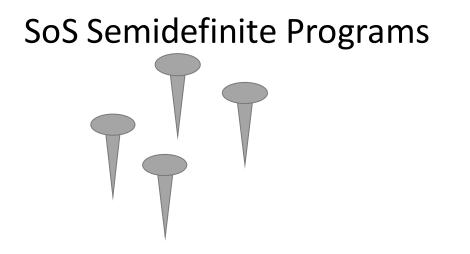
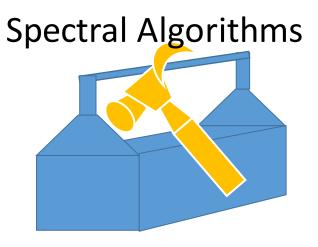
Sum-of-Squares and Spectral Algorithms

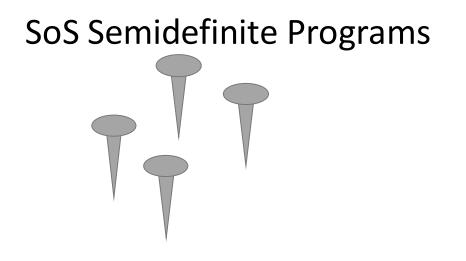
Tselil Schramm June 23, 2017 Workshop on SoS @ STOC 2017

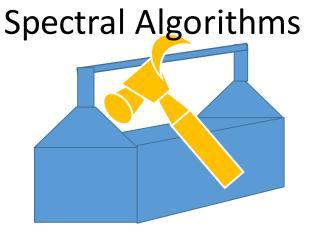
Spectral algorithms as a tool for analyzing SoS.





SoS suggests a new family of spectral algorithms!





Average-Case & Structured Instances

Average Case SoS/Spectral Algorithms

• Tensor Decomposition/Dictionary Learning

[Barak-Kelner-Steurer'14, Ge-Ma'15, Ma-Shi-Steurer'16]

- Planted Sparse Vector [Barak-Brandão-Harrow-Kelner-Steurer-Zhou'12, Barak-Kelner-Steurer'14]
- Tensor Completion [Barak-Moitra'16, Potechin-Steurer'17]
- Refuting Random CSPs [Allen-O'Donnell-Witmer'15, Raghavendra-Rao-S'17]
- Tensor Principal Components Analysis

[Hopkins-Shi-Steurer'15,Bhattiprolu-Guruswami-Lee'16, Raghavendra-Rao-S'17]

Average Case SoS/Spectral Algorithms

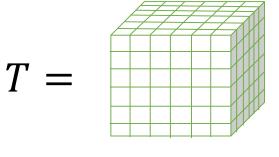
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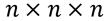
[Barak-Kelner-Steurer'14, Ge-Ma'15, Ma-Shi-Steurer'16]

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Tensor Principle Components Analysis (TPCA)





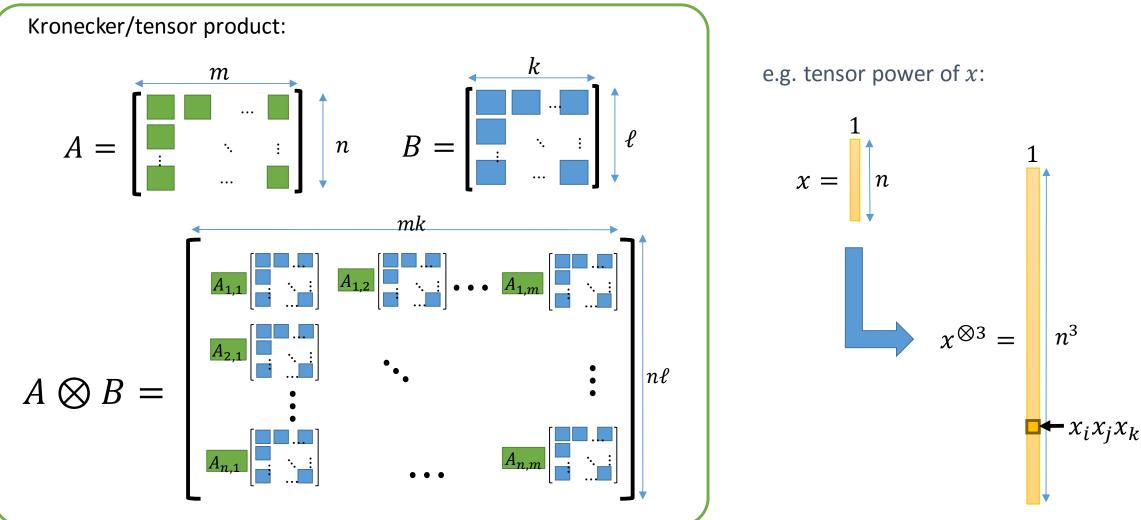
Want ``max tensor singular value/vector'':

$$\sigma^* = \max_{x \in \mathbb{S}_{n-1}} \langle T, x^{\otimes 3} \rangle \text{ and } x^* = \underset{x \in \mathbb{S}_{n-1}}{\operatorname{argmax}} \langle T, x^{\otimes 3} \rangle$$

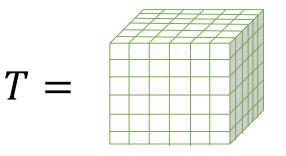
NP-hard in worst case.

This \bigotimes notation...

Definition



Tensor Principle Components Analysis (TPCA)



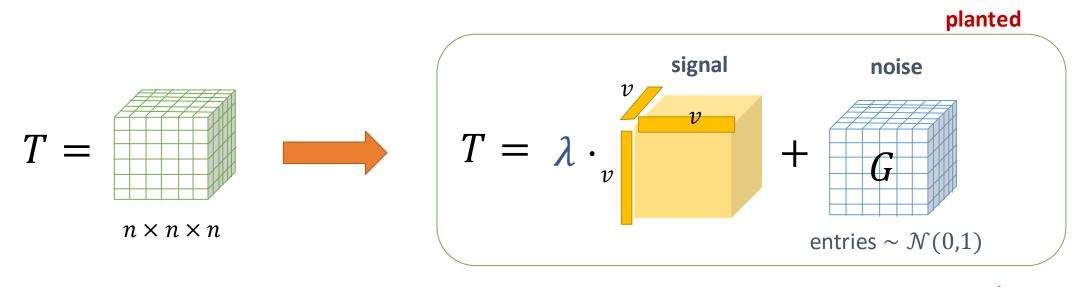
 $n \times n \times n$

Want ``max tensor singular value/vector'': NP-hard in worst case.

$$\sigma^{*} = \max_{x \in \mathbb{S}_{n-1}} \langle T, x^{\otimes 3} \rangle \text{ and } x^{*} = \operatorname*{argmax}_{x \in \mathbb{S}_{n-1}} \langle T, x^{\otimes 3} \rangle$$

$$\langle T, x^{\times 3} \rangle$$

"Spiked" tensor model for TPCA [Montanari-Richard'14]

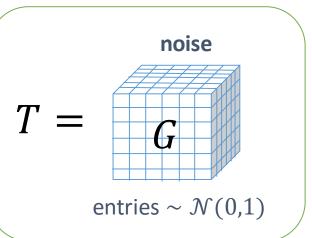




Search: find v in planted case

Distinguishing: planted or random case?

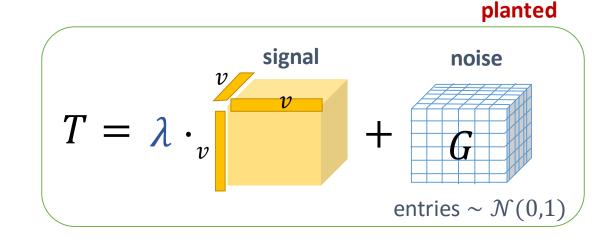
Refutation: certify upper bound on $\max_{x} \langle T, x^{\otimes 3} \rangle$ in random case

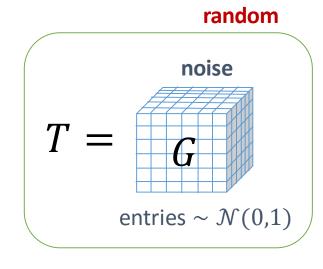


The Plan

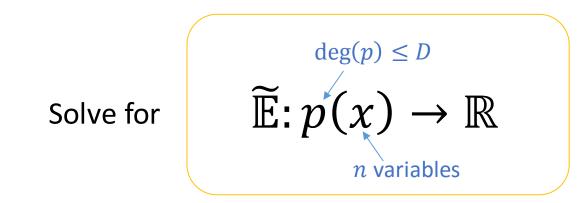
Refutation: certify upper bound on $\max_{x} \langle T, x^{\otimes 3} \rangle$ in random case

- 1. SoS suggests a family of spectral algorithms
- 2. Naïve spectral algorithm
- 3. Improving with SoS spectral algorithms
- Search: find v in planted case
- 4. Use SoS analysis to get fast algorithms





Degree-D SoS



Linearity:

$$\widetilde{\mathbb{E}}[a \cdot p(x) + b \cdot q(x)] = a \cdot \widetilde{\mathbb{E}}[p(x)] + b \cdot \widetilde{\mathbb{E}}[q(x)]$$

Fixed Scalars:

$$\widetilde{\mathbb{E}}[1] = 1$$

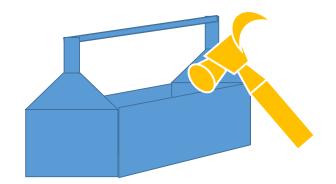
Non-negative squares:

$$\widetilde{\mathbb{E}}[q(x)^2] \ge 0 \operatorname{deg}(q) \le \frac{D}{2}$$

+ problem-specific constraints, e.g.

 $\widetilde{\mathbb{E}}[\|x\|^2] = 1$

SoS suggests spectral algorithms



If we want to bound f(x)... associate some matrix with f and then

Rearrange entries along "monomial symmetries"

Apply degree-*D* SoS polynomial inequalities

Cauchy-Schwarz, Jensen's Inequality (for squares), ...

Use problem-specific constraints (e.g. $x_i^2 = 1$)

SoS captures spectral algorithms

Theorem

$$\widetilde{\mathbb{E}}[f(x)] \le \lambda_{\max}(f)$$

Definition

$$\lambda_{\max}(f) = \underset{F \text{ symmetric}}{\operatorname{argmin}} \{\lambda_{\max}(F)\}$$

$$F = \langle F, x^{\otimes 2d} \rangle$$

symmetric
matrix representation
of
$$f(x)$$

 \downarrow
 $f(x) = \langle F, x^{\otimes 2d} \rangle$

e.g.
$$x_1^2 + 4x_1x_2 + x_2^2 = \left(\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \begin{bmatrix} x_1^2 & x_1x_2 \\ x_1x_2 & x_2^2 \end{bmatrix} \right)$$

.

SoS captures spectral algorithms

Theorem

$$\widetilde{\mathbb{E}}[f(x)] \le \lambda_{\max}(f)$$

symmetric matrix representation of f(x)

Proof

$$\widetilde{\mathbb{E}}[f(x)] = \widetilde{\mathbb{E}}[\langle F, x^{\otimes 2d} \rangle]$$

 $\lambda = \lambda_{\max}(F)$

$$\lambda = \lambda_{\max}(F) \qquad \geq 0 \\ 0 \leq \lambda \cdot Id - F = \sum \sigma_i u_i u_i^{\mathsf{T}} \qquad \text{if } 2d \leq D \\ \widetilde{\mathbb{E}} \langle \lambda \cdot Id - F, x^{\otimes 2d} \rangle = \widetilde{\mathbb{E}} \sum \left(\sqrt{\sigma_i} \cdot \langle u_i, x^{\otimes d} \rangle \right)^2 \geq 0$$

sum of degree-*d* squares

SoS captures spectral algorithms

Theorem

$$\widetilde{\mathbb{E}}[f(x)] \le \lambda_{\max}(f)$$

Proof

What kind of spectral algorithms?

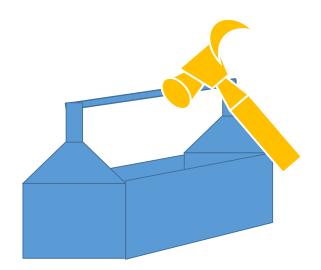
Choose best matrix representation *F* by:

Rearranging entries along "symmetries" of $x^{\otimes d}$

Applying degree-*D* SoS polynomial inequalities

Cauchy-Schwarz, Jensen's Inequality (for squares), ...

Problem-specific constraints (e.g. $x_i^2 = 1$)



What kind of spectral algorithms?

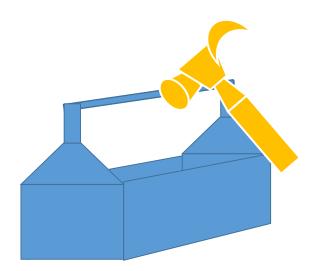
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Cauchy-Schwarz, Jensen's Inequality (for squares), ...

Problem-specific constraints (e.g. $x_i^2 = 1$)



$$\widetilde{\mathbb{E}}[f(x)] = \widetilde{\mathbb{E}}[\langle F, x^{\otimes 2d} \rangle] \leq \lambda \cdot \widetilde{\mathbb{E}}[\|x\|^{2d}]$$

choice of *F* may affect λ !

Claim

There exist f(x) with representations F_1, F_2 such that $f(x) = \langle F_1, x^{\otimes d} \rangle = \langle F_2, x^{\otimes d} \rangle$ but $\lambda(F_1) \gg \lambda(F_2)$.

$$f(x) = \mathbb{E}_{g \sim \mathcal{N}(0, Id)} [\langle x, g \rangle^4] = 3$$

Claim

There exist f(x) with representations F_1 , F_2 such that $f(x) = \langle F_1, x^{\otimes d} \rangle = \langle F_2, x^{\otimes d} \rangle$ but $\lambda(F_1) \gg \lambda(F_2)$.

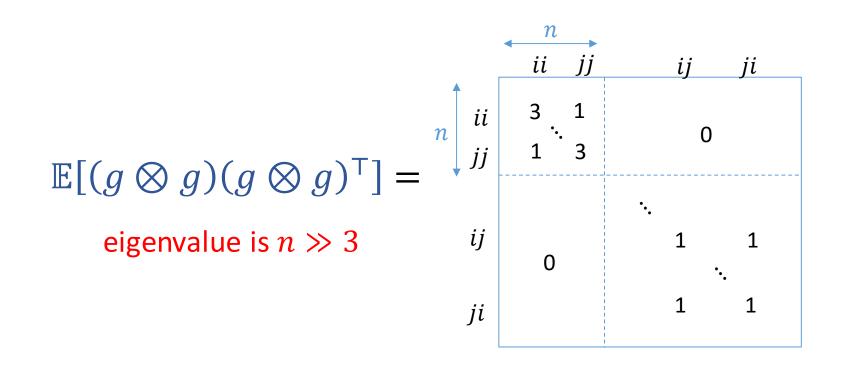
$$f(x) = \mathbb{E}_{g \sim \mathcal{N}(0, Id)} [\langle x, g \rangle^4] = \langle \mathbb{E}[g^{\otimes 4}], x^{\otimes 4} \rangle_{\sim \mathcal{N}(0, 1)}$$

 $\mathbb{E}[(g \otimes g)(g \otimes g)^{\mathsf{T}}]_{ij,k\ell} = \mathbb{E}[g_i g_j g_k g_\ell] = \begin{cases} 3 & i = j = k = \ell \\ 1 & i, j, k, \ell \text{ two distinct pairs} \\ 0 & \text{any index with odd multiplicity} \end{cases}$

Claim

There exist f(x) with representations F_1, F_2 such that $f(x) = \langle F_1, x^{\otimes d} \rangle = \langle F_2, x^{\otimes d} \rangle$ but $\lambda(F_1) \gg \lambda(F_2)$.

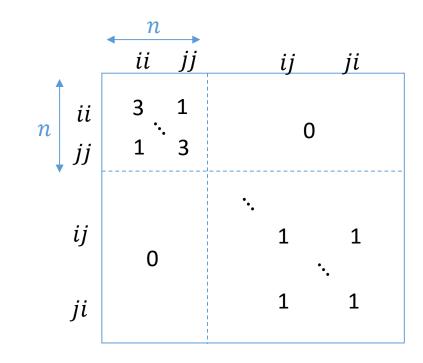
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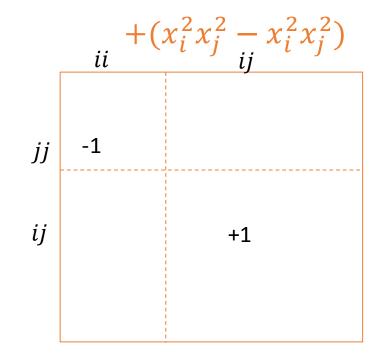


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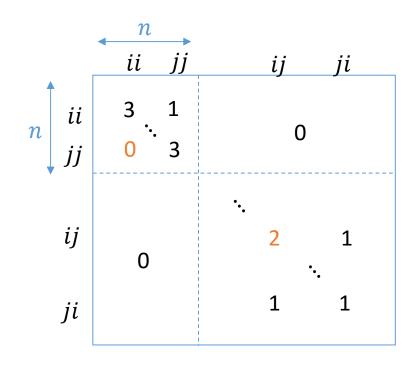


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1

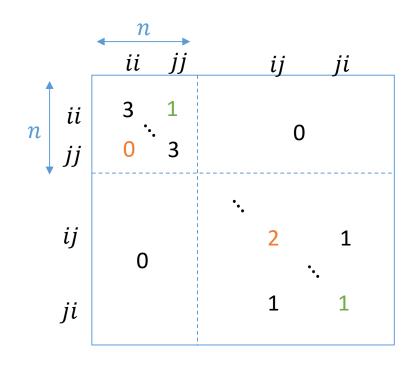


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1

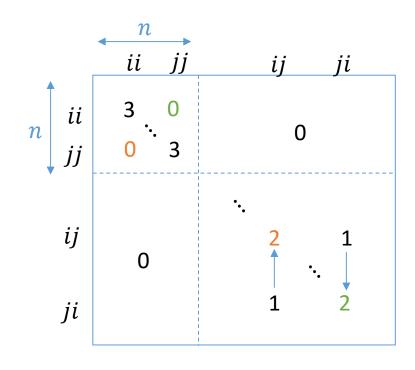


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1



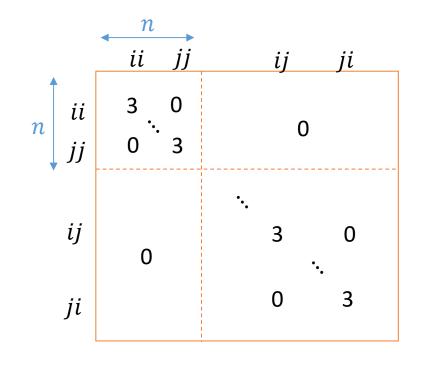
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$$= \langle \mathbb{E}[g^{\otimes 4}], x^{\otimes 4} \rangle^{\sim \mathcal{N}(0, 1)}$$

 $= 3 \cdot Id$

eigenvalues are 3!



Claim

There exist f(x) with representations F_1 , F_2 such that $f(x) = \langle F_1, x^{\otimes d} \rangle = \langle F_2, x^{\otimes d} \rangle$ but $\lambda(F_1) \gg \lambda(F_2)$.

 $f(x) = \mathbb{E}_{g \sim \mathcal{N}(0, Id)} [\langle x, g \rangle^4]$ $= \langle \mathbb{E}[g^{\otimes 4}], x^{\otimes 4} \rangle^{\sim \mathcal{N}(0, 1)}$

$$f(x) = \langle \mathbb{E}[g^{\otimes 4}], x^{\otimes 4} \rangle = \langle 3 \cdot Id, x^{\otimes 4} \rangle = 3 \quad \bigcirc$$

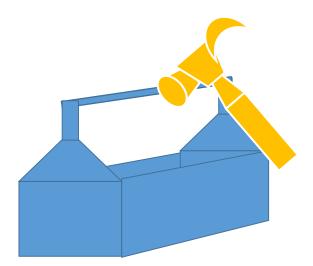
What kind of spectral algorithms?

Choose best matrix representation by:

M Rearranging entries along "symmetries" of $x^{\otimes d}$

Applying degree-*D* SoS polynomial inequalities

Cauchy-Schwarz, Jensen's Inequality (for squares), ...



Tensor Norm Refutation

random case, noise only

$$\max_{x \in \mathbb{S}_n} \left\langle G, x^{\otimes 3} \right\rangle \leq O(\sqrt{n}) \text{ with high probability over } G$$

Claim

"Simple" spectral algorithm can only certify O(n).

Proof:

$$\langle G, x^{\otimes 3} \rangle \leq \sigma_{\max}(F_G)$$

$$G$$
 n n

Representations all the same because *G* is symmetric with iid entries

Gordon's Theorem $\rightarrow \sigma_{\max}(G) \approx n$

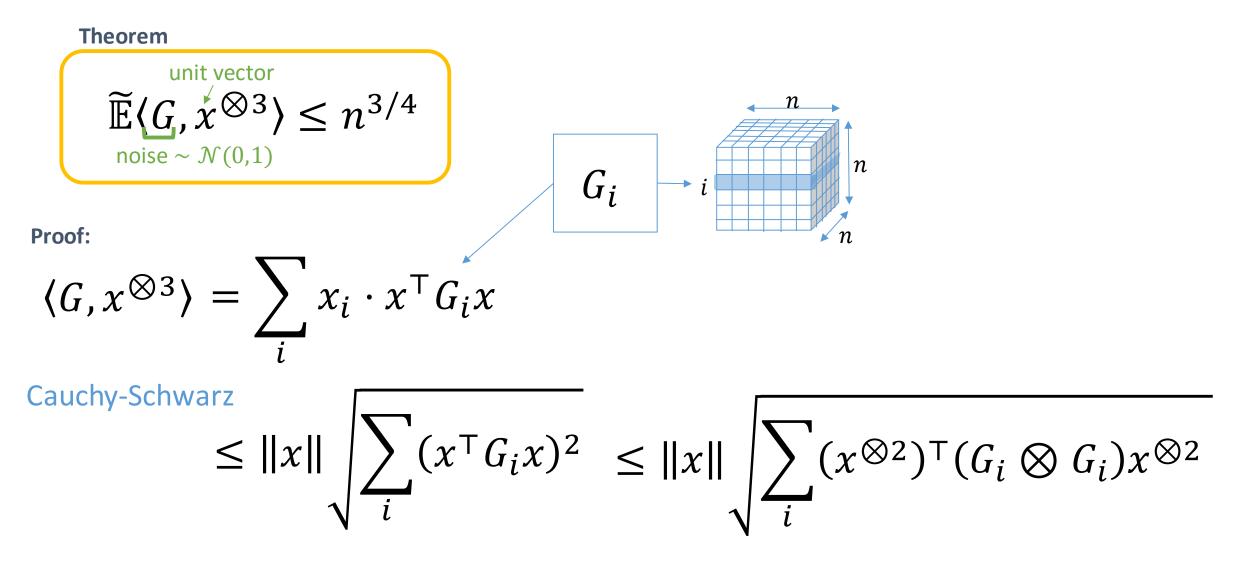
SoS Cauchy-Schwarz

$$\widetilde{\mathbb{E}}\langle f,g\rangle \leq \left(\widetilde{\mathbb{E}}\|g\|^2\right)^{1/2} \left(\widetilde{\mathbb{E}}\|f\|^2\right)^{1/2} \text{ if } D \geq 2\text{deg}(f), 2\text{deg}(g).$$

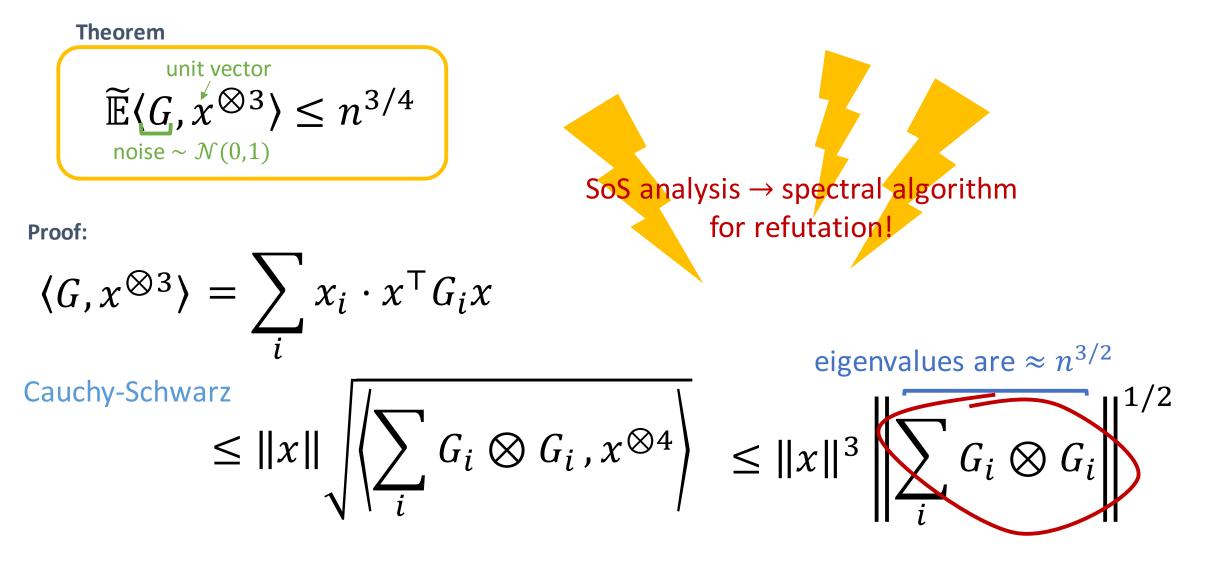
Proof:

$$\mathbb{E}\langle f,g\rangle \leq \frac{1}{2}\mathbb{E}||f||^{2} + \frac{1}{2}\mathbb{E}||g||^{2} \qquad \widetilde{\mathbb{E}}\langle f,g\rangle \leq \frac{1}{2}\widetilde{\mathbb{E}}||f||^{2} + \frac{1}{2}\widetilde{\mathbb{E}}||g||^{2}$$
$$\overset{\text{degree} \leq D \text{ square}}{0 \leq \frac{1}{2}||f-g||^{2}}$$

Cauchy-Schwarz for Tensor PCA Refutation



Cauchy-Schwarz for Tensor PCA Refutation

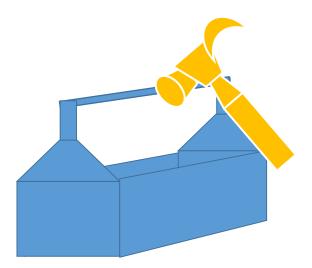


What kind of spectral algorithms?

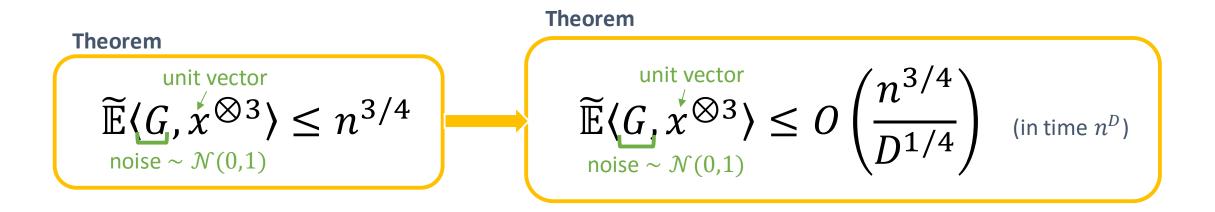
Choose best matrix representation by:

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Applying degree-*D* SoS polynomial inequalities Cauchy-Schwarz, Jensen's Inequality (for squares), ...



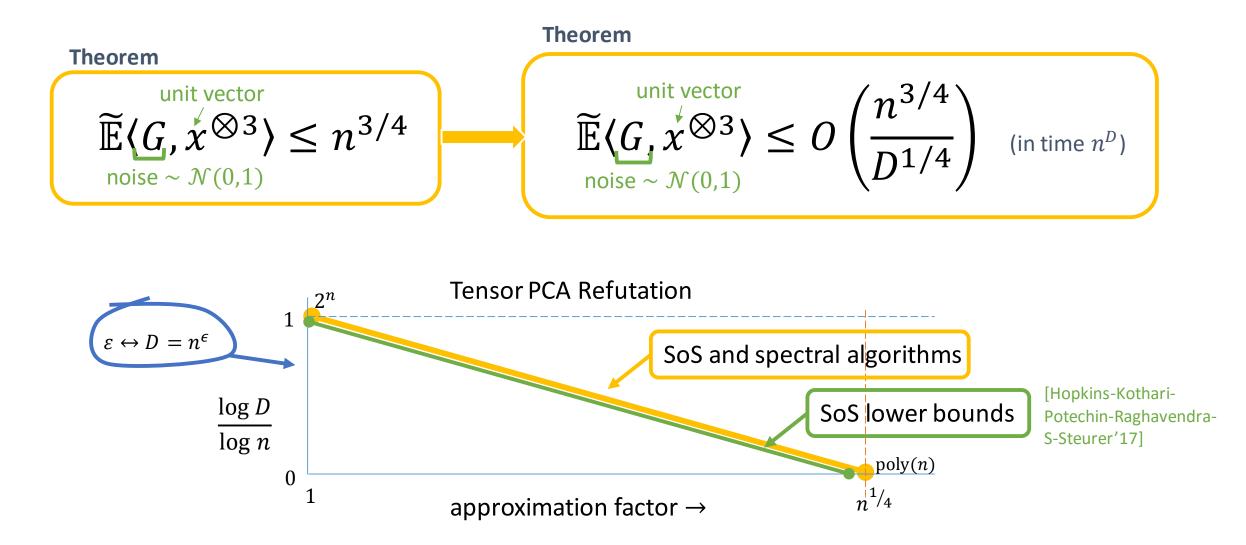
Better Approx (in more time)



But actually,
$$\max_{x \in S_n} \langle G, x^{\otimes 3} \rangle \leq O(\sqrt{n}).$$

Information-theoretically, can certify $\leq O(\sqrt{n})$ in time 2^n (epsilon net).

Better Approx (in more time)



Jensen's Inequality

For d a power of 2, $D \ge d \cdot \deg(f)$

$$\widetilde{\mathbb{E}}[f(x)] \leq \left(\widetilde{\mathbb{E}}[f(x)^d]\right)^{1/d}$$

Proof by induction on d...

$$\begin{split} 0 &\leq \widetilde{\mathbb{E}} \big(f(x)^d - \widetilde{\mathbb{E}} [f(x)^d] \big)^2 \\ \widetilde{\mathbb{E}} [f(x)^d]^2 &\leq \widetilde{\mathbb{E}} [f(x)^{2d}] \\ \widetilde{\mathbb{E}} [f(x)^d] &\leq \left(\widetilde{\mathbb{E}} [f(x)^{2d}] \right)^{1/2} \text{ apply inductive hypothesis} \end{split}$$

Jensen's Inequality

For d a power of 2, $D \ge d \cdot \deg(f)$

 $\widetilde{\mathbb{E}}[f(x)] \leq \left(\widetilde{\mathbb{E}}[f(x)^d]\right)^{1/d}$

We can take advantage of increased symmetry in higher-degree polynomials (more matrix representations)

Better Approximation

Theorem

$$\begin{array}{c} \text{unit vector} \\ \widetilde{\mathbb{E}}\langle G, x^{\bigotimes 3} \rangle \leq O\left(\frac{n^{3/4}}{D^{1/4}}\right) \quad (\text{in time } n^{D}) \\ \text{noise} \sim \mathcal{N}(0,1) \end{array}$$

1/2

Proof:

$$\widetilde{\mathbb{E}}\langle G, x^{\otimes 3} \rangle = \widetilde{\mathbb{E}} \sum_{i} x_{i} \cdot x^{\top} G_{i} x \leq \left(\widetilde{\mathbb{E}} \left| x^{\otimes 4}, \sum_{i} G_{i} \otimes G_{i} \right| \right)$$

Jensen's inequality for *d* some power of 2

$$\leq \left(\widetilde{\mathbb{E}} \left(x^{\otimes 4}, \sum_{i} G_{i} \otimes G_{i} \right)^{d} \right)^{1/2d}$$

Better Approximation

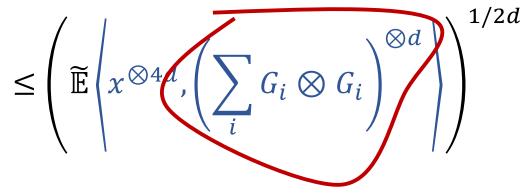
Theorem

$$\begin{array}{c} \text{unit vector} \\ \widetilde{\mathbb{E}}\langle G, \overset{\star}{x}^{\otimes 3} \rangle \leq O\left(\frac{n^{3/4}}{D^{1/4}}\right) \quad (\text{in time } n^{D}) \\ \text{noise} \sim \mathcal{N}(0,1) \end{array}$$

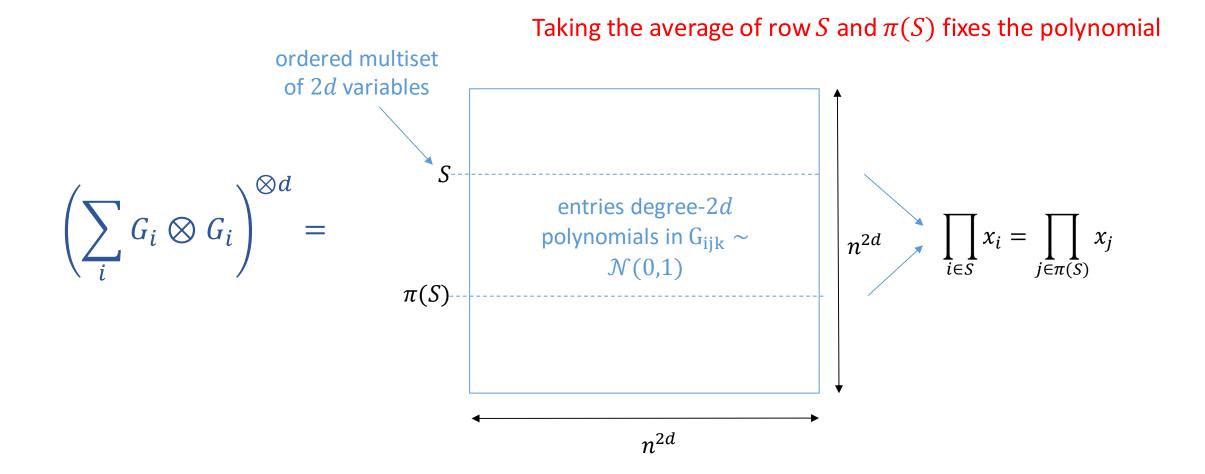
Proof:

$$\widetilde{\mathbb{E}}\langle G, x^{\otimes 3} \rangle = \widetilde{\mathbb{E}} \sum_{i} x_{i} \cdot x^{\top} G_{i} x \leq \left(\widetilde{\mathbb{E}} \left(x^{\otimes 4}, \sum_{i} G_{i} \otimes G_{i} \right) \right)^{1/2}$$

Jensen's inequality for *d* some power of 2

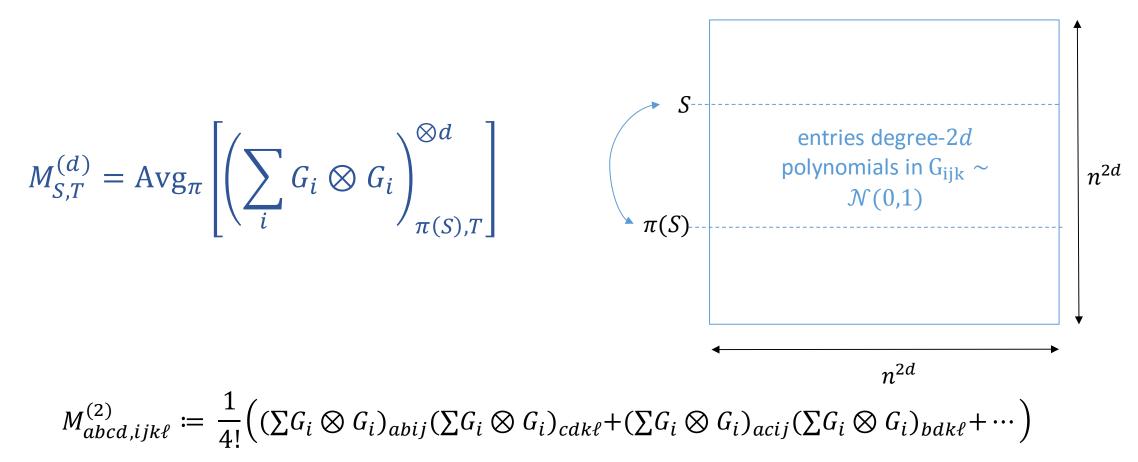


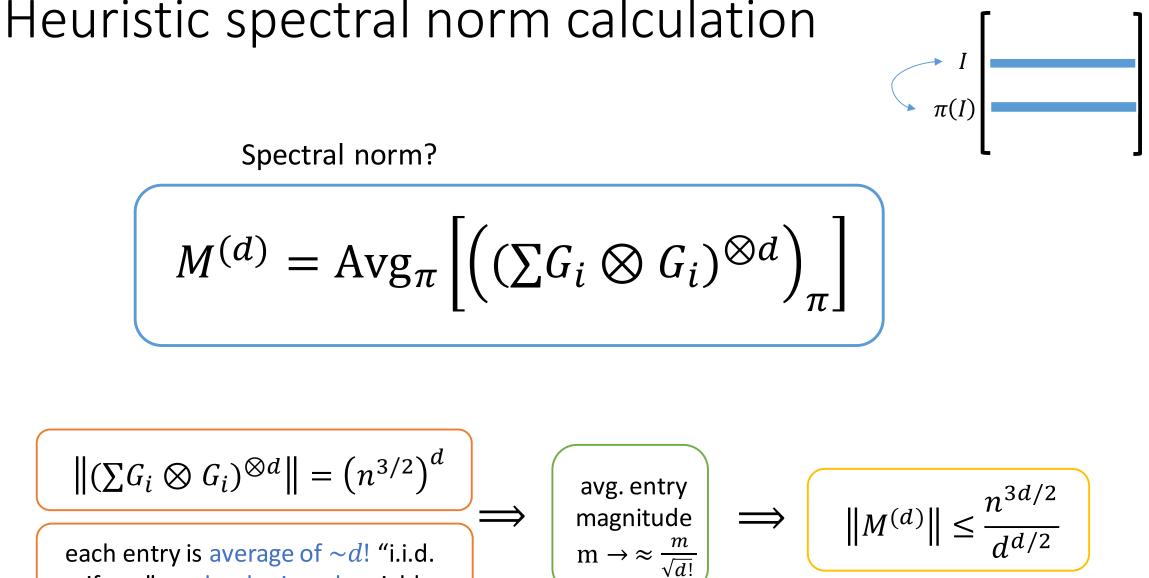
Symmetrize to improve eigenvalue



Symmetrizing to improve eigenvalue

Taking the average of row S and $\pi(S)$ fixes the polynomial





each entry is average of $\sim d!$ "i.i.d. uniform" randomly signed variables

Improving Tensor PCA noise parameter

$$\widetilde{\mathbb{E}}\langle G, x^{\otimes 3} \rangle \leq \left(\widetilde{\mathbb{E}} \left| x^{\otimes 4}, \sum_{i} G_{i} \otimes G_{i} \right| \right)^{1/2}$$

$$\widetilde{\mathbb{E}}\langle G, \overset{\checkmark}{x^{\otimes 3}} \rangle \leq O\left(\frac{n^{3/4}}{D^{1/4}}\right)$$
noise ~ $\mathcal{N}(0,1)$

Theorem

Jensen's inequality for *d* some power of 2 (if $D \ge 4d$)

$$\leq \left(\widetilde{\mathbb{E}} \left| x^{\otimes 4d}, \left(\sum_{i} G_{i} \otimes G_{i} \right)^{\otimes d} \right| \right)^{1/2}$$

Average over symmetries of $x^{\otimes 2d}$ to reduce matrix representation eigenvalues

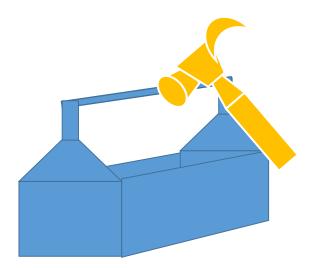
$$= \left(\widetilde{\mathbb{E}}\langle x^{\otimes 4d}, \underline{M}^{(d)}\rangle\right)^{1/2d} \leq \left\|M^{(d)}\right\|^{1/2d} \leq \frac{n^{3/4}}{d^{1/4}} \quad \text{w.h.p.}$$

What kind of spectral algorithms?

Choose best matrix representation by:

M Rearranging entries along "symmetries" of $x^{\otimes d}$

Applying degree-*D* SoS polynomial inequalities Cauchy-Schwarz, Jensen's Inequality (for squares), ...



Other SoS (via Spectral) Algorithms

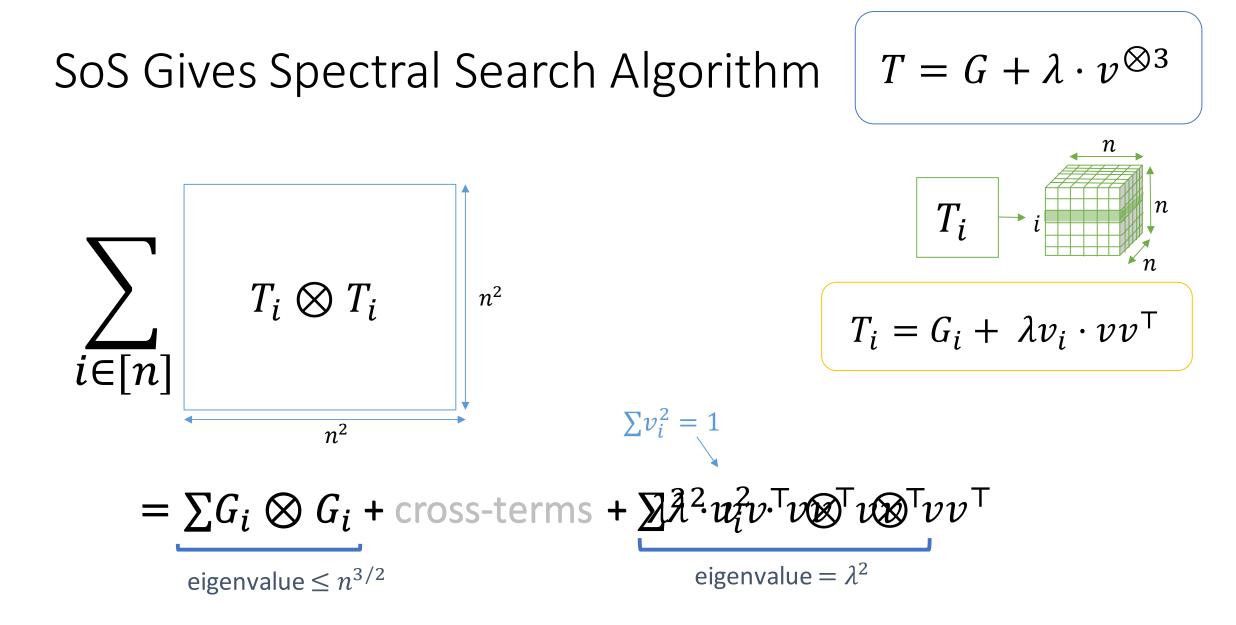
- Tensor Decomposition: symmetry, Cauchy-Schwarz, constant-d Jensen's
- Dictionary Learning: symmetry + tensor decomposition

[Barak-Kelner-Steurer'14, Ge-Ma'15, Ma-Shi-Steurer'16]

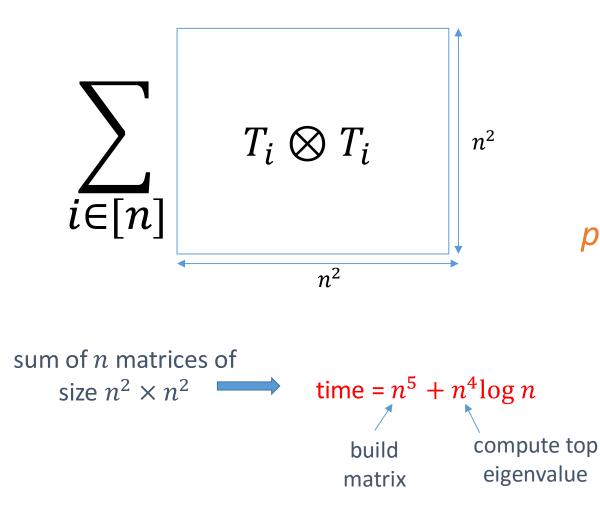
- Planted Sparse Vector: symmetry [Barak-Brandão-Harrow-Kelner-Steurer-Zhou'12, Barak-Kelner-Steurer'14]
- Tensor Completion: symmetry, Cauchy-Schwarz [Barak-Moitra'16, Potechin-Steurer'17]
- Refuting Random CSPs: symmetry, Cauchy-Schwarz, Jensen's, $(x_i^2 = 1)$ constraints [Allen-O'Donnell-Witmer'15, Raghavendra-Rao-S'17]
- Polynomial Maximization over S_n : symmetry, Cauchy-Schwarz, Jensen's, *worst case* [Bhattiprolu-Ghosh-Guruswami-E.Lee-Tulsiani'16]

Fast spectral algorithms from SoS Analyses

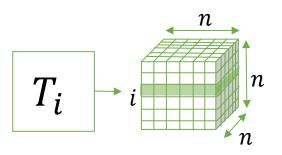
[Hopkins-S-Shi-Steurer'16]



Running in $O(n^5)$



 $T = G + \lambda \cdot v^{\otimes 3}$



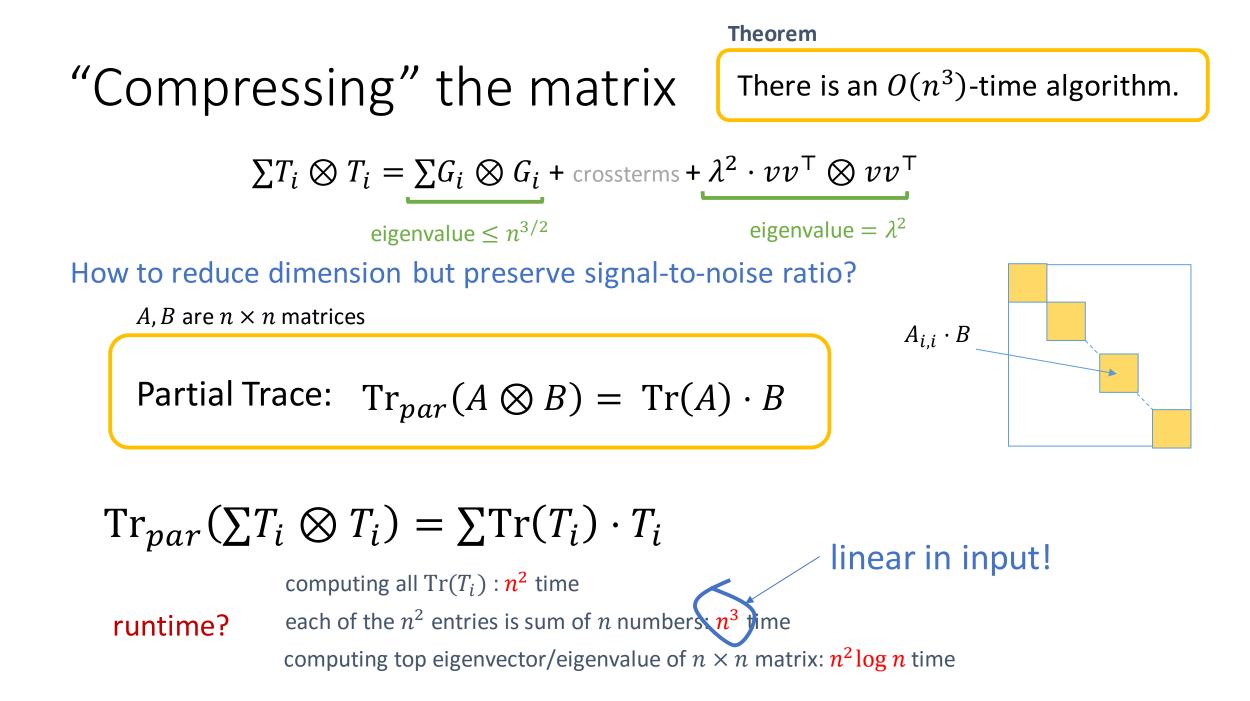
practical spectral algorithm?

Theorem

Can compress to get an $O(n^3)$ -time algorithm.

Theorem
"Compressing" the matrix There is an
$$O(n^3)$$
-time algorithm.

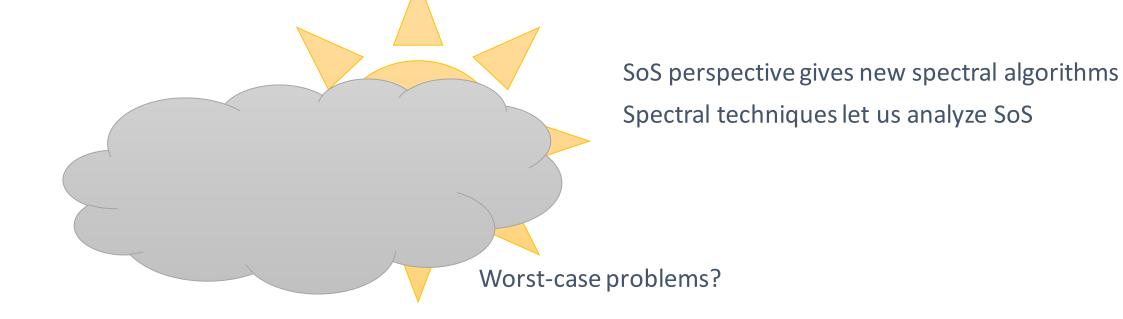
$$\sum T_i \otimes T_i = \sum G_i \otimes G_i + \operatorname{crossterms} + \lambda^2 \cdot vv^\top \otimes vv^\top$$
eigenvalue $\leq n^{3/2}$ eigenvalue $= \lambda^2$
How to reduce dimension but preserve signal-to-noise ratio?
 $A, B \text{ are } n \times n \text{ matrices}$
Partial Trace: $\operatorname{Tr}_{par}(A \otimes B) = \operatorname{Tr}(A) \cdot B$
 $\operatorname{Tr}_{par}(\lambda^2 vv^\top \otimes vv^\top) = \lambda^2 ||v||^2 \cdot vv^\top = \lambda^2 vv^\top$
 $\operatorname{Tr}_{par}(\sum G_i \otimes G_i) = \sum \operatorname{Tr}(G_i) \cdot G_i \to \operatorname{eigs} n^{3/2}$
 $\approx \pm n^{1/2}}$ signal-to-noise ratio preserved!



Fast Spectral Algorithms via SoS

Secret Sauce: apply partial trace to SoS matrix (in a way that enables fast power iteration)

- Tensor PCA [Hopkins-S-Shi-Steurer'16]
- Tensor decomposition [Hopkins-S-Shi-Steurer'16, S-Steurer'17]
- Planted Sparse Vector [Hopkins-S-Shi-Steurer'16]
- Tensor Completion [Montanari-Sun'17]



Spectral Algorithms

Sum-of-Squares Algorithms

