Lecture 1: Introduction to the Sum of Squares Hierarchy

Lecture Outline

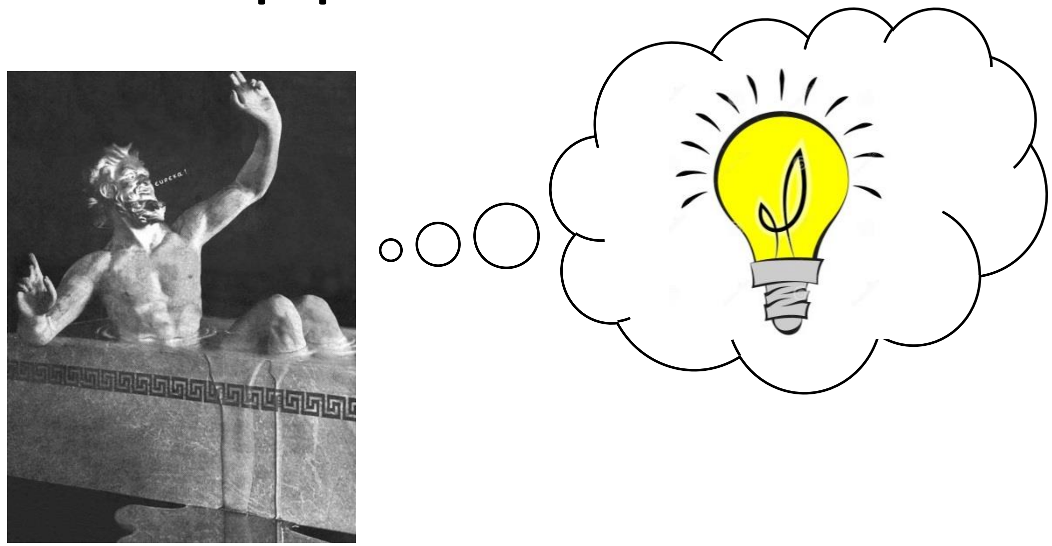
- Part I: Introduction/Motivation
- Part II: Planted Clique
- Part III: A Game for Sum of Squares (SOS)
- Part IV: SOS on General Equations
- Part V: Overview of SOS results and Seminar Plan

Part I: Introduction/Motivation

Goal of Complexity Theory

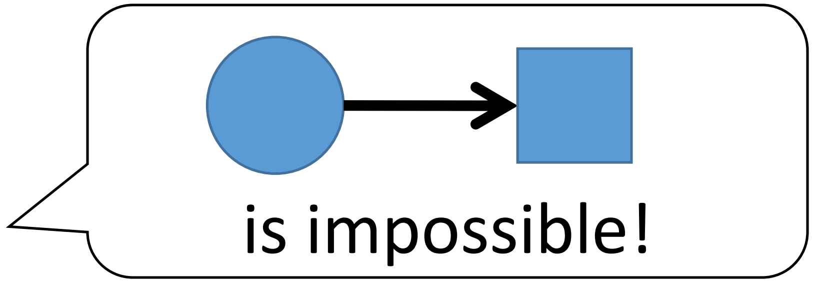
- Fundamental goal of complexity theory: Determine the computational resources (such as time and space) needed to solve problems
- Requires upper bounds and lower bounds

Upper Bounds



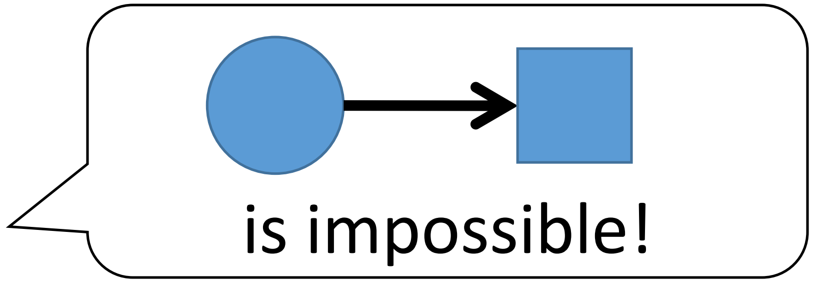
- Requires finding a good algorithm and analyzing its performance.
- Traditionally requires great ingenuity (but stay tuned!)

Lower Bounds



- Requires proving impossibility
- Notoriously hard to prove lower bounds on all algorithms (e.g. P versus NP)
- If we can't yet prove lower bounds on all algorithms, what can we do?

Lower Bounds: What we can do



Path #1

Conditional Lower Bounds: Assume one lower bound, see what follows (e.g. NP-hardness)

Path #2

Restricted Models: Prove lower bounds on restricted classes of algorithms

Both paths give a deep understanding and warn us what not to try when designing algorithms.

This seminar

- This seminar: Analyzing the Sum of Squares (SOS) Hierarchy (a restricted but powerful model)

Why Sum of Squares (SOS)?

- Broadly Applicable: Meta-algorithm (framework for designing algorithms) which can be applied to a wide variety of problems.
- Effective: Surprisingly powerful. Captures several well-known algorithms (max-cut [GW95], sparsest cut [ARV09], unique games [ABS10]) and is conjectured to be optimal for many combinatorial optimization problems!
- Simple: Essentially only uses the fact that squares are non-negative over the real numbers.

SOS for Optimists and Pessimists

- Upper bound side: SOS gives algorithms for a wide class of problems which may well be optimal.
- Lower bound side: SOS lower bounds give strong evidence of hardness

Part II: Planted Clique

SOS on planted clique

- As we'll see later in the course, SOS is not particularly effective on planted clique
- That said, it is an illustrative example for what SOS is.
- Also how I got interested in SOS.

Max Clique Problem

- Max clique: Given an input graph G, what is the size of the largest clique (set of vertices which are all adjacent to each other)?
- NP-hard, was in Karp's original list of NP-hard problems.
- This is worst case, how about average case?

Max Clique on Random Graphs

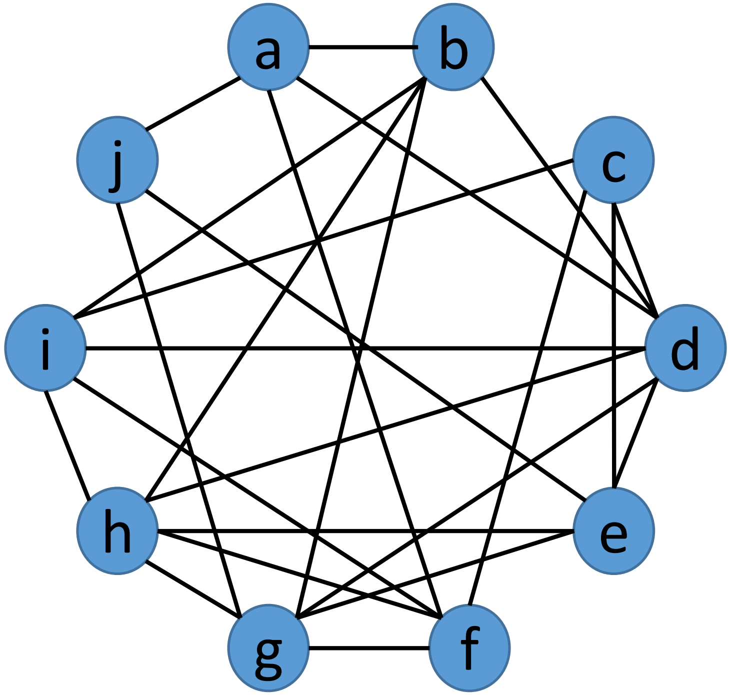
- If G is a random graph, w.h.p. (with high probability) the maximum size of a clique in G is $\left(2 \pm o(1)\right) \log_2 n$
- Idea: expected number of cliques of size k is $2^{-\binom{k}{2}}\binom{n}{k}$
- Solving for the k which makes this 1, we obtain that $k \approx 2 \log_2 n$.
- Open problem [Kar76]: Can we find a clique of size $(1 + \epsilon) \log_2 n$ in polynomial time?

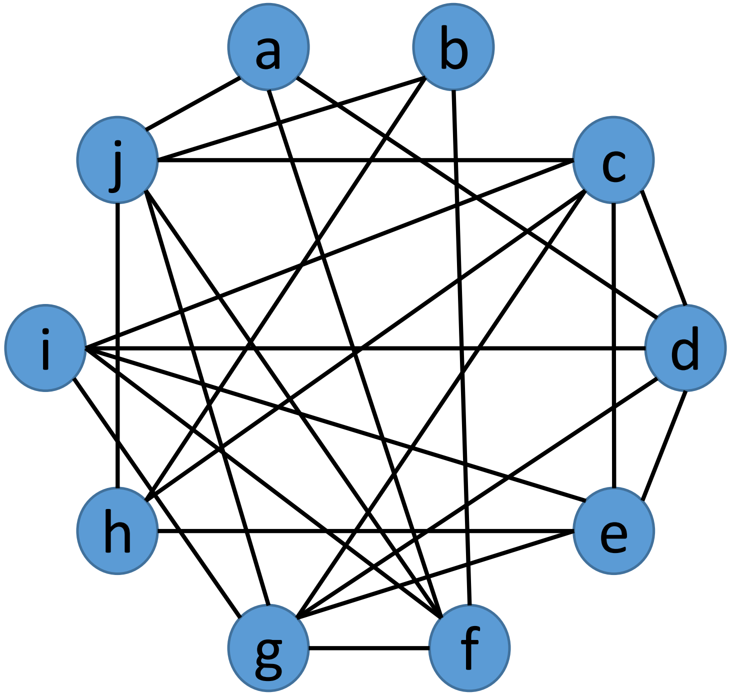
Planted Clique

- Introduced by Jerrum [Jer92] and Kucera [Kuc95]
- Instead of looking for the largest clique in a random graph G, what happens if we plant a clique of size $k \gg 2\log_2 n$ in G by taking k vertices in $V(G)$ and making them all adjacent to each other?
- Can we find such a planted k-clique? Can we tell if a k-clique has been planted?
- Proof complexity analogue: Can we prove that a random graph has no clique of size k?
- Best known algorithm: $k = \Omega(\sqrt{n})$ [AKS98]

Planted Clique Example

- Random instance: $G\left(n, \frac{1}{2}\right)$
- Planted instance: $G\left(n, \frac{1}{2}\right) + K_k$
- Example: Which graph has a planted 5-clique?





Planted Clique Example

- Random instance: $G\left(n, \frac{1}{2}\right)$
- Planted instance: $G\left(n, \frac{1}{2}\right) + K_k$
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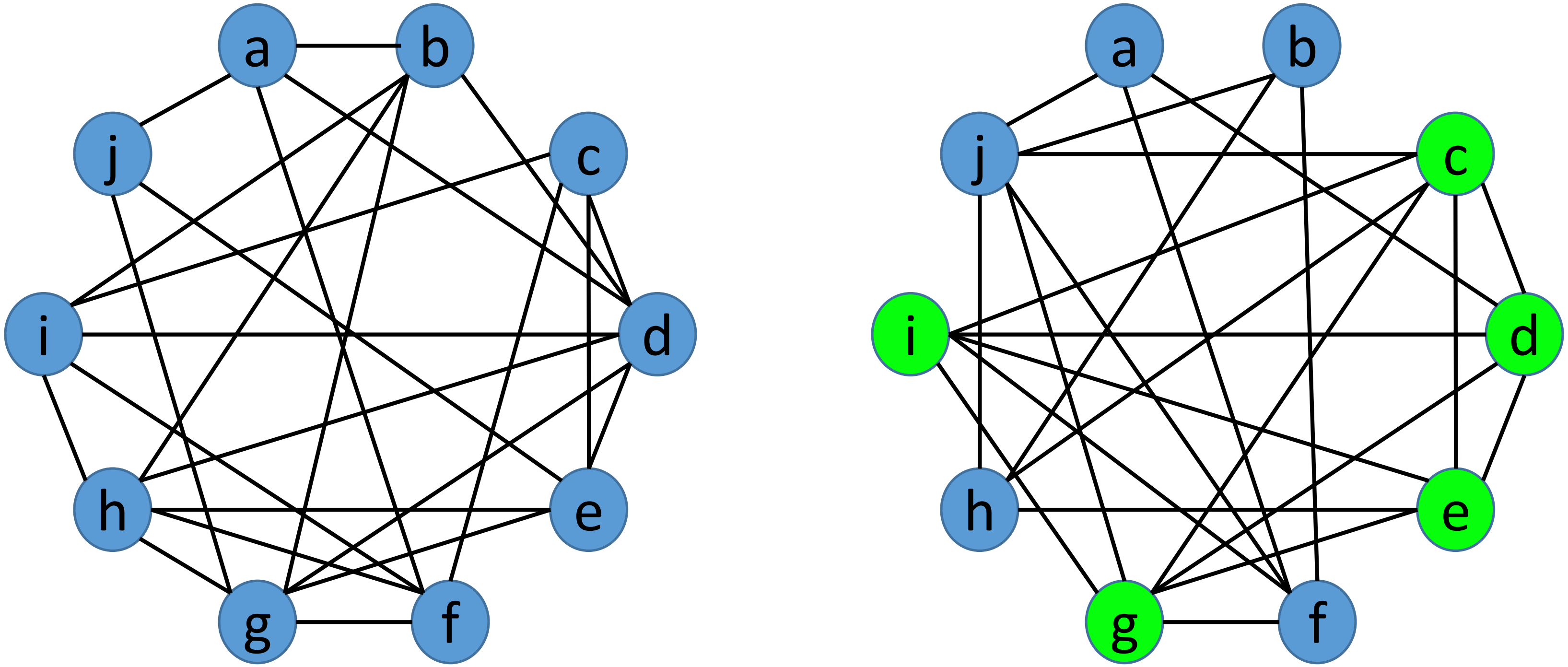


Part III:
A Game for Sum of Squares (SOS)

Distinguishing via Equations

- Recall: Want to distinguish between a random graph and a graph with a planted clique.
- Possible method: Write equations for k-clique (k=planted clique size), use a feasibility test to determine if these equations are solvable.
- SOS gives a feasibility test for equations.

Equations for k-Clique

- Variable x_i for each vertex i in G.
- Want $x_i = 1$ if i is in the clique.
- Want $x_i = 0$ if i is not in the clique.
- Equations:

$x_i^2 = x_i$ for all i.

$x_i x_j = 0$ if $(i, j) \notin E(G)$

$\sum_i x_i = k$

These equations are feasible precisely when G contains a k-clique.

A Game for the Sum of Squares Hierarchy

- SOS hierarchy: feasibility test for equations, expressible with the following game.
- Two players, Optimist and Pessimist
- Optimist: Says answer is YES, gives some evidence
- Pessimist: Tries to refute Optimist's evidence
- SOS hierarchy computes who wins this game (with optimal play)

What evidence should we ask for?

Choice #1: Optimist must give the values for all variables.

How do I find what the variables are?

Optimist

Checking this is easy!

Pessimist

What evidence should we ask for?

Choice #2: No evidence at all.

Yeah, that's solvable!

How do I show this is unsolvable?

Optimist

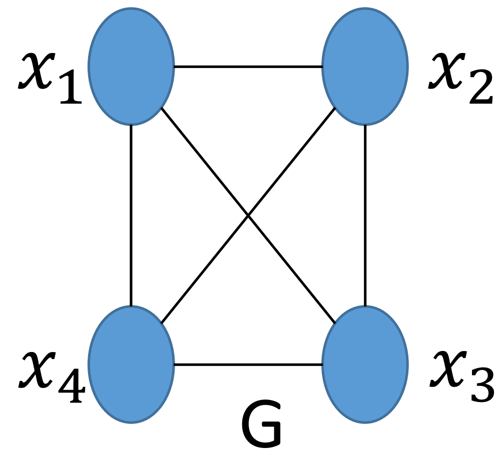
Pessimist

What evidence should we ask for?

- We want something in the middle.
- Optimist's evidence for degree d SOS hierarchy: expectation values of all monomials up to degree d over some distribution of solutions.

Example: Does K_4 Have a Triangle?

Recall equations:
Want $x_i = 1$ if $i \in$ triangle, 0 otherwise.
$\forall i, x_i^2 = x_i$
$\sum_i x_i = 3$



Example: Does K_4 Have a Triangle?

One option: Optimist can take the trivial distribution with the single solution

$x_1 = x_2 = x_3 = 1, x_4 = 0$

and give the corresponding values of all monomials up to degree d.

Values for $d = 2$:

E[1] = 1

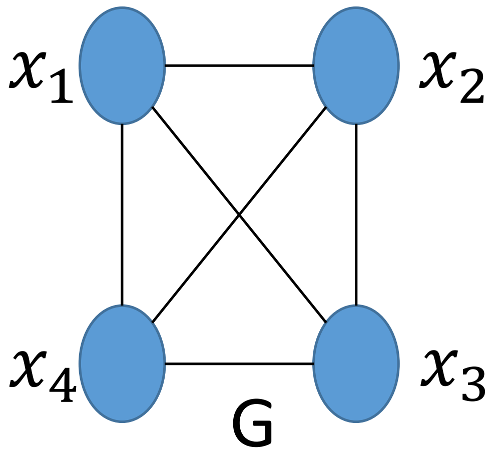
E[x_1] = E[x_2] = E[x_3] = 1

E[x_1^2] = E[x_2^2] = E[x_3^2] = 1

E[$x_1 x_2$] = E[$x_1 x_3$] = E[$x_2 x_3$] = 1

E[x_4^2] = E[x_4] = 0

E[$x_1 x_4$] = E[$x_2 x_4$] = E[$x_3 x_4$] = 0.



Example: Does K_4 Have a Triangle?

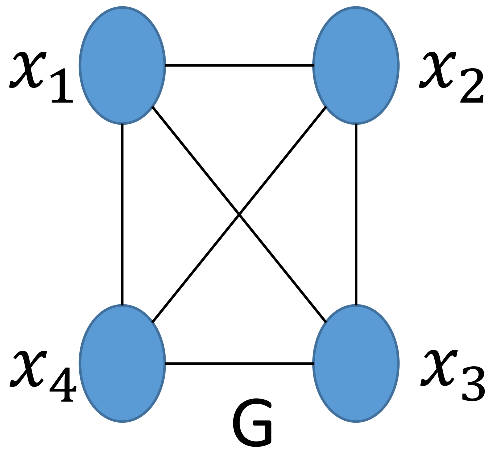
Another option: Optimist can take each of the 4 triangles in G with probability ¼ (uniform distribution on solutions)

Values for $d = 2$:

E[1] = 1

$\forall i$, $E[x_i^2] = E[x_i] = \frac{3}{4}$

$\forall i \neq j$, $E[x_i x_j] = \frac{1}{2}$



Example: Does C_4 Have a Triangle?

Recall equations:

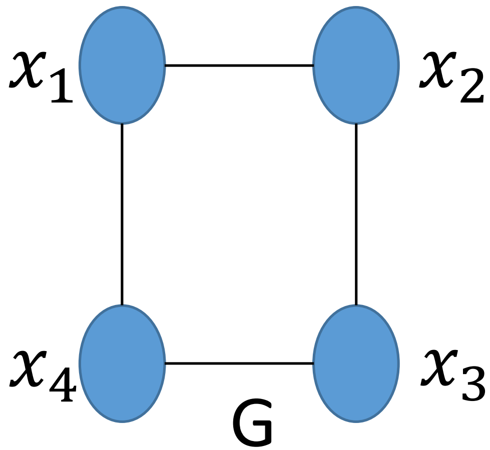
Want $x_i = 1$ if $i \in$ triangle, 0 otherwise.

$\forall i, x_i^2 = x_i$

$\sum_i x_i = 3$

$x_1 x_3 = x_2 x_4 = 0$

Here there is no solution, so Optimist has to bluff



Optimist Bluffs

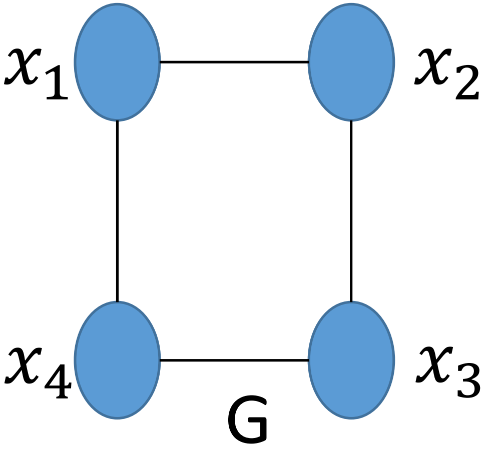
Optimist could give the following pseudo-expectation values as "evidence":

$\tilde{E}[1] = 1$

$\forall i, \tilde{E}\left[x_i^2\right] = \tilde{E}[x_i] = \frac{3}{4}$

$\tilde{E}[x_1x_2] = \tilde{E}[x_2x_3] = \tilde{E}[x_3x_4] = \tilde{E}[x_1x_4] = \frac{3}{4}$

$\tilde{E}[x_1x_3] = \tilde{E}[x_2x_4] = 0$



Detecting Lies

How can Pessimist detect lies systematically?

Method 1: Check equations!

Let's check some: (all vertices and edges have pseudo-expectation value 3/4)

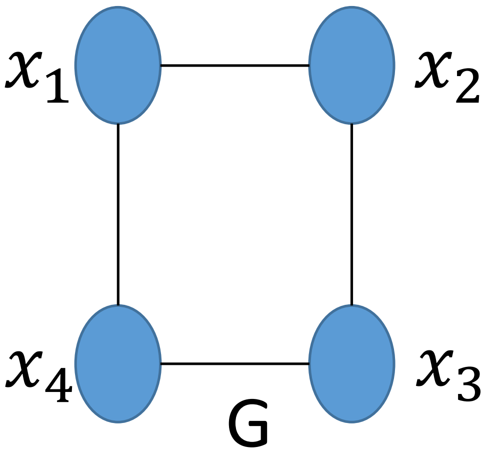
$x_1 + x_2 + x_3 + x_4 = 3$

$\tilde{E}[x_1] + \tilde{E}[x_2] + \tilde{E}[x_3] + \tilde{E}[x_4] = 4 \cdot \frac{3}{4} = 3$

$x_1^2 + x_1x_2 + x_1x_3 + x_1x_4 = 3x_1$

$\tilde{E}[x_1^2] + \tilde{E}[x_1\ x_2] + \tilde{E}[x_1x_3] + \tilde{E}[x_1x_4]$
$= 3/4 + 3/4 + 0 + 3/4 = 9/4 = 3\tilde{E}[x_1]$

Equations are satisfied, need something more…



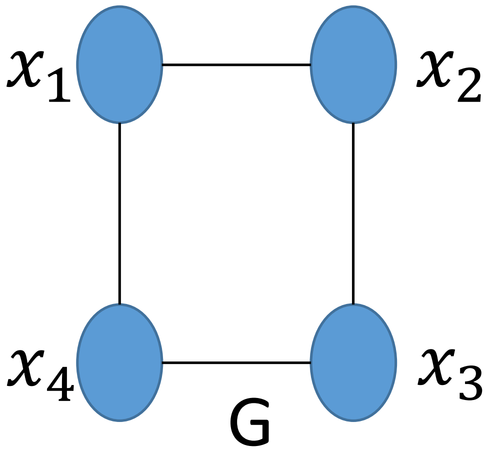
Detecting Lies

How else can Pessimist detect lies?

Method 2: Check non-negativity of squares!

$\tilde{E}[(x_1 + x_3 - x_2 - x_4)^2] =$
$\tilde{E}[x_1^2] + \tilde{E}[x_3^2] + \tilde{E}[x_2^2] + \tilde{E}[x_4^2]$
$+ 2\tilde{E}[x_1 x_3] - 2\tilde{E}[x_1 x_2] - 2\tilde{E}[x_1 x_4]$
$- 2\tilde{E}[x_3 x_2] - 2\tilde{E}[x_3 x_4] + 2\tilde{E}[x_2 x_4]$
$= 3/4 + 3/4 + 3/4 + 3/4 + 0$
$- 3/2 - 3/2 - 3/2 - 3/2 + 0 = -3$

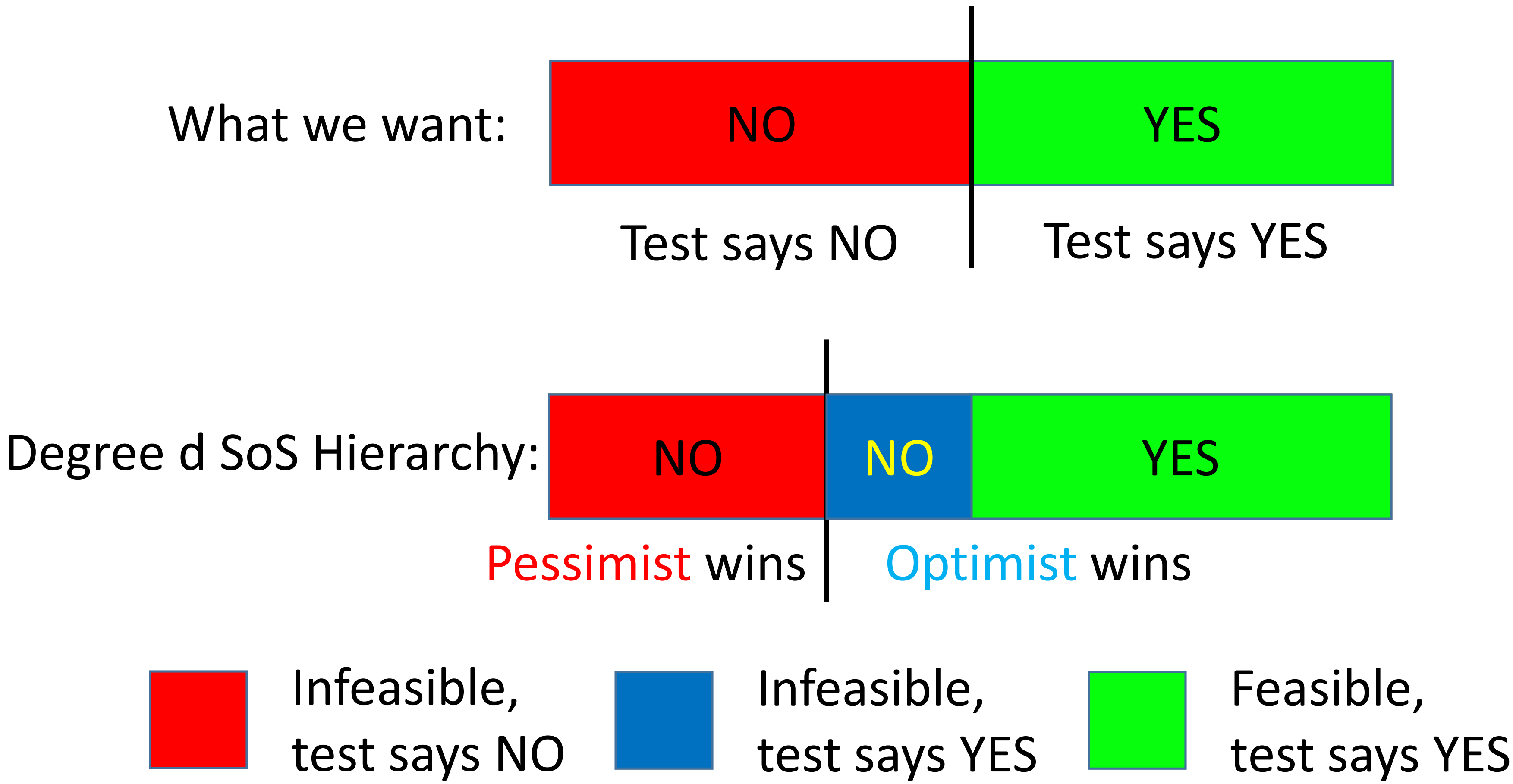
Nonsense!



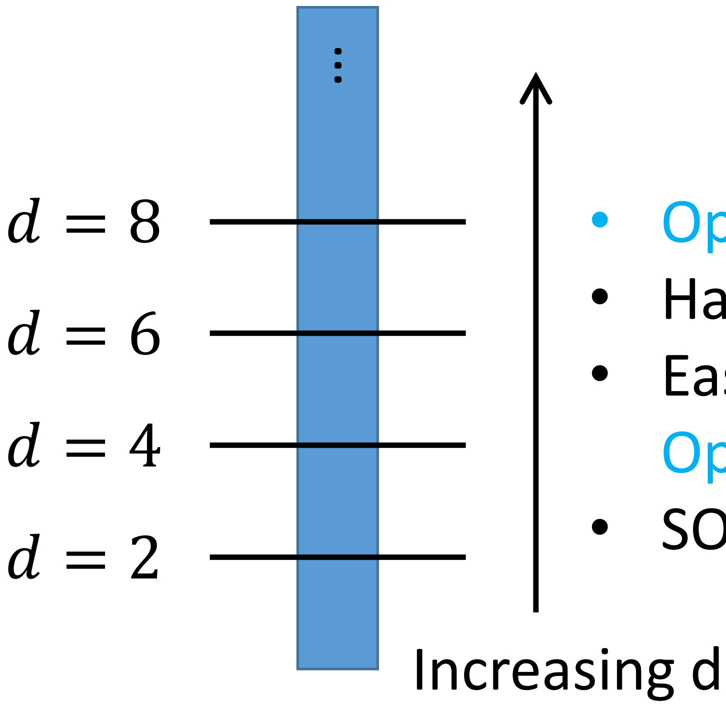
Degree d SoS Hierarchy

- We restrict Pessimist to these two methods.
- Optimist wins if he can come up with pseudo-expectation values $\tilde{E}$ (up to degree d) which obey all of the required equations and have non-negative value on all squares.
- Otherwise, Pessimist wins.
- Degree d SOS hierarchy says YES if Optimist wins and NO if Pessimist wins, this gives a feasibility test.

Feasibility Testing with SOS



SOS Hierarchy



- Optimist must give more values
- Harder for Optimist to bluff
- Easier for Pessimist to refute Optimist and win
- SOS takes longer to compute winner

Part IV:
SOS on general equations

General Setup

- Want to know if polynomial equations

$s_1(x_1, \ldots, x_n) = 0, s_2(x_1, \ldots, x_n) = 0, \ldots$

can be solved simultaneously over $\mathbb{R}$.

- Actually quite general, most problems can be formulated in terms of polynomial equations

Optimist's strategy: Pseudo-expectation values

- Recall: trying to solve equations $s_1(x_1, \dots, x_n) = 0, s_2(x_1, \dots, x_n) = 0, \dots$
- Pseudo-expectation values are a linear mapping $\tilde{E}$ from polynomials of degree $\leq d$ to $\mathbb{R}$ satisfying the following conditions (which would be satisfied by any real expectation over a distribution of solutions):
  1. $\tilde{\mathrm{E}}[1] = 1$
  2. $\tilde{\mathrm{E}}[f s_i] = 0$ whenever $\deg(f) + \deg(s_i) \leq d$
  3. $\tilde{\mathrm{E}}\left[g^2\right] \geq 0$ whenever $\deg(g) \leq \frac{d}{2}$

Pessimist's Strategy: Positivstellensatz/SoS Proofs

- Can $s_1(x_1, \ldots, x_n) = 0, s_2(x_1, \ldots, x_n) = 0, \ldots$ be solved simultaneously over $\mathbb{R}$?
- There is a degree d Positivstellensatz/SoS proof of infeasibility if $\exists$ polynomials f_i, g_j such that
  1. $-1 = \sum_i f_i s_i + \sum_j g_j^2$
  2. $\forall i, \deg(f_i) + \deg(s_i) \leq d$
  3. $\forall j, \deg(g_j) \leq \frac{d}{2}$

Duality

- Degree d Positivstellensatz proof:

$$-1 = \sum_i f_i s_i + \sum_j g_j^2$$

- Pseudo-expectation values:

$$\tilde{\mathrm{E}}[1] = 1$$

$$\tilde{\mathrm{E}}[f_i s_i] = 0$$

$$\tilde{\mathrm{E}}\left[g_j^2\right] \geq 0$$

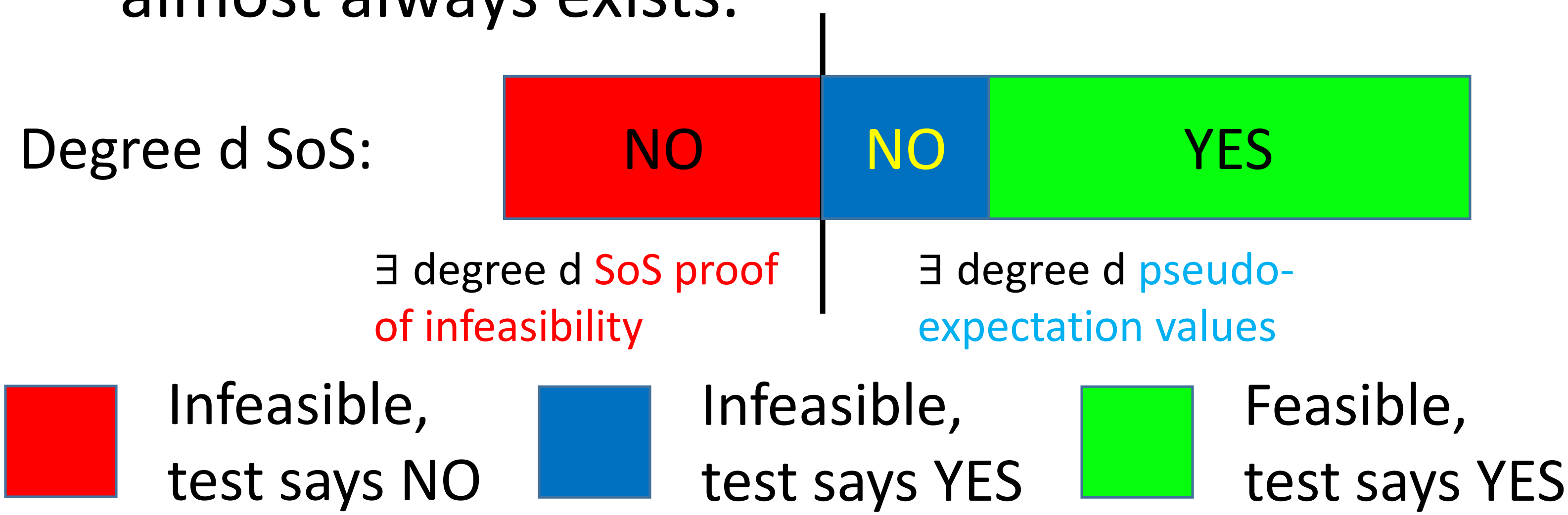
Cannot both exist, otherwise

$$-1 = \tilde{\mathrm{E}}[-1] = \sum_i \tilde{\mathrm{E}}[f_i s_i] + \sum_j \tilde{\mathrm{E}}[g_j^2] \geq 0$$

- Almost always, one or the other will exist.
- SoS hierarchy determines which one exists.

Summary: Feasibility Testing with SoS

- Degree d SoS hierarchy: Returns YES if there are degree d pseudo-expectation values, returns NO if there is a degree d Positivstellensatz/SoS proof of infeasibility,
- Duality: Cannot both exist, one or the other almost always exists.



Fundamental Research Questions

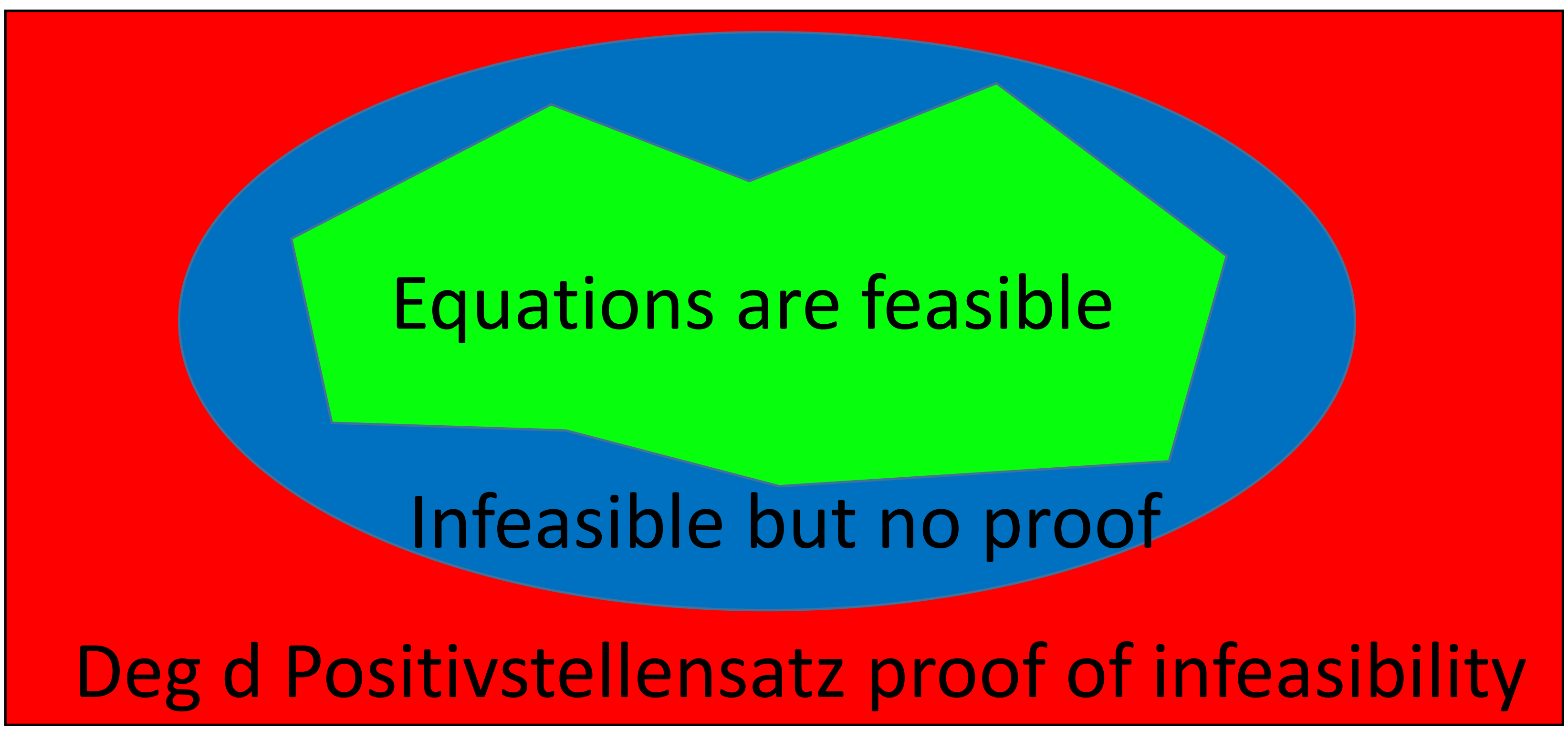
- Which sets of infeasible equations can SOS refute at a given degree d?
- For a given set of infeasible equations, how high does the degree d need to be before SOS can refute it?

Optimization with SoS

- How can we use SoS for optimization and approximation algorithms?
- Equations often have parameter(s) we are trying to optimize
- Example:
  - $\forall i, x_i^2 = x_i$
  - $x_i\, x_j = 0$ if $(i, j) \notin E(G)$
  - $\sum_i x_i = k$
- Can use SoS to estimate the optimal value of k

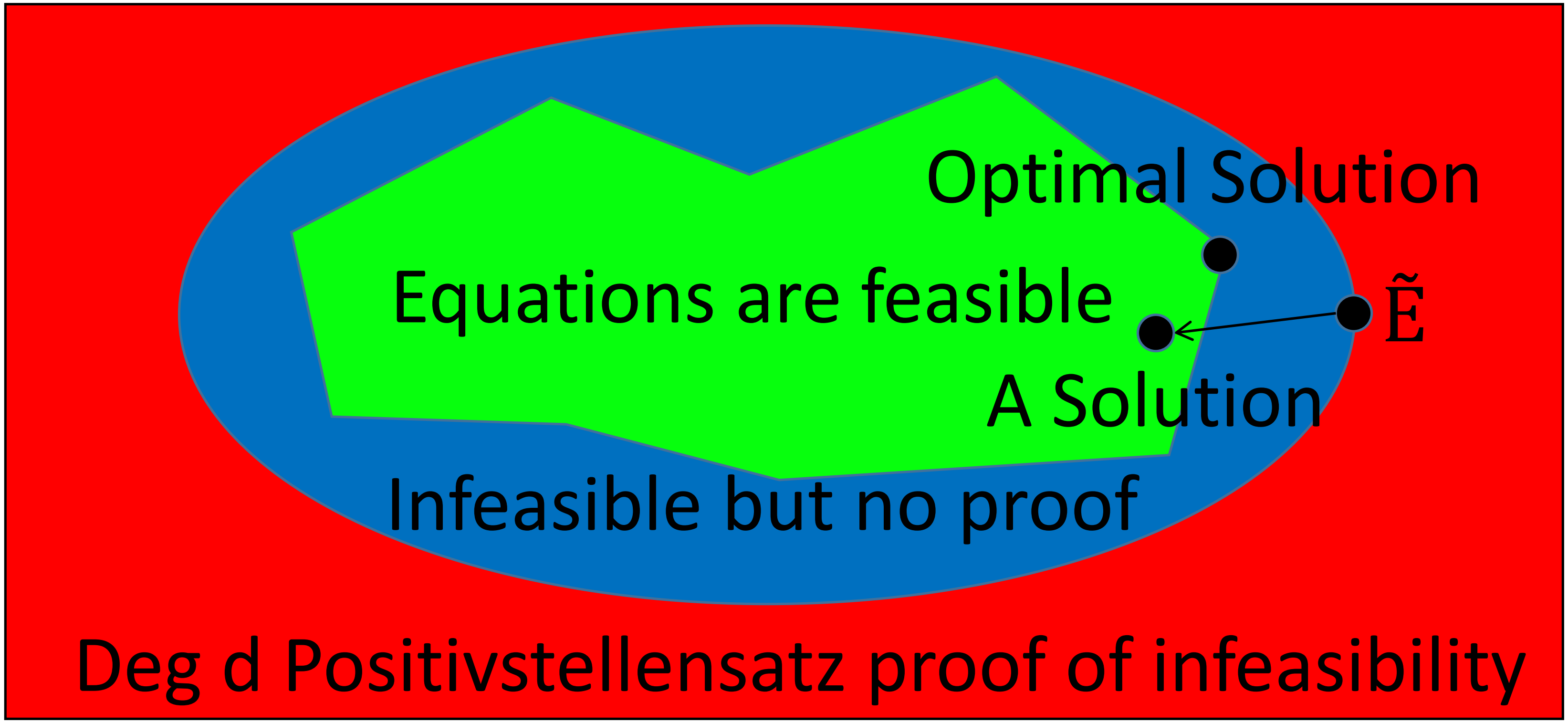
Optimization with SoS

- Want to optimize parameters (such as k) over green region, SOS optimizes over the blue and green regions.
- As we increase the degree d, the blue region shrinks



Approximation Algorithms with SoS

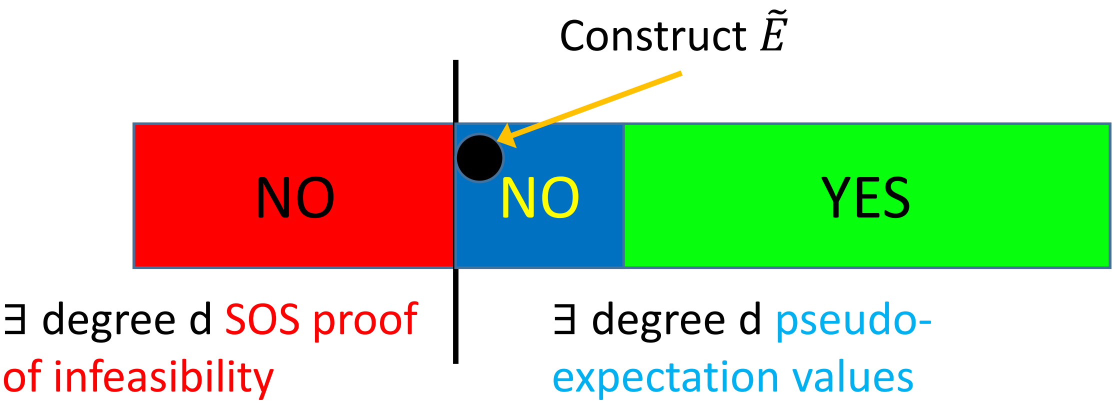
- If there is a method for rounding the pseudo-expectation values $\tilde{\mathrm{E}}$ into an actual solution (with worse parameters), this gives an approximation algorithm.



Lower Bound Strategy for SoS

1. Construct pseudo-expectation values $\tilde{\mathrm{E}}$
2. Show that $\tilde{\mathrm{E}}$ obeys the required equalities and is non-negative on squares.

Degree d SoS:



Part V: Overview of SOS results and Seminar Plan

Mathematical Questions on SOS

- Hilbert's 17th problem: Can every non-negative polynomial be written as a sum of squares of rational functions?
- Resolved affirmitavely by Emil Artin [Art27] in 1927
- Closely related to completeness of the Positivstellensatz proof system (Stengle's Positivstellensatz [Kri64],[Ste74] gives full proof).
- Note: Hilbert [Hil1888] had already showed that not every non-negative polynomial can be written as a sum of squares. Motzkin [Mot67] gave the first explicit example.

Mathematical Questions on SOS

- Lots of further research on non-negative polynomials and sums of squares. Two examples:
- Blekherman [Ble06] showed that there are significantly more non-negative polynomials than polynomials which are sums of squares of polynomials.
- Open problem: How many squares of rational functions are required to obtain a given non-negative polynomial? Best known bound: 2^n by Pfister [Pfi67]

SOS hierarchy in Computer Science

- SOS hierarchy was investigated independently by Grigoriev [Gri01a,Gri01b], Lasserre [Las01], Nesterov [Nes00], Parrilo [Par00], and Shor [Sho87]
- SOS was first used in practice for control theory, where the number of variables is small and we can afford a relatively high degree.
- Theoretically, SOS has been investigated for both algorithms and lower bounds.

Algorithms Captured By SOS

- Several algorithms were discovered by other means then shown to be captured by SOS. Examples are:
  1. Goemans-Williamson for MAX CUT [GW95]
  2. The Arora-Rao-Vazirani analysis for sparsest cut [ARV09]
  3. The sub-exponential time algorithm for unique games [ABS10]

Further Algorithms

- More recently, SOS has given algorithms for several problems directly. Examples are:
  1. Planted Sparse Vector [BKS14] and dictionary learning [BKS15]
  2. Tensor Decomposition [GM15], [BKS15], [MSS16], [HSSS16] and Tensor Completion [BM16], [PS17].
  3. Subexponential time algorithm for quantum separability [BKS17].

SOS Lower Bounds

- Grigoriev [Gri01a], [Gri01b] proved SOS lower bounds for random 3-XOR and knapsack. The 3-XOR lower bound was later independently rediscovered by Schoenebeck [Sch08]
- Tulsiani [Tul09] adapted gadget reductions to SOS to prove SOS lower bounds on many NP-hard problems
- Recently, a series of works [MPW15], [DM15], [HKPRS16], [BHKKMP16] proved SOS lower bounds on planted clique

Further SOS Lower Bounds

- Now have SOS bounds for general CSPs [BCK15], [KMDW17]
- Planted clique lower bound has been generalized to other planted problems including tensor PCA [HKPRSS17]
- Actually, we don’t know that much more for lower bounds, we’re in need of another breakthrough…

SOS and Unique Games

- The unique games conjecture [Kho02], which says that the unique games problem is NP-hard, is an extremely important conjecture in complexity theory and inapproximability theory.
- SOS is a leading candidate for refuting the unique games conjecture
- Difficulty in proving lower bounds: many potential hard examples are broken by SOS because SOS captures our bounds on their value [BBH+12]!
- Summary: We conjecture unique games is hard but can’t prove that constant degree SOS fails.

Other SOS topics

- SOS and symmetry: Can symmetry be used to simplify the sum of squares program and its analysis? Answer: Yes [GP04], [RSST16]
- Extension complexity: SOS only looks at degree, can we bound the size of any semidefinite program solving a problem? Answer: Yes, at least for some problems [LRS15]

Covered

Hope you'll present much of this

Can present on this if you'd like to

What we'll cover

Mathematical questions on non-negative polynomials and SOS

Other

Other Topics
- Symmetry and SOS
- Extension Complexity
- Counterexamples broken by SOS

SOS

SOS Lower Bounds
- Knapsack
- 3-XOR
- NP-hard problems
- Planted Clique

SOS Algorithms
- MAX CUT
- Sparsest Cut
- Planted sparse vector
- Tensor decomposition and completion
- Unique Games

Control theory and other applications

Further lower bounds
- General CSPs
- More general planted problems

Further algorithms
- Quantum separability
- Dictionary learning

Seminar Plan

- Part I: Background
- Part II: Upper Bounds for SOS
- Part III: Lower Bounds for SOS
- Part IV: Further SOS upper bounds (including unique games)
- Part V: Presentations
- See schedule for more information.

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