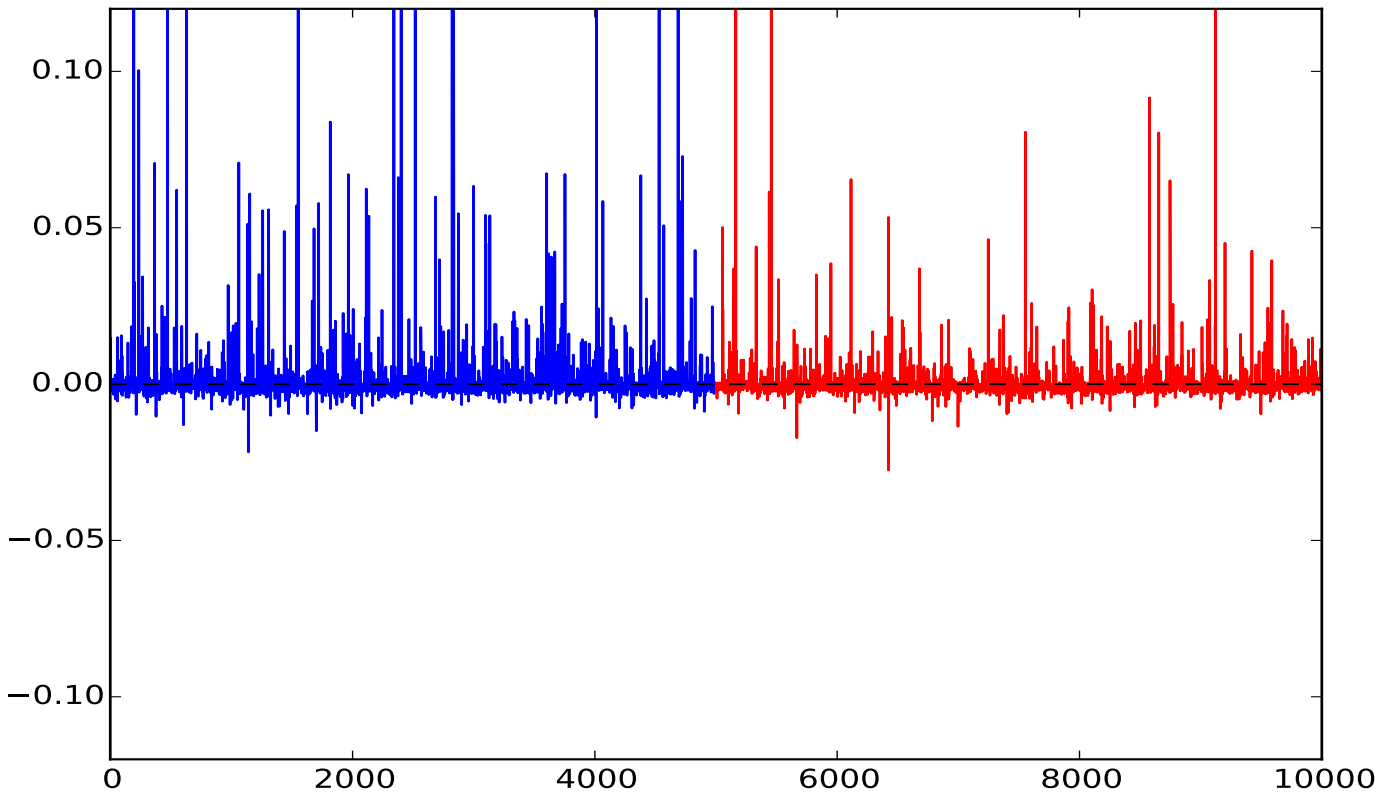
$$\lambda_{\max}(\boldsymbol{A}^{cen}/\sqrt{d}) = \begin{cases} 2\,(1+o(1)) & \text{if } d \gg (\log n)^4, \\ C\sqrt{\log n/(\log\log n)}(1+o(1)) & \text{if } d = O(1). \end{cases}$$

Example: $d = 20$, $\lambda = 1.2$, $n = 10^4$



$v_1(A^{\text{cen}})$

Example: $d = 3$, $\lambda = 1.2$, $n = 10^4$



$v_1(A^{\text{cen}})$

Why should SDP work better?

$$\begin{aligned} \text{maximize} \quad & \langle \boldsymbol{A}^{\text{cen}}, \boldsymbol{X} \rangle \,, \\ \text{subject to} \quad & \boldsymbol{X} \in \mathbb{R}^{n \times n}, \ \boldsymbol{X} \succeq 0 \,, \\ & X_{ii} = 1 \,. \end{aligned}$$

Recall the ultimate limit

$\mathsf{G}(n, d, \lambda)$ graph distribution with parameters

$$d = \frac{a+b}{2} > 1\,, \qquad \lambda = \frac{a-b}{\sqrt{2(a+b)}}$$

Theorem (Mossel, Neeman, Sly, 2012)

If $\lambda < 1$, then

$$\lim\sup_{n\to\infty} \left\|\mathsf{G}(n, d, 0) - \mathsf{G}(n, d, \lambda)\right\|_{\mathrm{TV}} < 1\,.$$

If $\lambda > 1$, then

$$\lim_{n\to\infty} \left\|\mathsf{G}(n, d, 0) - \mathsf{G}(n, d, \lambda)\right\|_{\mathrm{TV}} = 1\,.$$

SDP has nearly optimal threshold

Theorem (Montanari, Sen 2015)

Assume $G \sim \mathsf{G}(n, d, \lambda)$.
If $\lambda \leq 1$, *then, with high probability,*

$$\frac{1}{n\sqrt{d}}\mathsf{SDP}(\boldsymbol{A}_G^{cen}) = 2 + o_d(1)\,.$$

If $\lambda > 1$, *then there exists* $\Delta(\lambda) > 0$ *such that, with high probability,*

$$\frac{1}{n\sqrt{d}}\mathsf{SDP}(\boldsymbol{A}_G^{cen}) = 2 + \Delta(\lambda) + o_d(1)\,.$$

Consequence

$$T_{\mathsf{SDP}}(G) = \begin{cases} 1 & \text{if } \mathsf{SDP}(\boldsymbol{A}_G^{\text{cen}}) \geq (2+\delta)n\sqrt{d}, \\ 0 & \text{otherwise.} \end{cases}$$

Corollary (Montanari, Sen 2015)

Assume $\lambda \geq 1+\varepsilon$. Then there exists $d_0(\varepsilon)$ and $\delta(\varepsilon)$ such that the SDP-based test succeeds with high probability, provided $d \geq d_0(\varepsilon)$. Namely

$$\lim_{n\to\infty} \left[\mathbb{P}_0(T_{\mathsf{SDP}}(G)=1) + \mathbb{P}_1(T_{\mathsf{SDP}}(G)=0)\right] = 0\,.$$

Earlier/related work

Optimal spectral tests

- Massoulie 2013
- Mossel, Neeman, Sly, 2013
- Bordenave, Lelarge, Massoulie, 2015

SDP, $d = \Theta(\log n)$

- Abbe, Bandeira, Hall 2014
- Hajek, Wu, Xu 2015

SDP, detection

- Guédon, Vershynin, 2015 (requires $\lambda \geq 10^4$, very different proof)

How does SDP work 'in practice'?

Thresholds

- $\lambda_c^{\rm opt}(d) \equiv$ Threshold for optimal test
- $\lambda_c^{\rm SDP}(d) \equiv$ Threshold for SDP-based test

What we know

- $\lambda_c^{\rm opt}(d) = 1$ [Mossel, Neeman, Sly, 2013]
- $\lambda_c^{\rm SDP}(d) = 1 + o_d(1)$ [Montanari, Sen, 2015]

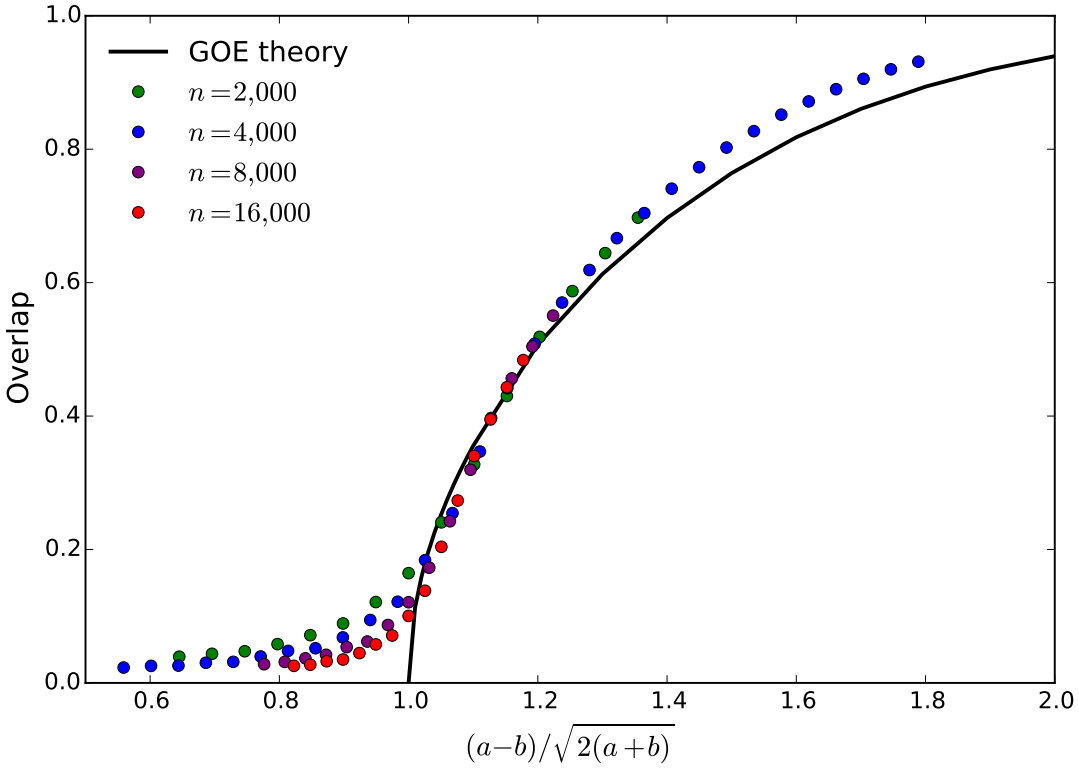
How big is the $o_d(1)$ gap?

What we know

- $\lambda_c^{\rm opt}(d) = 1$ [Mossel, Neeman, Sly, 2013]
- $\lambda_c^{\rm SDP}(d) = 1 + o_d(1)$ [Montanari, Sen, 2015]

How big is the $o_d(1)$ gap?

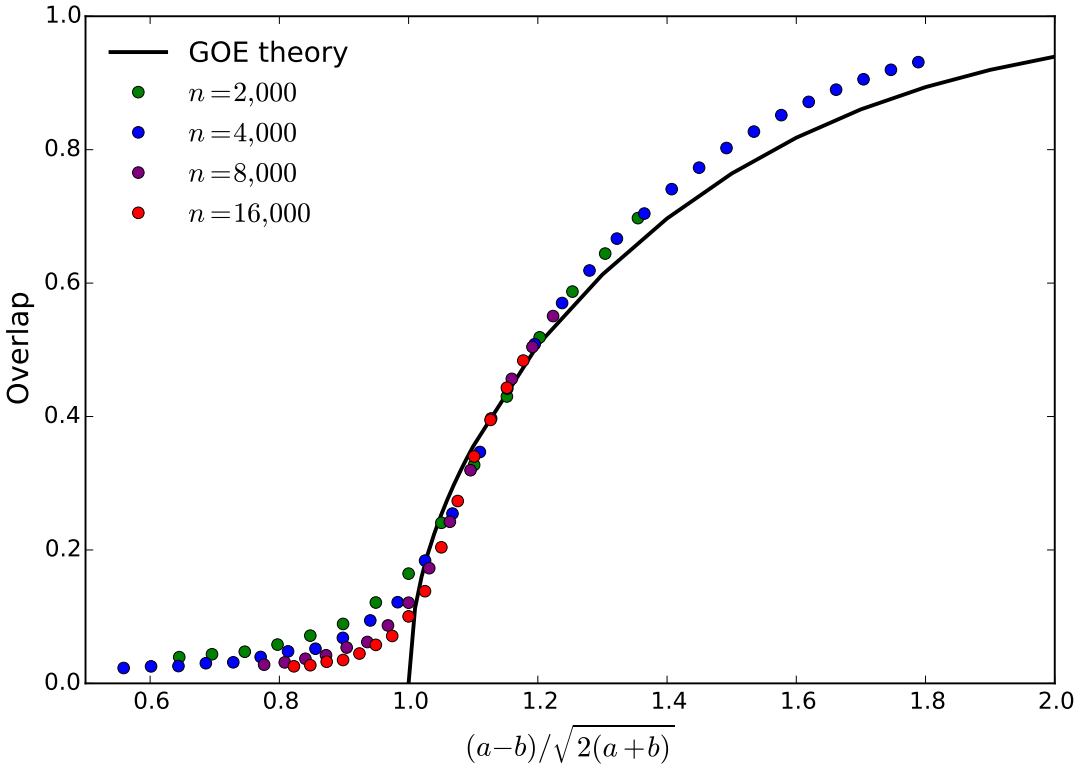
Simulations: $d = 5$, $N_{\text{sample}} = 500$ (with Javanmard and Ricci)



SDP estimator $\hat{\boldsymbol{x}}^{\mathbf{SDP}} \in \{+1, -1\}^n$

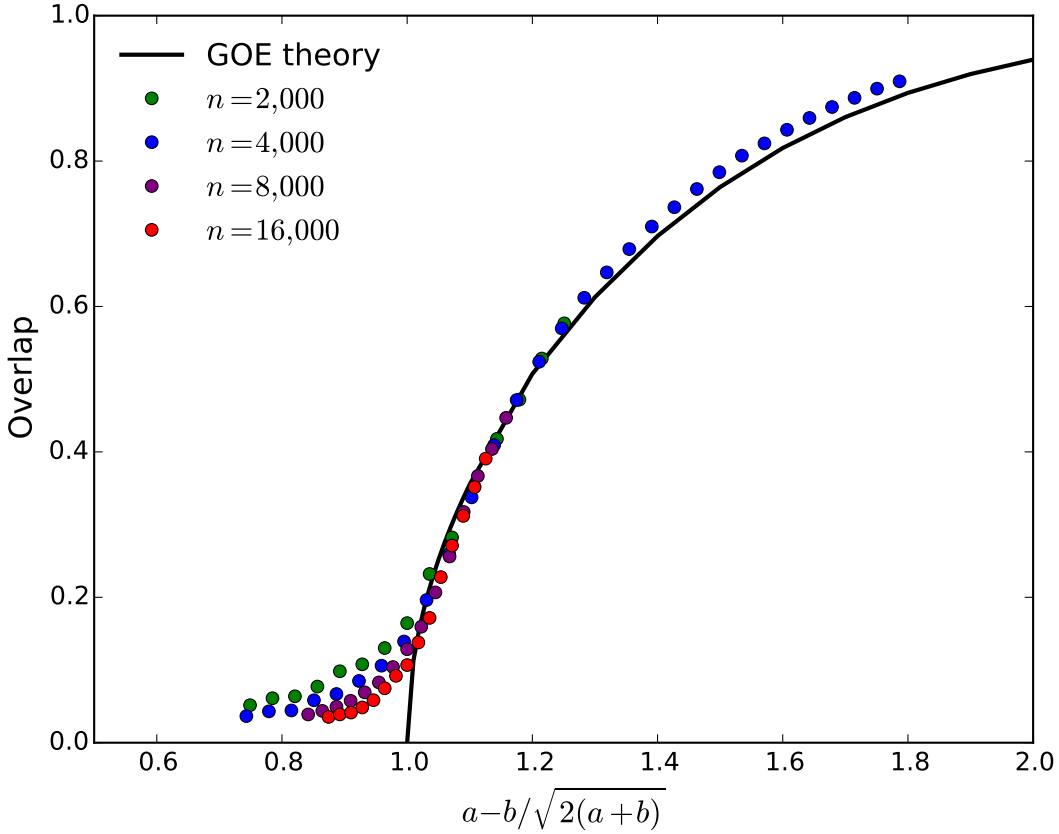
$$\text{Overlap}_n(\widehat{\mathrm{x}}) = \frac{1}{n}\mathbb{E}\{|\langle \hat{\boldsymbol{x}}^{\text{SDP}}(G), \boldsymbol{x_0}\rangle|\}\,.$$

Simulations: $d = 5$, $N_{\text{sample}} = 500$



$$\lambda_c^{\text{SDP}}(d = 5) \approx 1\,.$$

Simulations: $d = 10$, $N_{\text{sample}} = 500$



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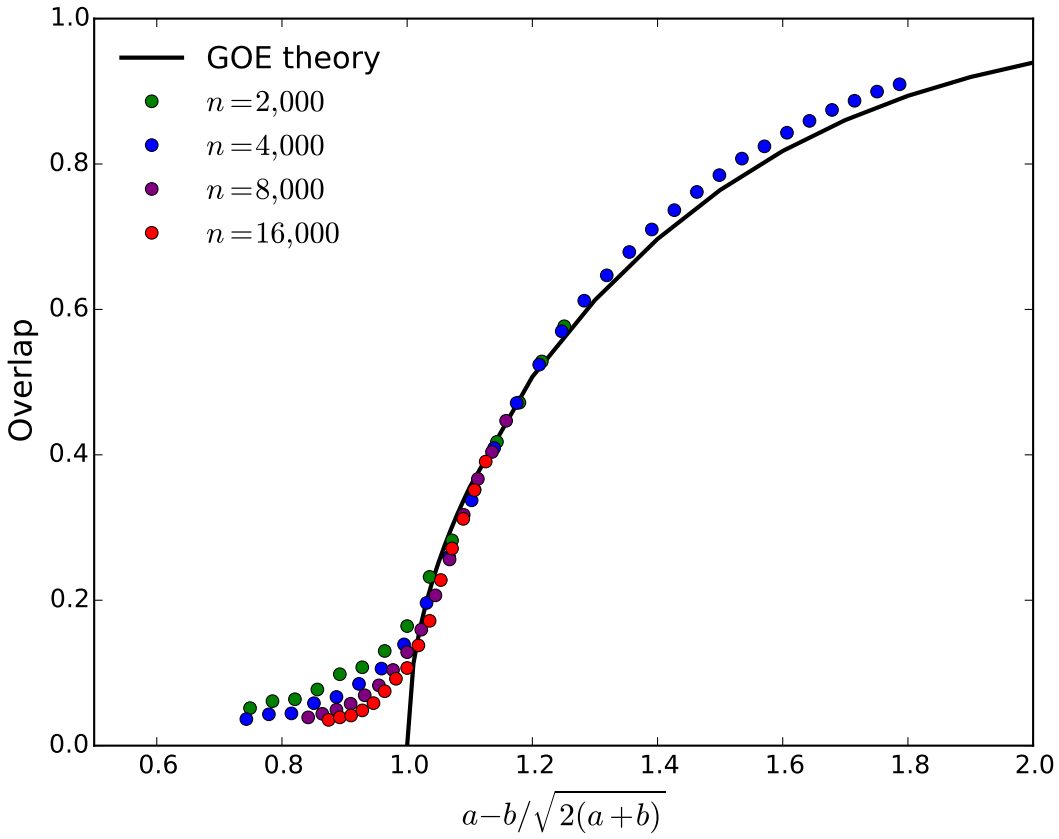

How to estimate $\lambda_c^{SDP}(d)$ from data?

A technique from physics: Binder cumulant

$$Q(G) \equiv \frac{1}{n}\langle \hat{\boldsymbol{x}}^{\rm SDP}(G), \boldsymbol{x}_{\mathbf{0}}\rangle\,,$$

$$\mathsf{Bind}(n,\lambda,d) \equiv \frac{\mathbb{E}\{Q(G)^4\}}{\mathbb{E}\{Q(G)^2\}^2}$$

CLT heuristics

$$\lim_{n\to\infty}\mathsf{Bind}(n,\lambda,d) = \begin{cases} 3 & \text{if } \lambda < \lambda_c^{\rm SDP}(d),\\ 1 & \text{if } \lambda > \lambda_c^{\rm SDP}(d).\end{cases}$$

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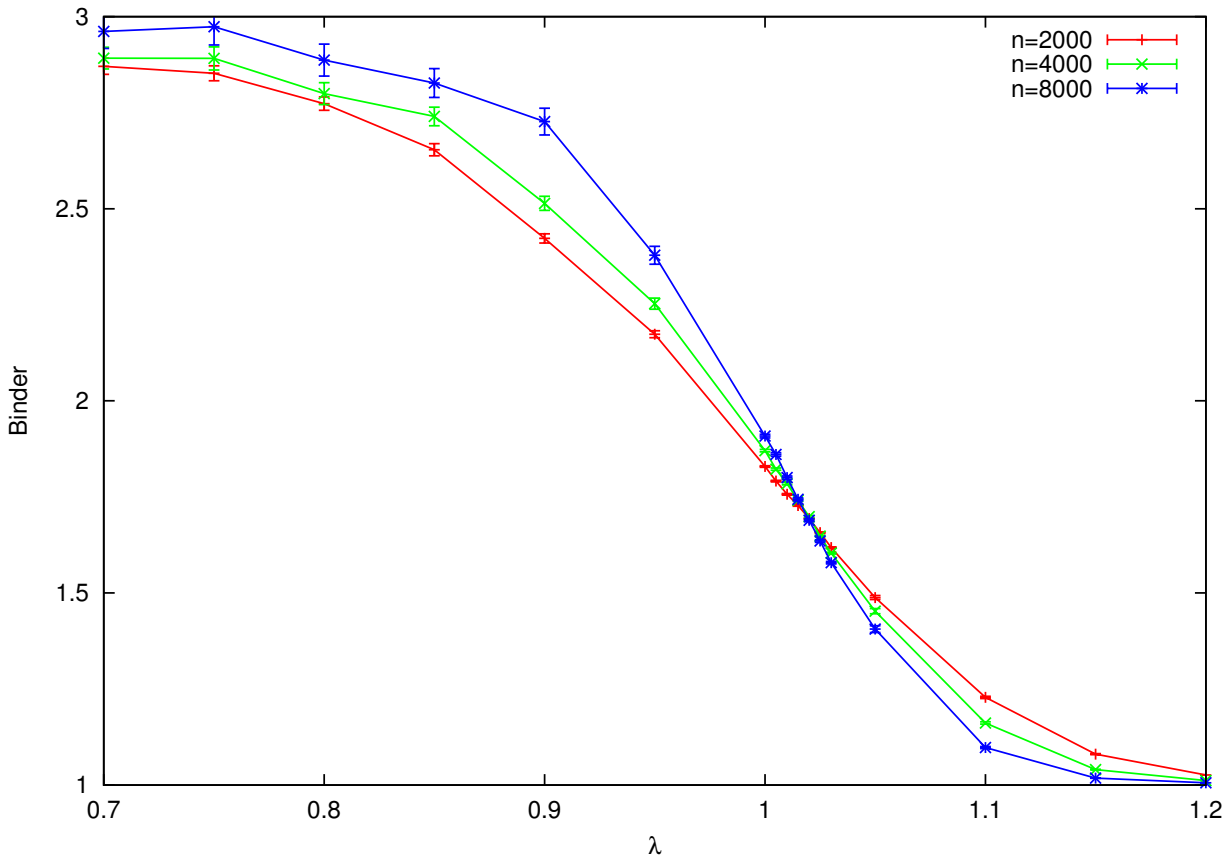
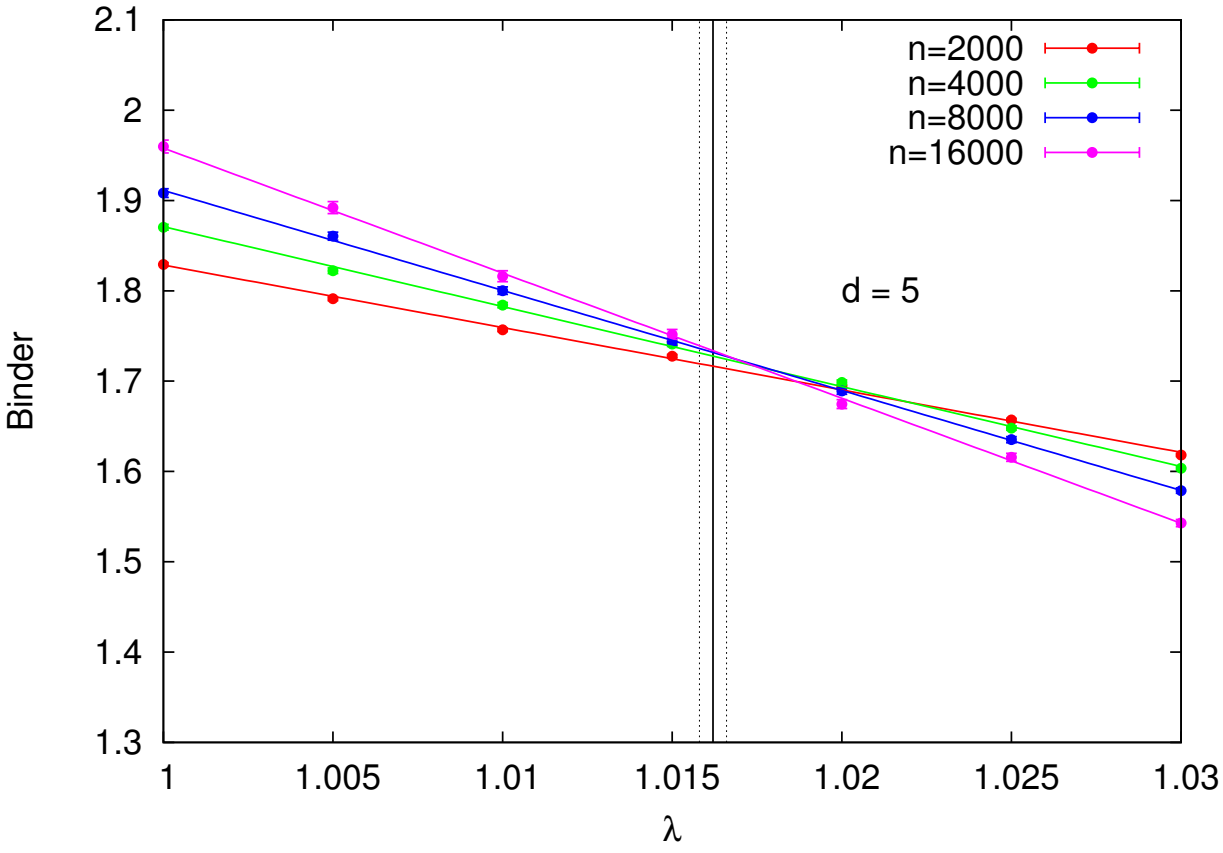
Simulations: $d = 5$, $N_{\text{sample}} \geq 10^5$!



Zoom

(∼ 2 years CPU time)



Estimate $\lambda_c^{\rm SDP}(d)$ by the crossing point

Zoom

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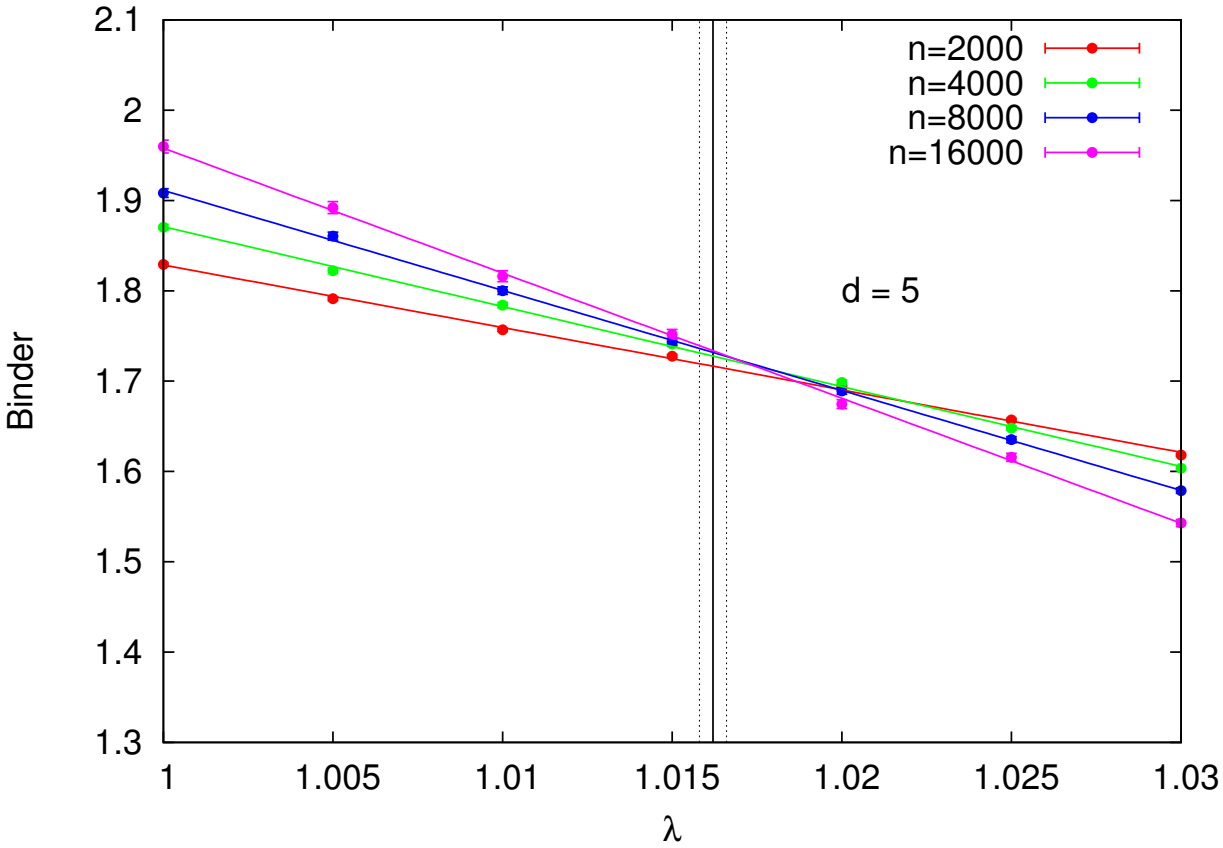

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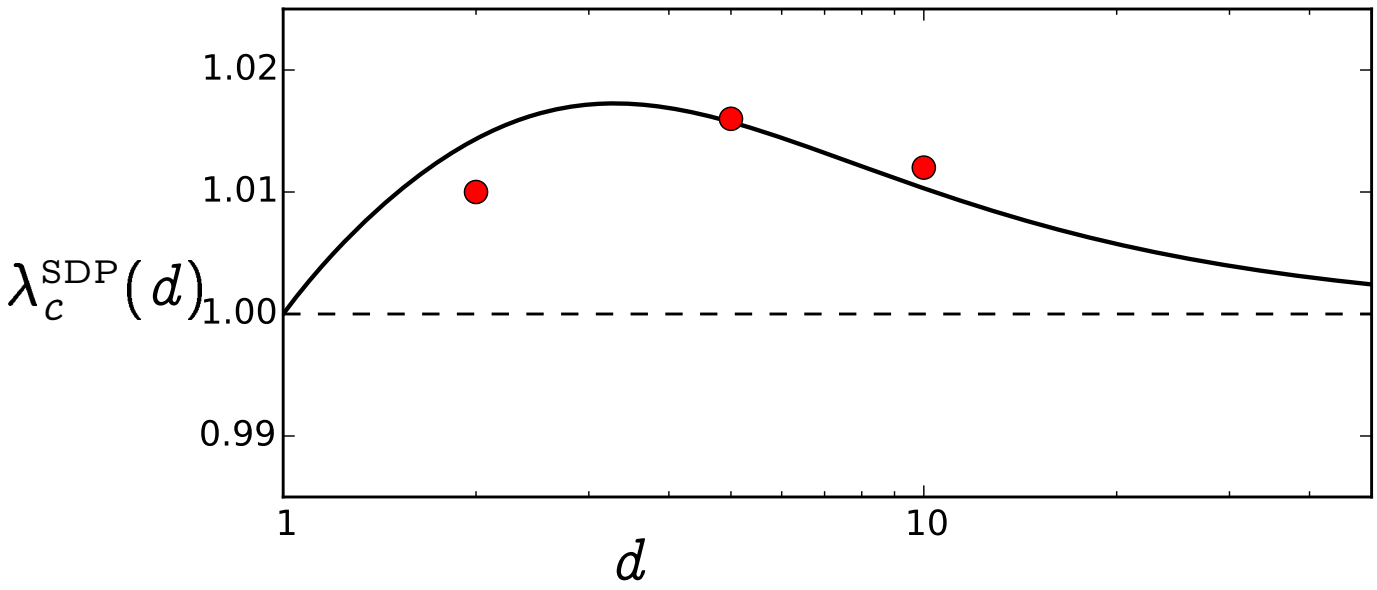
$\lambda_c^{\mathrm{SDP}}(d)$



- Dots: Numerical estimates
- Line: Non-rigorous analytical approximation (using statistical physics)
- **At most 2% sub-optimal!**

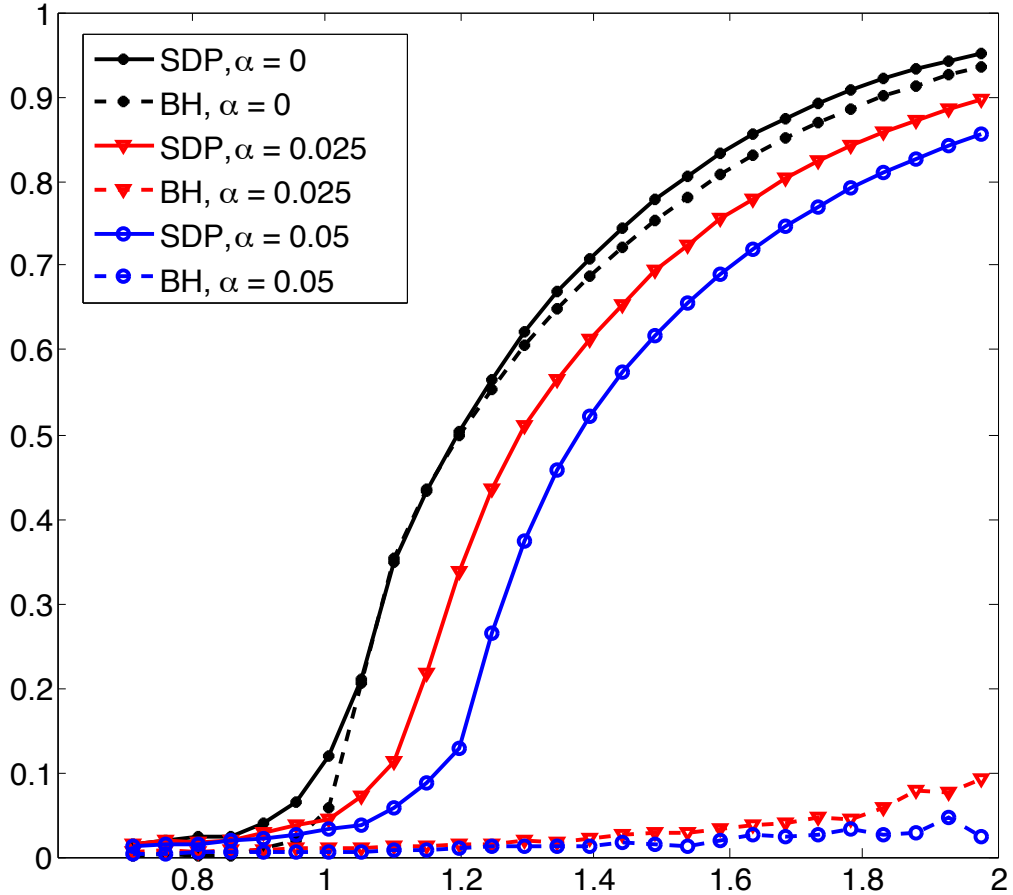
One last question

Is this approach robust to model miss-specifications?

An experiment

- Select $S \subseteq V$ uniformly at random. with $|S| = n\alpha$.
- For each $i \in S$, connect all of its neighbors.

An experiment



- Solid line:SDP
- Dashed line: Spectral
  (Non-backtracking walk [Krzakala, Moore, Mossel, Neeman, Sly, Zdeborova, Zhang, 2013])

A simple robustness result

Lemma (Montanari, Sen, 2015)

If $\widetilde{G}$ is obtained from the hidden partition model by flipping at most $n\varepsilon$ edges, then

$$\left|\tilde{\lambda}_c^{SDP}(d) - \lambda_c^{SDP}(d)\right| \leq \delta(\varepsilon)\,.$$

Proof ideas

What we want to prove

Theorem (Montanari, Sen 2015)

Assume $G \sim \mathsf{G}(n, d, \lambda)$.
If $\lambda \leq 1$, *then, with high probability,*

$$\frac{1}{n\sqrt{d}}\mathsf{SDP}(\boldsymbol{A}_G^{cen}) = 2 + o_d(1)\,.$$

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Strategy

I. Prove equivalence to Gaussian model

II. Analyze Gaussian model

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Gaussian model: $\boldsymbol{x_0} \in \{+1, -1\}^n$

$$\boldsymbol{B}(\lambda) \equiv \frac{\lambda}{n}\, \boldsymbol{x_0}\boldsymbol{x_0}^{\mathsf{T}} + \boldsymbol{W}\,.$$

$\boldsymbol{W} \sim \mathsf{GOE}(n)$:

- $(W_{ij})_{i<j} \sim_{iid} \mathrm{N}(0, 1/n)$
- $\boldsymbol{W} = \boldsymbol{W}^{\mathsf{T}}$

- *A lot is known about spectral properties of* $\boldsymbol{B}$

Need to characterize the SDP value with Gaussian data

Gaussian model: $\boldsymbol{x_0} \in \{+1, -1\}^n$

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Need to characterize the SDP value with Gaussian data

Notation

$$\bar{\mathsf{s}}(\lambda) \equiv \lim \sup_{n\to\infty} \frac{1}{n}\mathsf{SDP}(\boldsymbol{B}(\lambda))\,,$$

$$\underline{\mathsf{s}}(\lambda) \equiv \lim \inf_{n\to\infty} \frac{1}{n}\mathsf{SDP}(\boldsymbol{B}(\lambda))\,.$$

$$\mathsf{SDP}(\boldsymbol{B}) \equiv \max\left\{\langle \boldsymbol{B}, \boldsymbol{X}\rangle :\ \boldsymbol{X} \succeq 0, X_{ii} = 1\,\forall i\right\}$$

Phase transition at $\lambda = 1$!

Theorem (Montanari, Sen, 2015)

The following holds almost surely

$$\lambda \in [0,1] \Rightarrow \quad \underline{s}(\lambda) = \bar{s}(\lambda) = 2\,,$$

$$\lambda \in (1,\infty) \Rightarrow \quad \underline{s}(\lambda) > 2 \quad \textit{(strictly)}\,.$$

For explicit probability bounds, see the paper

Proof of Gaussian phase transition

Simple facts:

- $$\bar{\mathsf{s}}(\lambda) \le \lim_{n\to\infty} \sigma_{\max}(\boldsymbol{B}(\lambda)) = \begin{cases} 2 & \text{if } \lambda \in [0,1], \\ \lambda + \lambda^{-1} & \text{if } \lambda \in (1,\infty). \end{cases}$$

  [Baik, Ben Arous, Peche, 2005]

- $$\underline{\mathsf{s}}(\lambda) \le \lim_{n\to\infty} \frac{1}{n}\langle \mathbf{1}, \boldsymbol{B}(\lambda)\mathbf{1}\rangle = \lambda$$

- $\underline{\mathsf{s}}(\lambda)$, $\bar{\mathsf{s}}(\lambda)$ are non-random, non-decreasing

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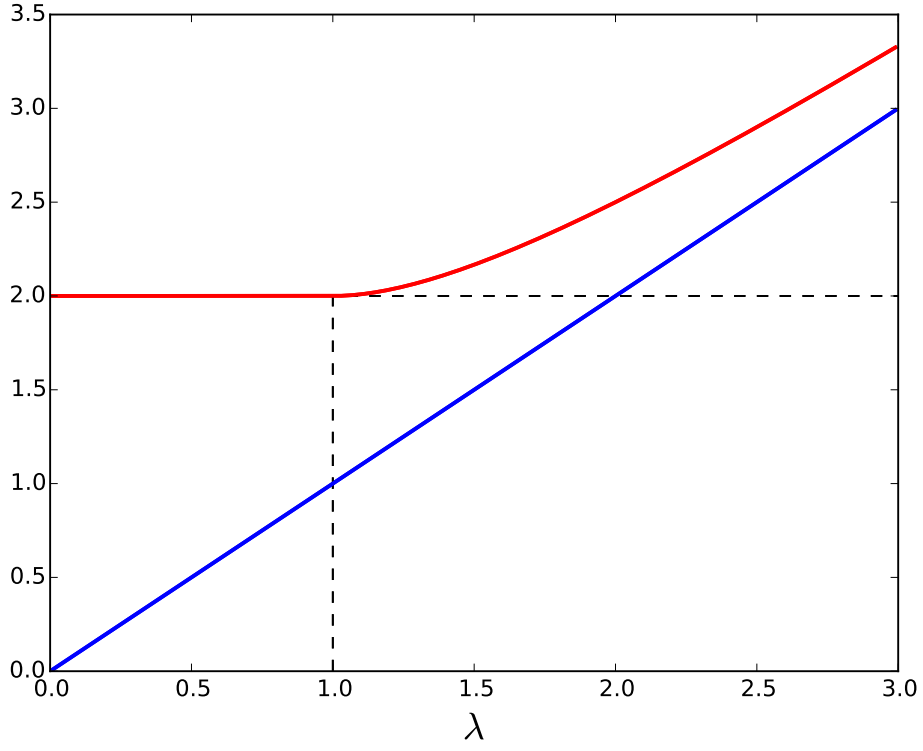
Summarizing



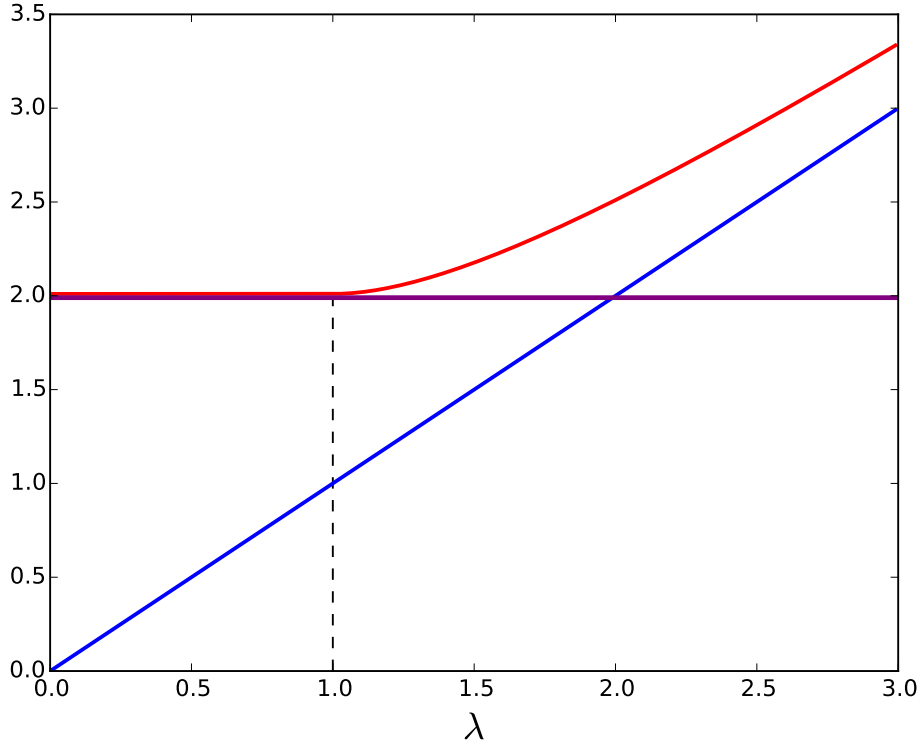
- Red: Upper bound
- Blue: Lower bound

Proof of Gaussian phase transition

Part 1:

Prove that $\underline{s}(\lambda = 0) \geq 2$

Hence



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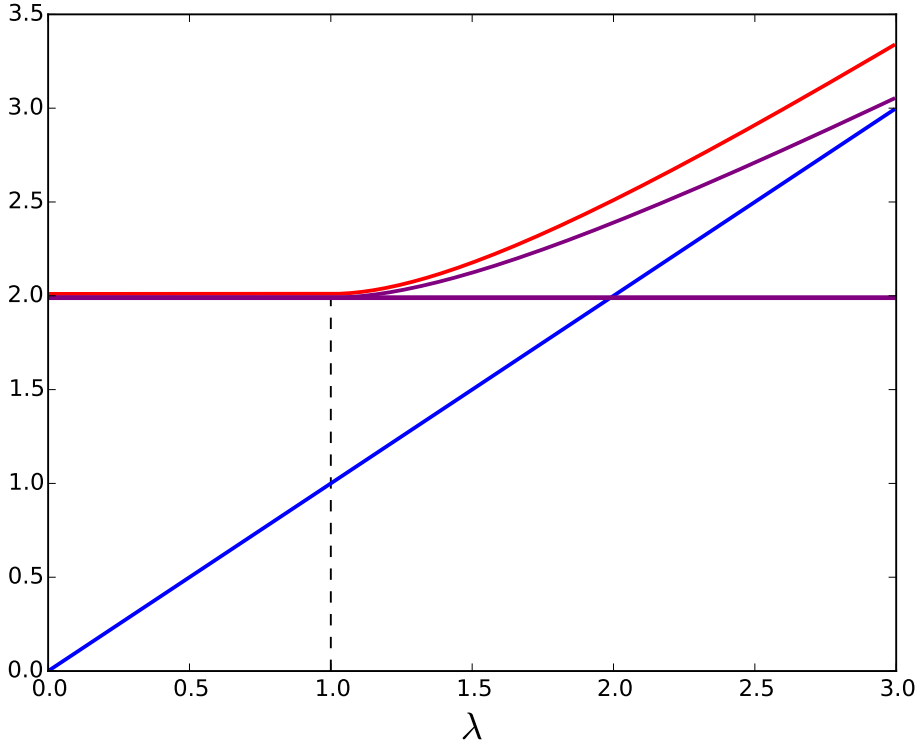

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Proof of Gaussian phase transition

Part 1:

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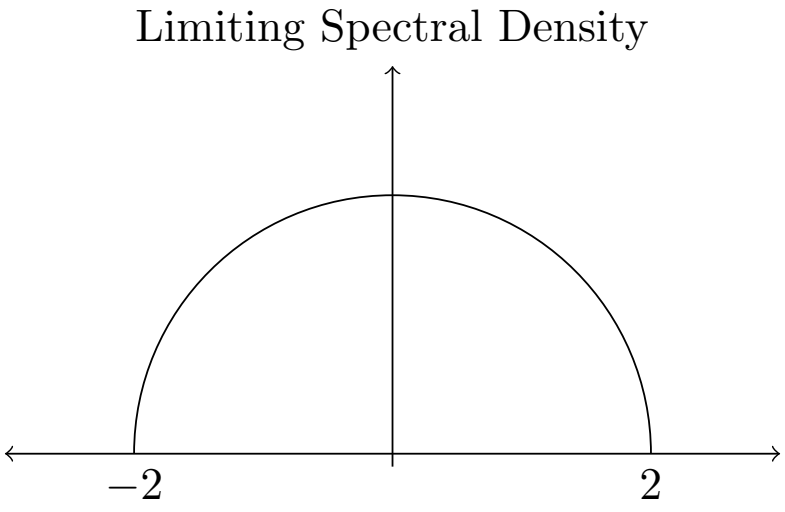
Technique: Construct feasible $\boldsymbol{X}$, such that $\langle \boldsymbol{A}, \boldsymbol{X} \rangle \geq \dots$.

Part 1: $\lambda = 0$



First idea:

- $\boldsymbol{v}_1 = \boldsymbol{v}_1(\boldsymbol{B}) \equiv$ principal eginvector of $\boldsymbol{B}$
- Take $\boldsymbol{X} = n\, \boldsymbol{v}_1 \boldsymbol{v}_1^{\mathsf{T}}$
- **Wrong:** $X_{ii} \approx \mathrm{N}(0,1)^2 \neq 1$

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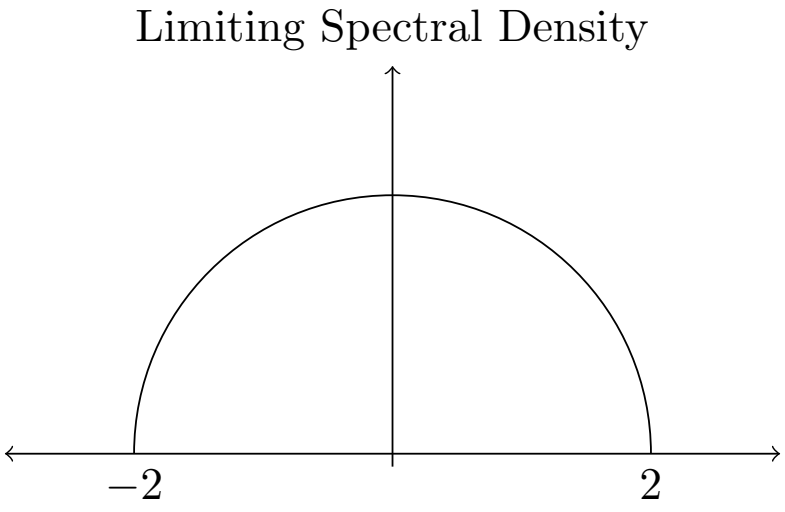

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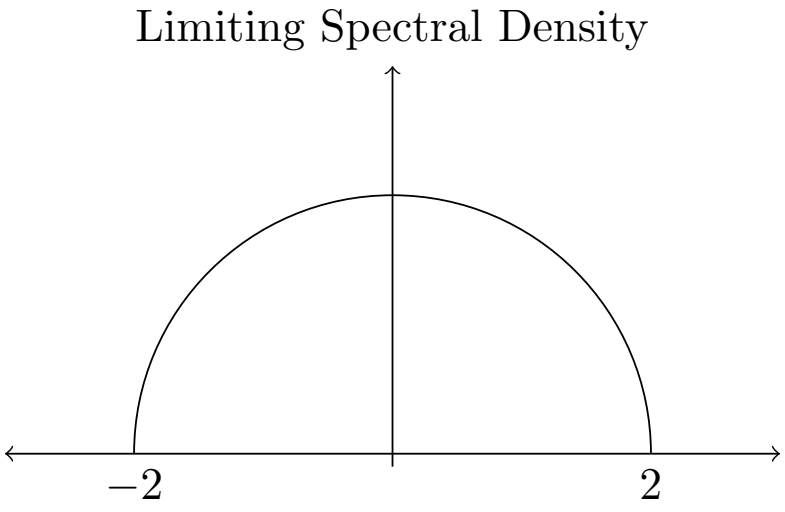

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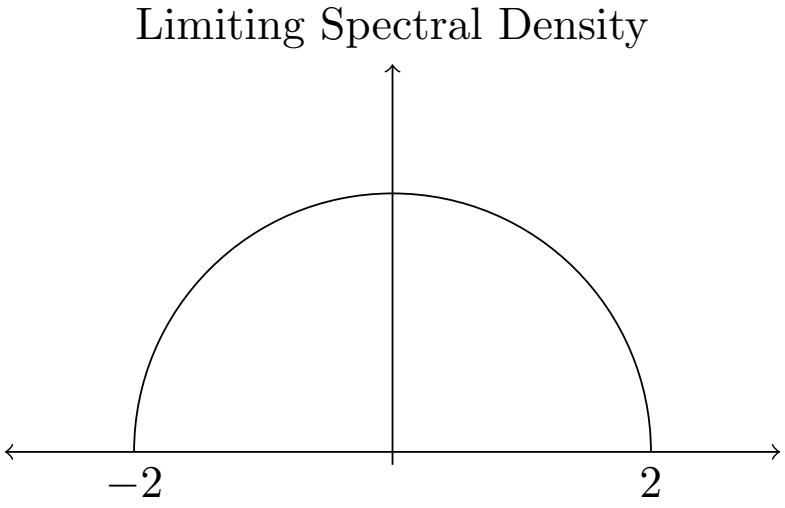

Good idea:

- Let $\boldsymbol{U} = [\boldsymbol{v}_1|\boldsymbol{v}_2|\cdots|\boldsymbol{v}_{n\delta}] \in \mathbb{R}^{n\times n\delta}$, δ small.
- $\boldsymbol{D} \equiv \mathrm{Diag}(\boldsymbol{U}\,\boldsymbol{U}^{\mathsf{T}}) \in \mathbb{R}^{n\times n}$. Claim $\boldsymbol{D} \approx \delta\,\mathbf{I}$ $(D_{ii} \sim n^{-1}\chi_{n\delta})$
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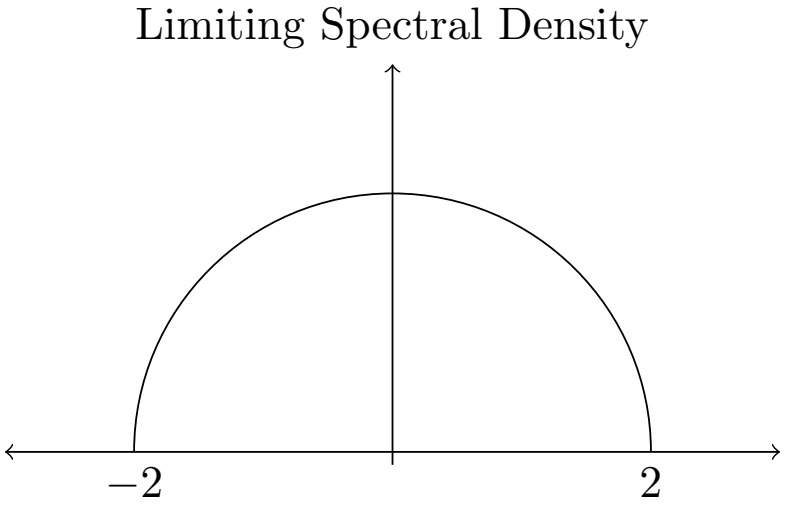

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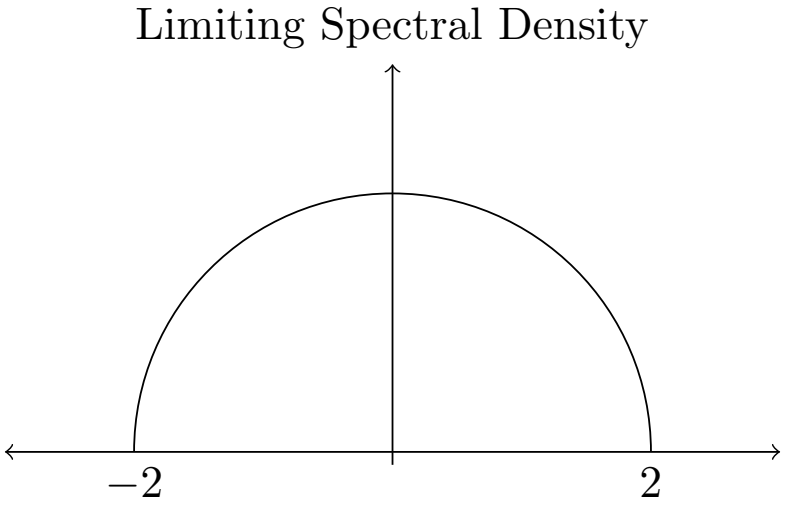

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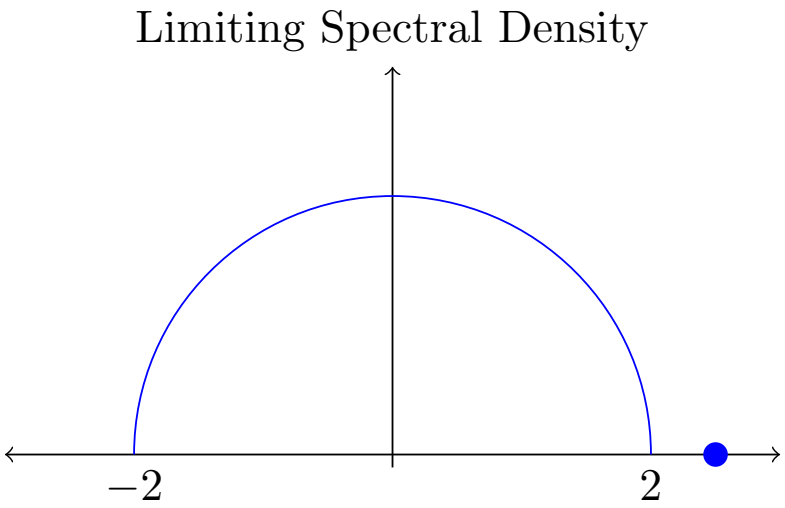

Construction:

- $T(x) \equiv \max(\min(x, +1), -1)$, $\varphi \in \mathbb{R}^n$

$$\varphi_i \equiv T(\varepsilon\sqrt{n}\, v_{1,i})\,.$$

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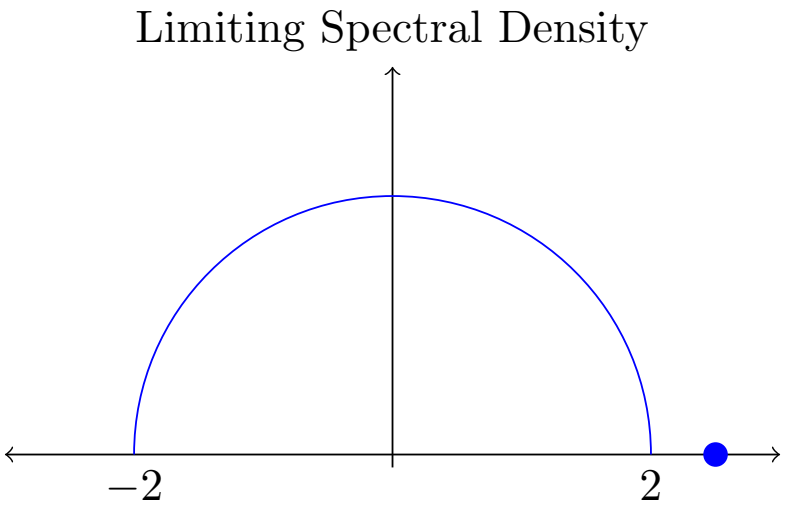

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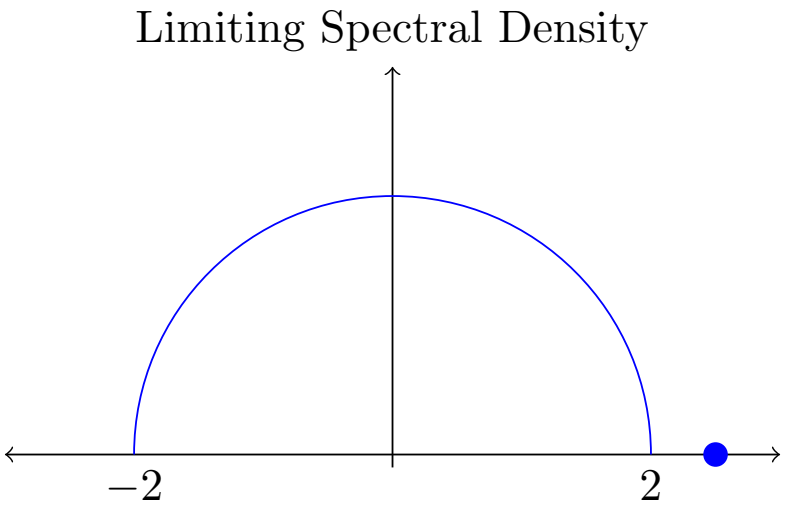

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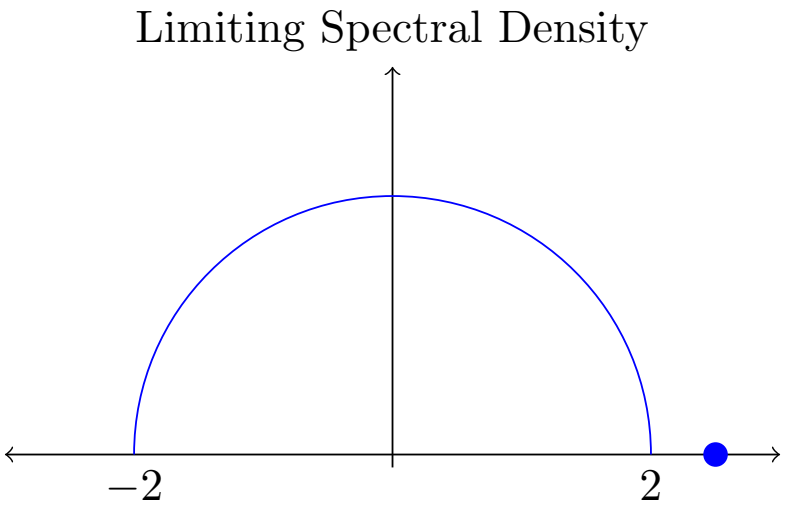

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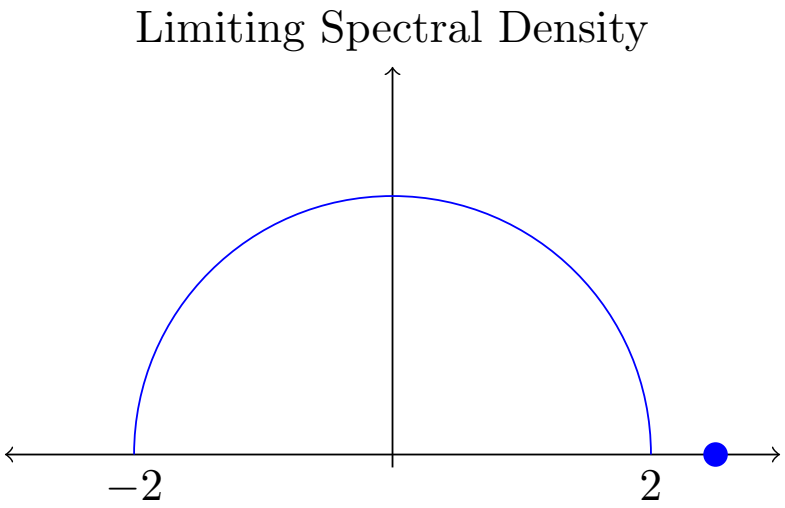

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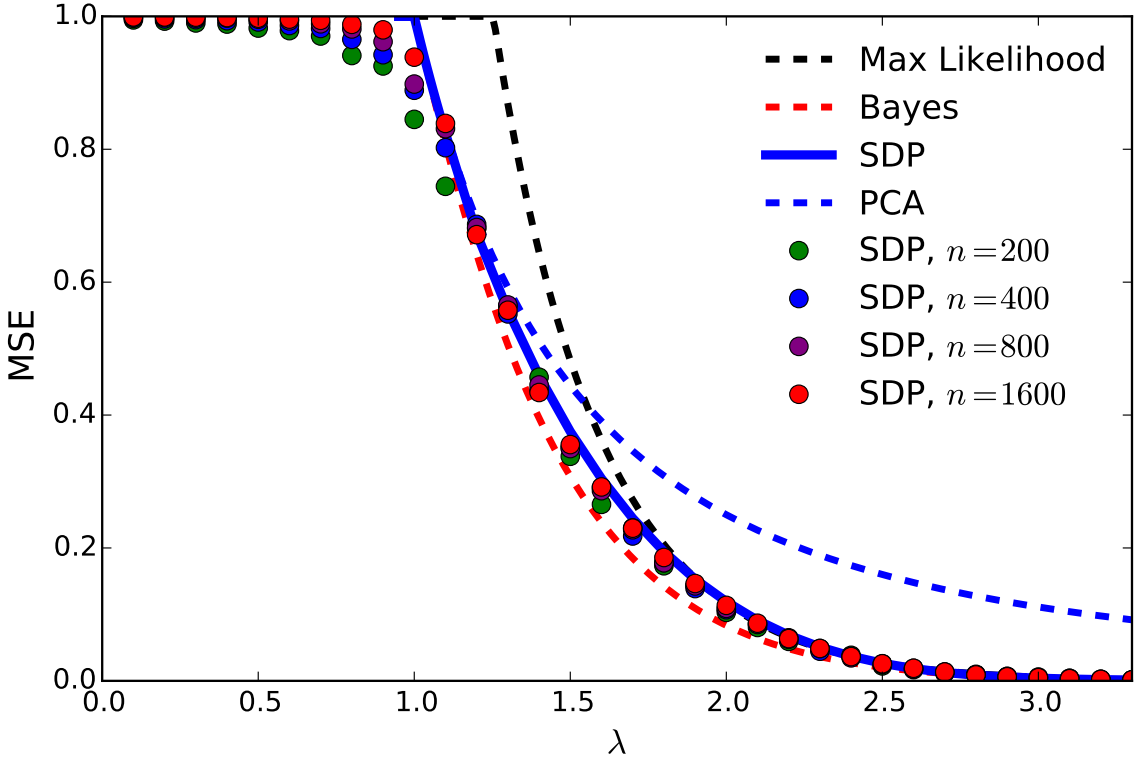
A parenthesis

The Gaussian model is very interesting



Strategy

I. Prove equivalence to Gaussian model

II. Analyze Gaussian model

We want to prove

$$\frac{1}{\sqrt{d}}\mathsf{SDP}(\boldsymbol{A}^{\rm cen}) \approx \mathsf{SDP}(\boldsymbol{B}(\lambda))$$

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A simple Lindeberg lemma

- $X_1, X_2, \dots X_M$ iid

$$X_i = \begin{cases} \frac{1}{\sqrt{d}}\left(1 - \frac{d}{n}\right) & \text{with probability } \frac{d}{n}\,, \\ -\frac{\sqrt{d}}{n} & \text{with probability } \left(1 - \frac{d}{n}\right). \end{cases}$$

$\mathbb{E}\{X_i\} = 0$, $\mathbb{E}\{X_i^2\} = (1/n) - (d/n^2)$

- $Z_1, Z_2, \dots Z_M \sim_{i.i.d.} \mathrm{N}(0, 1/n)$

Lemma

Assume $M = n(n-1)/2$, $F \in C_3(\mathbb{R}^M)$, $d \le n^{2/3}/10$. Then

$$\left|\mathbb{E}F(\boldsymbol{X}) - \mathbb{E}F(\boldsymbol{Z})\right| \le \frac{n}{3\sqrt{d}} \max_{i\in[M]} \left(\|\partial_i^2 F\|_\infty \vee \|\partial_i^3 F\|_\infty\right).$$

where $\partial_i^\ell F(\boldsymbol{x}) \equiv \frac{\partial^\ell F}{\partial x_i^\ell}$, and $\|\partial_i^\ell F\|_\infty \equiv \sup_{\boldsymbol{x}\in\mathbb{R}^M} |\partial_i^\ell F(\boldsymbol{x})|$.

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Smoothing

SDP($\boldsymbol{A}$):

$$\begin{aligned} \text{maximize} \quad & \sum_{i,j=1}^{n} A_{ij} \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle \,, \\ \text{subject to} \quad & \boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \dots, \boldsymbol{\sigma}_n)^{\mathsf{T}} \in \mathbb{R}^{n \times n} \,, \\ & \boldsymbol{\sigma}_i \in \mathbb{R}^n \,, \quad \|\boldsymbol{\sigma}_i\|_2 = 1 \,. \end{aligned}$$

Free energy

$$\Phi_k(\beta, k; \boldsymbol{A}) \equiv \frac{1}{\beta} \log \left\{ \int \exp\left(\beta \sum_{i,j=1}^{n} A_{i,j} \langle \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j \rangle \right) \nu_{0,k}(\mathrm{d}\boldsymbol{\sigma}) \right\}$$

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- Sharp information about eigenvalues of random matrices
- A lot of work on SDP with random data

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