Optimality and Sub-optimality of Principal Component Analysis for Spiked Random Matrices

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MIT

Joint work with:
Amelia Perry (MIT), Afonso Bandeira (Courant NYU), Ankur Moitra (MIT)

Random Matrices

Wigner Matrix

$$\frac{1}{\sqrt{n}}W \in \mathbb{R}^{n\times n} \text{ symmetric,}$$
$$W_{ij} \sim \mathcal{N}(0,1)$$

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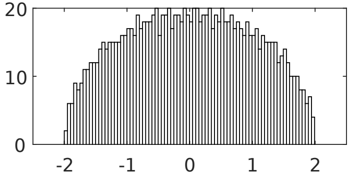

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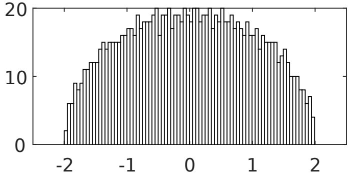

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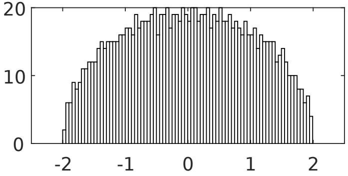

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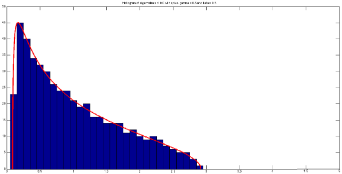

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$$Y = \frac{1}{\sqrt{n}}W + \lambda x x^T$$

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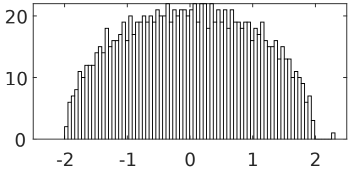

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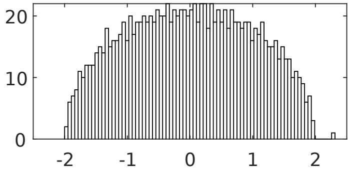

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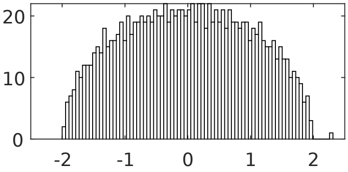

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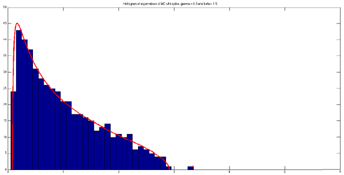

Visible on the largest eigenvalue when

$$|\beta| > \sqrt{\gamma}, \ \gamma = \frac{n}{N}, \ \beta \in [-1, \infty)$$

Statistical Questions

- Detection: distinguish reliably (error prob $\to 0$)

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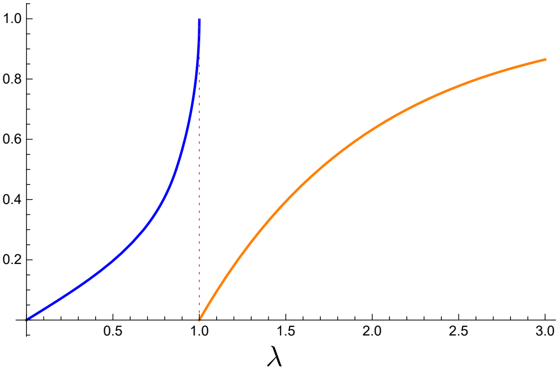
- Need a prior on the spike $x \in \mathbb{R}^n$
  - unit sphere
  - i.i.d. ± 1
  - sparse ± 1

Detection vs Recovery

Hypothesis testing power   Recovery quality



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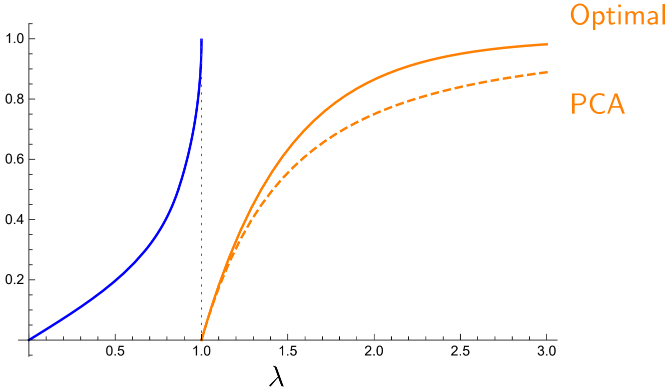

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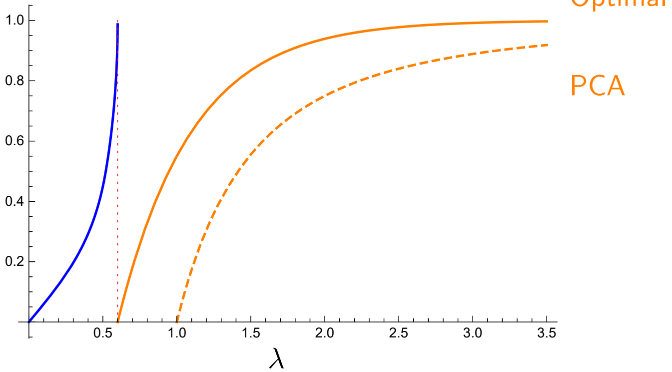

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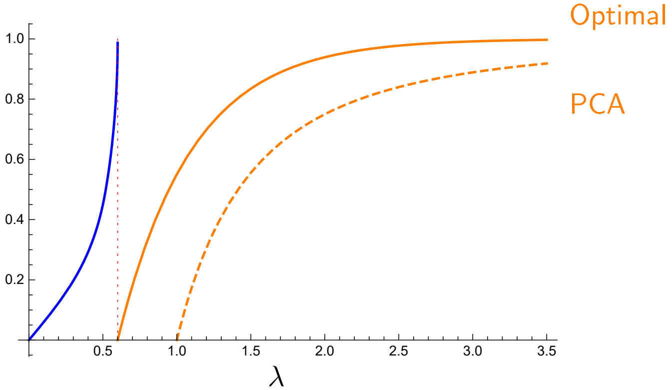

"PCA is sub-optimal"

This talk: focus on detection threshold
(also hypothesis testing bounds, recovery threshold)

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3. Can beat PCA, but only with an inefficient algorithm
   (e.g. sparse priors; Wishart)

Tool: Contiguity

- Sequence of distributions P_n is contiguous to Q_n if for any sequence of events A_n,

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- E.g. if P_n, Q_n have densities p_n, q_n:
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But what about when we know more about the spike?

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- But for sparse priors, with enough sparsity, PCA is no longer optimal.

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$$\frac{1}{N}\sum_{k=1}^{N} y_k y_k^T$$

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- But... for $\gamma > 0.698$ there exists a computationally inefficient procedure that distinguishes the two models for some $\beta \in (-\sqrt{\gamma}, 0)$ (below the spectral threshold).

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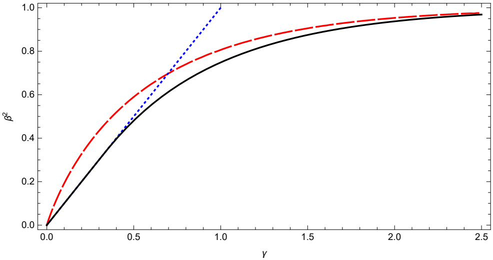
Is there a computational gap?

Rademacher Wishart, Negative β



- PCA: succeeds above the line
- inefficient algorithm: succeeds above the line
- contiguity lower bound: impossible below the line

Back to Wigner: What if noise is not Gaussian?

$$Y = \frac{1}{\sqrt{n}} W + \lambda x x^T$$

$x \sim \mathrm{Unif}\{\mathbb{S}^{n-1}\}$, $W \in \mathbb{R}^{n \times n}$
but $W_{ij} \sim p(w)$ such that $\mathbb{E}w = 0$, $\mathbb{E}w^2 = 1$.

D. Feral, S. Peche, CMP 2006.

T. Tao, V. Vu, MAoRMT 2012.

Back to Wigner: What if noise is not Gaussian?

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Universality: spectral properties are unchanged...

D. Feral, S. Peche, CMP 2006.

T. Tao, V. Vu, MAoRMT 2012.

Can you tell which one is which?

For $W_{ij} \sim \mathrm{Unif}(\pm 1)$, $\lambda < 1$

$$W + \lambda\sqrt{n}xx^T \quad \text{vs} \quad W$$

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-1.0000	1.0000	-1.0000	-1.0000	1.0000	-1.0000
1.0000	1.0000	1.0000	-1.0000	-1.0000	1.0000
-1.0000	1.0000	1.0000	-1.0000	-1.0000	-1.0000
-1.0000	-1.0000	-1.0000	1.0000	-1.0000	1.0000
1.0000	-1.0000	-1.0000	-1.0000	-1.0000	1.0000
-1.0000	1.0000	-1.0000	1.0000	1.0000	1.0000

vs

-0.9988	1.0011	-1.0007	-0.9997	0.9990	-1.0014
1.0011	1.0010	0.9993	-0.9997	-1.0010	0.9987
-1.0007	0.9993	1.0004	-1.0002	-0.9994	-0.9991
-0.9997	-0.9997	-1.0002	1.0001	-1.0002	0.9997
0.9990	-1.0010	-0.9994	-1.0002	-0.9991	1.0012
-1.0014	0.9987	-0.9991	0.9997	1.0012	1.0017

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1.0000	1.0000	1.0000	-1.0000	-1.0000	1.0000
-1.0000	1.0000	1.0000	-1.0000	-1.0000	-1.0000
-1.0000	-1.0000	-1.0000	1.0000	-1.0000	1.0000
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Let's restrict ourselves to when the density $p(w)$ is smooth.

Entrywise function

If noise drawn from non-Gaussian $p(w)$: we will beat PCA by applying some function $f : \mathbb{R} \to \mathbb{R}$ entrywise to our matrix $Y = W + \lambda\sqrt{n}xx^\top$, followed by PCA.

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$$\begin{aligned} f(Y_{ij}) &= f\left(W_{ij} + \lambda\sqrt{n}x_i x_j\right) \\ &\approx f\left(W_{ij}\right) + f'\left(W_{ij}\right)\lambda\sqrt{n}x_i x_j \end{aligned}$$

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- It is (close to) a new spiked Wigner matrix with

$$
\lambda' = \frac{\lambda\mathbb{E}f'\left(W_{ij}\right)}{\sqrt{\mathbb{E}f^2\left(W_{ij}\right)}}.
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- Calculus of variations gives optimal choice of f:

$$f(w) = \frac{-p'(w)}{p(w)}$$

Pre-transformed PCA

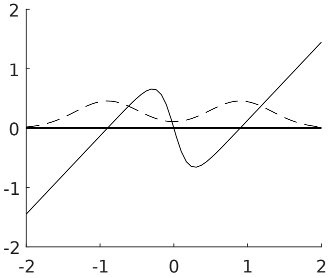
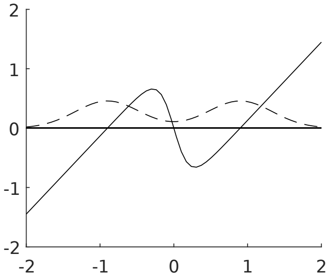


Figure: Dashed: $p(w)$,
Solid: $f(w) = -p'(w)/p(w)$

T. Lesieur, F. Krzakala, L. Zdeborová, Allerton 2015.

F. Krzakala, J. Xu, L. Zdeborová, 2016.

Pre-transformed PCA



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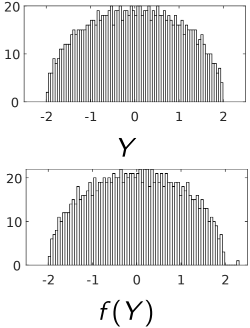

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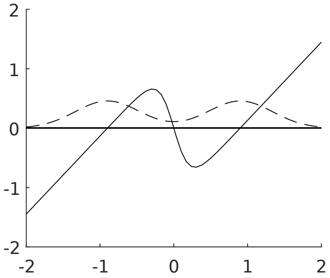

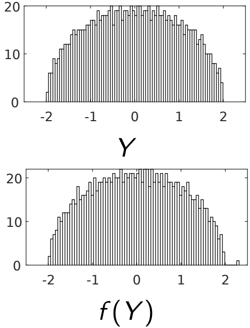

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- New threshold at $\lambda = \frac{1}{\sqrt{F_p}}$, $\quad F_p = \mathbb{E}_p \left(\frac{p'(w)}{p(w)}\right)^2 \geq 1.$

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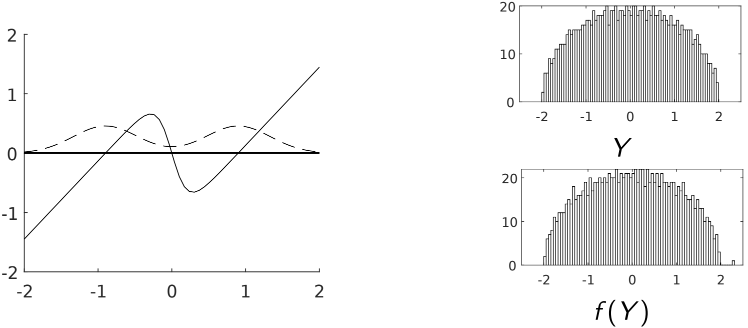

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Gaussian is hardest.

T. Lesieur, F. Krzakala, L. Zdeborová, Allerton 2015.

F. Krzakala, J. Xu, L. Zdeborová, 2016.

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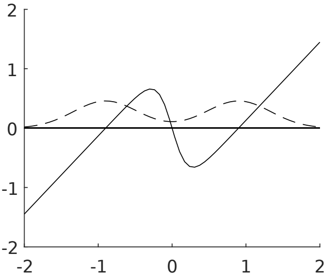

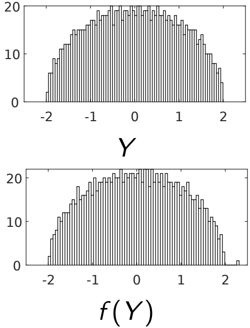

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- Contiguity shows this is optimal!

T. Lesieur, F. Krzakala, L. Zdeborová, Allerton 2015.

F. Krzakala, J. Xu, L. Zdeborová, 2016.

Proof Details: Bounding the (Wigner) Second Moment

$$\mathbb{E}_{Q_n}\left(\frac{dP_n}{dQ_n}\right)^2 \quad = \quad \mathbb{E}\, exp\left(\frac{\lambda^2 n}{2}\langle x, x'\rangle^2\right) \qquad x, x' \sim \mathcal{X}$$

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&= 2\int_0^1 \Pr\left[\langle x, x'\rangle \geq u\right] \exp\left(\frac{\lambda^2 n}{2}u^2\right) \lambda^2 n\, u\, du
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In other words: $\Pr\left[\langle x, x'\rangle \geq u\right] \approx \exp(-n\, R(u))$

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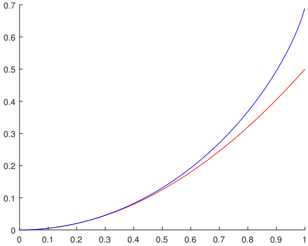
- Bounded iff $\frac{\lambda^2}{2}u^2 - R(u) < 0$ for all $u \in (0,1)$
- How big a parabola can you fit underneath the rate function?
- E.g. Rademacher prior (± 1) has $R(u) = \log 2 - h\left(\frac{1+u}{2}\right)$ where $h(p) = -p\log p - (1-p)\log(1-p)$



$R(u)$

$\frac{1}{2}u^2$ $\quad (\lambda = 1)$

Improvement: Conditioning

J. Banks, C. Moore, J. Neeman, P. Netrapalli, COLT 2016.

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- Goal: P_n contiguous to Q_n: $Q_n(A_n) \to 0 \;\Rightarrow\; P_n(A_n) \to 0$

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- Condition away from rare bad events

J. Banks, C. Moore, J. Neeman, P. Netrapalli, COLT 2016.

Conditioning Example: Sparse Rademacher Prior

J. Banks, C. Moore, R. Vershynin, J. Xu, 2016.

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- Sparsity $\rho \in [0, 1]$

J. Banks, C. Moore, R. Vershynin, J. Xu, 2016.

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- Prior $\mathcal{X}_\rho$: i.i.d. $x_i \sim \frac{1}{\sqrt{\rho n}} \begin{cases} +1 & \text{w.p. } \rho/2 \\ -1 & \text{w.p. } \rho/2 \\ 0 & \text{w.p. } 1-\rho \end{cases}$

J. Banks, C. Moore, R. Vershynin, J. Xu, 2016.

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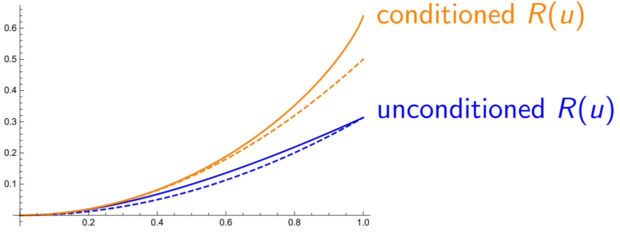
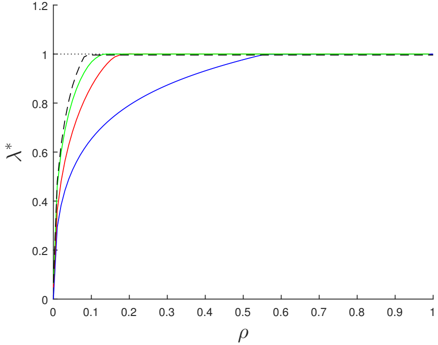


Figure: $\rho = 0.2$

J. Banks, C. Moore, R. Vershynin, J. Xu, 2016.

Sparse Rademacher: Results



- unconditioned
- conditioned
- noise-conditioned (upcoming)
- replica prediction (truth)

Summary

Summary

- 3 scenarios:

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  - PCA optimal (Wigner with spherical or Rademacher prior)

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  - PCA optimal (Wigner with spherical or Rademacher prior)
  - PCA beaten efficiently (non-Gaussian Wigner)
  - PCA beaten inefficiently (Rademacher Wishart; sparse Rademacher Wigner)
- Second moment method: simple, widely-applicable technique to show non-detection lower bounds

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Thanks! Questions?