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

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MIT

Joint work with:
Alex Wein (MIT), Afonso Bandeira (Courant/CDS), 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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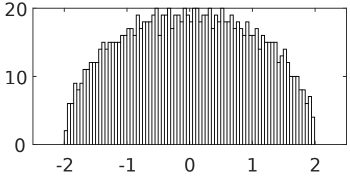

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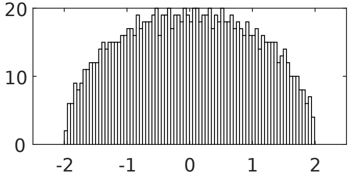

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$\frac{1}{N} \sum_{k=1}^{N} y_k y_k^T$
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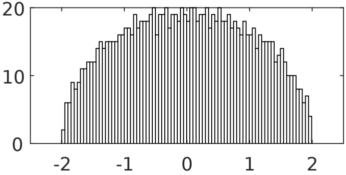

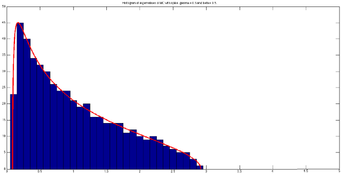

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Spiked Models

Spiked Wigner Matrix

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

$\frac{1}{\sqrt{n}}W$ Wigner, $\|x\| = 1$.

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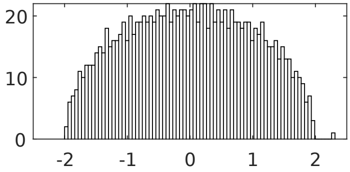

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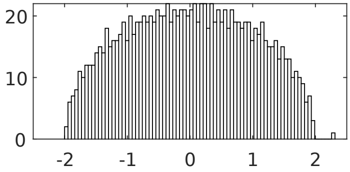

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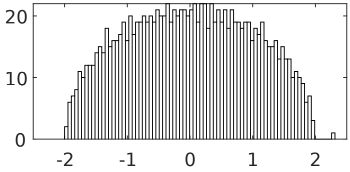

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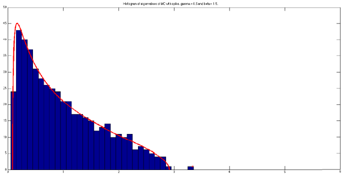

Visible on the largest eigenvalue when

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

Statistical Questions

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

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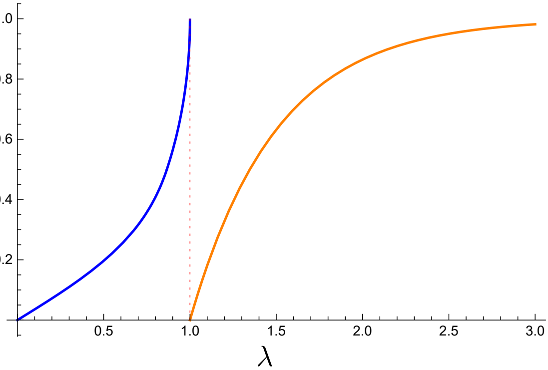
- Need a prior on the spike $x \in \mathbb{R}^n$
  - unit sphere
  - i.i.d. ± 1
  - sparse ± 1

Detection vs Recovery

Hypothesis testing power   Recovery quality



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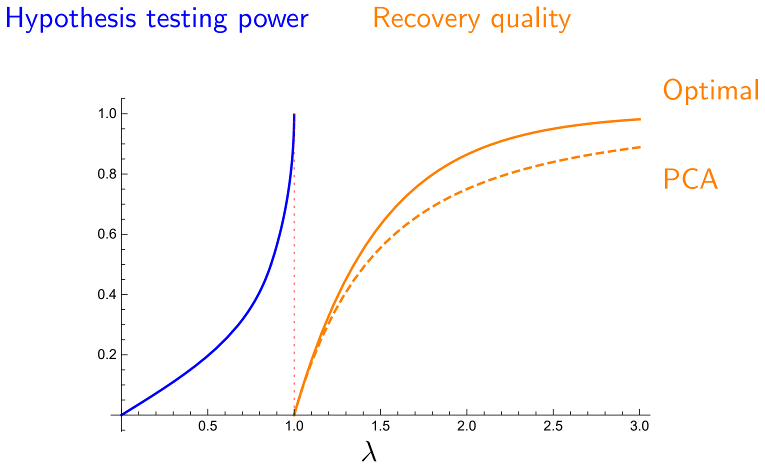

“PCA is optimal”

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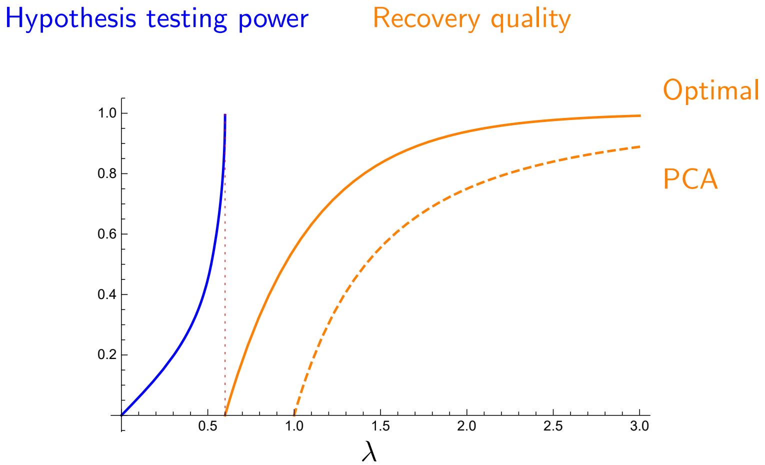

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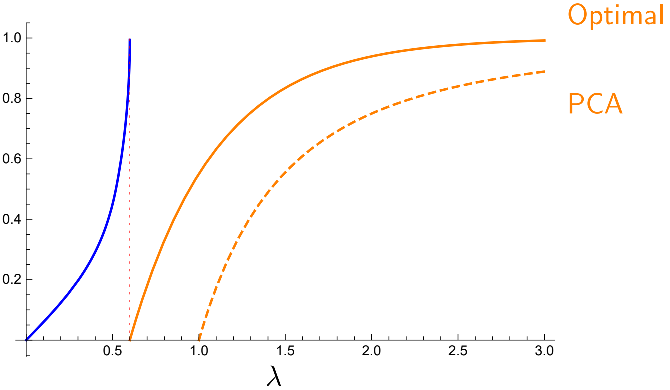

"PCA is sub-optimal"

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

Our Results: 3 Scenarios

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

Lower Bound Concept: Contiguity

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

$$\lim_{n\to\infty} Q_n(A_n) = 0 \quad \Rightarrow \quad \lim_{n\to\infty} P_n(A_n) = 0.$$

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If $\mathbb{E}_{Q_n}\left(\frac{dP_n}{dQ_n}\right)^2 = O(1)$, *then P_n is contiguous to Q_n.*

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Case 1: PCA is optimal

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- Taking $P_n : \frac{1}{\sqrt{n}} W + \lambda x x^T$ with $x \sim \mathcal{X}$, and $Q_n : \frac{1}{\sqrt{n}} W$

[MRZ15] A. Montanari, D. Reichman, O. Zeitouni, NIPS 2015.

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But what about when we know more about the spike?

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Wigner, Rademacher Prior

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

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- Contiguity argument goes through for a general class of priors!

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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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$$\begin{aligned}\mathbb{E}_{Q_n}\left(\frac{dP_n}{dQ_n}\right)^2 &= \mathbb{E}\exp\left(\frac{\lambda^2 n}{2}\langle x, x'\rangle^2\right) \qquad x, x' \sim \mathcal{X} \\ &= \int_0^\infty \Pr\left[\exp\left(\frac{\lambda^2 n}{2}\langle x, x'\rangle^2\right) \geq t\right] dt\end{aligned}$$

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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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$$\mathbb{E}_{Q_n}\left(\frac{dP_n}{dQ_n}\right)^2 \quad \to \quad 2\int_0^1 \lambda^2 n\, u \exp\left[n\left(\frac{\lambda^2}{2}u^2 - R(u)\right)\right] du$$

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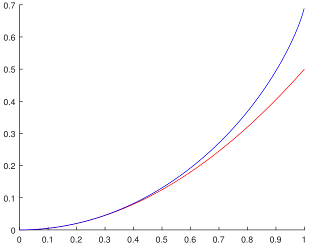
- How big a parabola can you fit underneath the rate function?
- E.g. Rademacher prior (± 1) has $R(u) = \log 2 - h\left(\frac{1+u}{2}\right)$ where $h(p) = -p\log p - (1-p)\log(1-p)$



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

Case 2: PCA can be efficiently beaten

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 $\mathbb{E}w = 0$, $\mathbb{E}w^2 = 1$.

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Universality: spectral properties are unchanged...

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Can you tell which one is which?

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

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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

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

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- Calculus of variations gives optimal choice of f:

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

Pre-transformed PCA

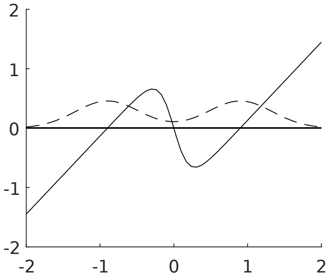

Figure: Dashed: $p(w)$,
Solid: $f(w) = -p'(w)/p(w)$

Related: T. Lesieur, F. Krzakala, L. Zdeborová, Allerton 2015;
F. Krzakala, J. Xu, L. Zdeborová, 2016.

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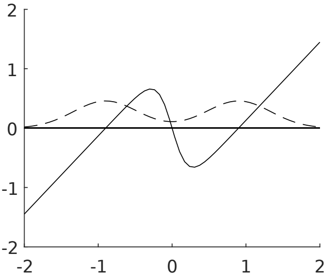

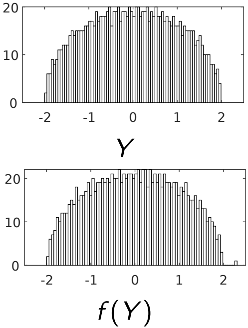

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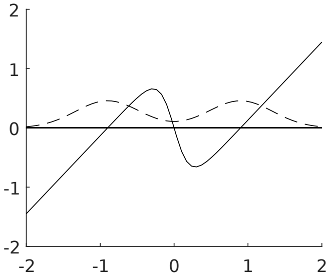

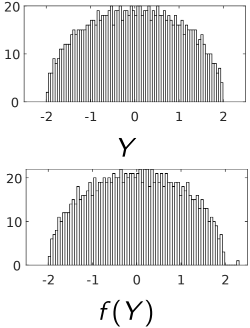

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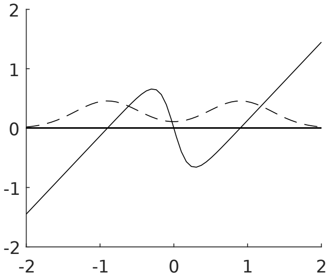

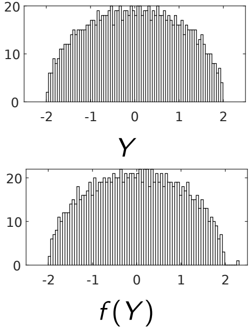

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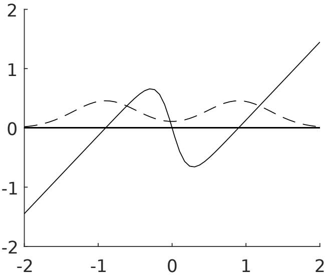

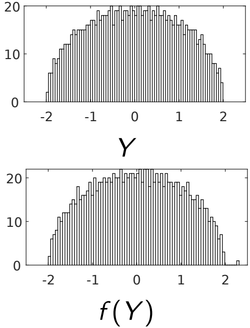

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- Theorem: detection is impossible below this threshold!

Related: T. Lesieur, F. Krzakala, L. Zdeborová, Allerton 2015;
F. Krzakala, J. Xu, L. Zdeborová, 2016.

Case 3: PCA can be inefficiently beaten

Spiked Wishart model, Rademacher prior

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

$y_k \sim \mathcal{N}(0, I_n)$ vs $y_k \sim \mathcal{N}\left(0, I_n + \beta x x^T\right)$, $x \sim \mathrm{Unif}\left\{\pm \frac{1}{\sqrt{n}}\right\}^n$

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Is there a computational gap?

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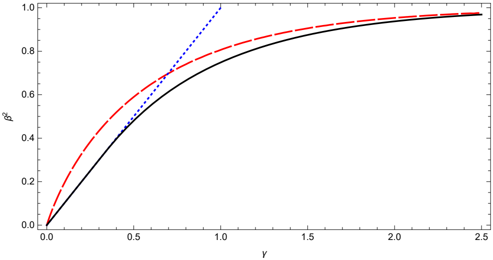
Rademacher Spiked Wishart, Negative β



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

Improvement: Conditioning

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

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

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- Condition away from rare bad events

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

Wigner with Sparse Rademacher Prior

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

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

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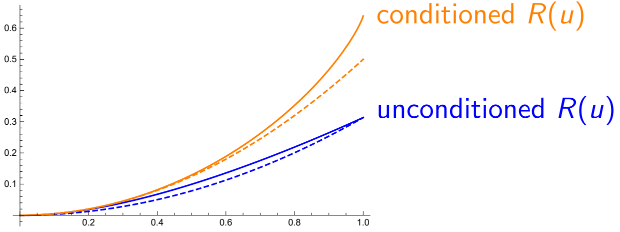
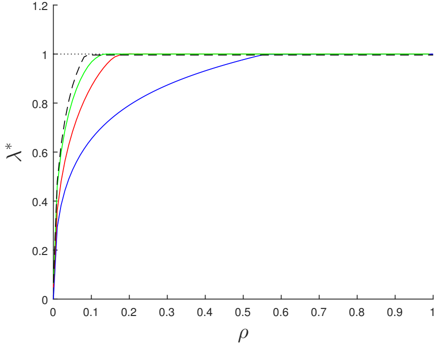


Figure: $\rho = 0.2$

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

Sparse Rademacher: Results



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

Summary

- 3 scenarios:

A. Perry, A. S. Wein, A. S. Bandeira, A. Moitra, "Optimality and Sub-optimality of PCA for Spiked Random Matrices and Synchronization," 2016.

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Thanks! Questions?

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