

# Convex optimization and quantum information theory

Hamza Fawzi

Department of Applied Mathematics and Theoretical Physics  
University of Cambridge

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Tutorial

# Convex optimization

- Basics, semidefinite programs
- Algorithms (Newton, interior-point)
- Convex relaxations for polynomial optimization

# Quantum information

- Entropies
- Separable states and sums of squares

# Convex optimization

- Solve/study optimization problem

$$\min_{x \in C} f(x)$$

where  $f$  convex function and  $C$  convex set.

- Can be easy or hard depending on  $f$  and  $C$

# Examples

- Capacity of a cq-channel

$$\max H\left(\sum_{i=1}^n p_i \sigma_i\right) - \sum_{i=1}^n p_i H(\sigma_i) \quad \text{s.t.} \quad p \in \Delta^{n-1}$$

where  $H(\sigma) = -\text{tr}[\sigma \log \sigma]$  von Neumann entropy,  
 $\Delta^{n-1} = \{p \geq 0, \sum_i p_i = 1\}$ .

## Examples

- Capacity of a cq-channel

$$\max H \left( \sum_{i=1}^n p_i \sigma_i \right) - \sum_{i=1}^n p_i H(\sigma_i) \quad \text{s.t.} \quad \rho \in \Delta^{n-1}$$

where  $H(\sigma) = -\text{tr}[\sigma \log \sigma]$  von Neumann entropy,  
 $\Delta^{n-1} = \{\rho \geq 0, \sum_i p_i = 1\}$ .

- Relative entropy of PPT, for fixed  $\rho \in \mathbf{H}^{nm}$

$$\min D(\rho \parallel \sigma) \quad \text{s.t.} \quad \sigma \in \text{PPT}$$

where  $D(\rho \parallel \sigma) = \text{tr}[\rho(\log \rho - \log \sigma)]$ , and

$$\text{PPT} = \{\rho \succeq 0, \text{tr}[\rho] = 1, \text{ and } (I \otimes T)(\rho) \succeq 0\}.$$

## Examples 2

- Best separable state

$$\max \operatorname{tr}[M\sigma] \quad \text{s.t.} \quad \sigma \in \text{Sep}$$

where  $M \in \mathbf{H}^{n^2}$ , and  $\text{Sep} = \operatorname{conv}\{xx^\dagger \otimes yy^\dagger : x, y \in (\mathbb{C}^n)^2, |x| = |y| = 1\}$ .

## Examples 2

- Best separable state

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- Nonlocal games, Bell inequalities

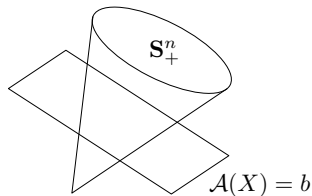
$$\max \sum_{abxy} w(ab|xy)p(ab|xy) \quad \text{s.t.} \quad (p(ab|xy))_{ab|xy} \in C_q$$

where  $C_q$  is the set of quantum correlations

$$C_q = \left\{ p(a, b|x, y) = \langle \psi, (F_a^x \otimes G_b^y) \psi \rangle : d \in \mathbb{N}, \psi \in \mathbb{C}^d, F_a^x \in \mathbf{H}_+^d, G_b^y \in \mathbf{H}_+^d \right. \\ \left. \sum_{1 \leq a \leq m} F_a^x = I, \sum_{1 \leq b \leq m} G_b^y = I \quad \forall 1 \leq x, y \leq n \right\}.$$

# Semidefinite programming

$$\begin{array}{ll} \min & \langle C, X \rangle \\ \text{s.t.} & X \succeq 0 \\ & \langle A_i, X \rangle = b_i \quad (i = 1, \dots, m) \end{array}$$





# Duality

$$\begin{aligned} p^* = \min \quad & \langle C, X \rangle \\ \text{s.t.} \quad & X \succeq 0 \\ & \langle A_i, X \rangle = b_i \quad (i = 1, \dots, m) \end{aligned}$$

$$\begin{aligned} d^* = \max \quad & \langle b, z \rangle \\ \text{s.t.} \quad & C - \sum_{i=1}^m z_i A_i \succeq 0. \end{aligned}$$

- Weak duality:  $p^* \geq d^*$
  
  
  
  
  
  
  
  
  
  
- Strong duality:  $p^* = d^*$ , holds assuming e.g., primal or dual problem are strictly feasible (Slater's condition)

# Duality

$$\begin{aligned} p^* = \min \quad & \text{tr}(CX) \\ \text{s.t.} \quad & X \succeq 0 \\ & \text{tr}(A_i X) = b_i \quad (i = 1, \dots, m) \end{aligned}$$

$$\begin{aligned} d^* = \max \quad & \langle b, z \rangle \\ \text{s.t.} \quad & C - \sum_{i=1}^m z_i A_i \succeq 0. \end{aligned}$$

KKT conditions of optimality:

$$\begin{cases} X \succeq 0, \quad \text{tr}(A_i X) = b_i \quad (i = 1, \dots, m) \\ S \succeq 0, \quad S = C - \sum_{i=1}^m z_i A_i \\ XS = 0. \end{cases}$$

Nonlinear system in the unknowns  $(X, S, z)$

# Algorithms

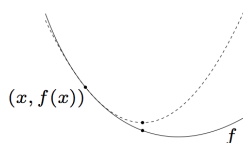
- Newton's method (unconstrained)
- Path-following methods

# Newton's method

$$\min_{x \in \mathbb{R}^n} f(x)$$

- At iteration  $x_k$ , form quadratic approximation of  $f$

$$f(x_k + h) \approx f(x_k) + \nabla f(x_k)^T h + \frac{1}{2} h^T \nabla^2 f(x_k) h$$



- If  $f$  strongly convex then  $\nabla^2 f(x_k)$  positive definite, and quadratic approximation has a unique minimum, attained by taking

$$h^* = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

# Newton's method

$$x_{k+1} = x_k + t_k h^* = x_k - t_k [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

where  $t_k > 0$  step size (default step size  $t_k = 1$ ).

- Computational complexity: at each step need to solve the linear system

$$\nabla^2 f(x_k) h = \nabla f(x_k)$$

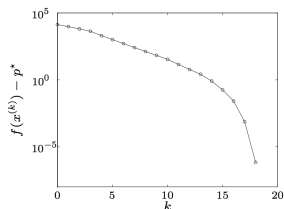
$O(n^3)$  flops for unstructured systems. Limiting factor when  $n$  large.

- Compare to gradient method where each iteration takes  $O(n)$  flops.
- Method invariant under change of basis  $\tilde{x} = Px$  where  $P$  invertible.

# Convergence of Newton's method

$$x_{k+1} = x_k - t_k [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

- Extremely fast when close to optimal solution



- Quadratic convergence:  $r_{k+1} \leq r_k^2$  for some measure of the residual  $r_k$ . If  $r_0 < 1$  this is extremely fast convergence:  $r_k \leq (r_0)^{2^k}$ .

Quadratic convergence region is  $\{x \in \text{dom}(f) : r_0 < 1\}$ .

# Quadratic convergence

- *Standard analysis of Newton's method:* Assume  $f$  is such that  $\nabla^2 f(x) \succeq ml$ , and  $\nabla^2 f$  is  $M$ -Lipschitz (in the operator norm). Then with  $r_k = \frac{M}{2m^2} \|\nabla f(x_k)\|_2$  we have  $r_{k+1} \leq r_k^2$ .

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- *Nesterov & Nemirovski:* **Self-concordant** functions  $f$ , defined by a Lipschitz condition on  $\nabla^2 f$  **with respect to local metric**

$$\|v\|_x = \sqrt{v^T \nabla^2 f(x) v}$$

Self-concordance:  $\|H_x(y) - H_x(x)\|_x \leq \phi(\|y - x\|_x)$

where  $\phi(t) = 1/(1 - t)^2 - 1$ .



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$$\text{Self-concordance: } \|H_x(y) - H_x(x)\|_x \leq \phi(\|y - x\|_x)$$

where  $\phi(t) = 1/(1 - t)^2 - 1$ .

- Advantage of self-concordance: analysis of Newton's method does not depend on any constants, and is invariant under change of coordinates:

$$\lambda(x_{k+1}) \leq \frac{\lambda(x_k)^2}{(1 - \lambda(x_k))^2}$$

where  $\lambda(x) = \|g_x(x)\|_x$ .

## Relationship with Newton-Raphson method

- Newton-Raphson method to solve a system of nonlinear equations,  $F(x) = 0$  where  $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$

- Linearize at  $x_k$

$$F(y) \approx F(x_k) + DF(x_k)(y - x_k)$$

- Equate right-hand side to zero to get

$$x_{k+1} = x_k - (DF(x_k))^{-1}F(x_k)$$

- Newton's method for optimization is Newton-Raphson applied to the system  $\nabla f(x) = 0$ .

# Constrained problems

$$\min_{x \in C} \langle c, x \rangle$$

Let  $B(x)$  be a convex barrier function for  $C$  so that  $B(x) \rightarrow +\infty$  as  $x \rightarrow \partial C$ . For example if  $C = \{x : \langle a_i, x \rangle \leq b_i\}$  then we choose

$$B(x) = - \sum_i \log(b_i - \langle a_i, x \rangle).$$

We consider, for  $t > 0$ :

$$x^*(t) = \operatorname{argmin}_x t \langle c, x \rangle + B(x).$$

This traces out a path in the interior of  $C$ . Can show that

$$\langle c, x^* \rangle \leq \langle c, x^*(t) \rangle \leq \langle c, x^* \rangle + \theta/t$$

where  $\theta$  is some parameter that depends on  $B$ .

Goal: trace out the path with  $t \rightarrow \infty$

# Central path

$$x^*(t) = \operatorname{argmin}_x B_t(x)$$

where  $B_t(x) = t\langle c, x \rangle + B(x)$ .

Barrier method, assuming initial point  $x^*(t_0)$  for  $t_0 > 0$  given:

- Let  $t = t_0$ ,  $x = x^*(t_0)$
- While not converged ( $t < \theta/\epsilon$ ):
  - Set  $t^+ \leftarrow \alpha t$  for some  $\alpha > 1$
  - Compute  $x^*(t^+)$  by using Newton's method starting from  $x^*(t)$
  - Update  $t \leftarrow t^+$

How to choose  $\alpha$ ? We want:

$x^*(t)$  is in the quadratic convergence region of  $B_{\alpha t}$

# Illustration

- Theory tells us that  $\alpha \approx 1 + 1/\sqrt{\theta}$  works. This leads to a number of iterations  $\approx \sqrt{\theta}$
- Practice: such  $\alpha$  is too small. Use “predictor-corrector” approach where one predicts at each iteration how large  $\alpha$  can you choose.

# Application to SDPs

## Dual SDP

$$\max \langle b, z \rangle \quad \text{s.t.} \quad C - \sum_{i=1}^m z_i A_i \succeq 0.$$

Barrier function  $B(z) = \log \det (C - \sum_{i=1}^m z_i A_i)$ .

$$\max \quad t \langle b, z \rangle + B(z)$$

Need to compute  $\nabla B_t$  and  $\nabla^2 B_t$ . If we let  $S = C - \sum_{i=1}^m z_i A_i \succ 0$ , then

$$\begin{aligned} [\nabla B_t(z)]_i &= t b_i - \langle A_i, S^{-1} \rangle \\ [\nabla^2 B_t(z)]_{ij} &= -\text{tr}[S^{-1} A_i S^{-1} A_j]. \end{aligned}$$

Cost of forming the Hessian is  $\approx mn^3 + m^2 n^2$ , and cost of solving linear system for Newton's method is  $m^3$ .

## Barrier path and KKT equations

At “time  $t$ ” of central path we have  $\nabla B_t(z) = 0$  i.e.,

$$b_i = \frac{1}{t} \langle A_i, S^{-1} \rangle.$$

If we call  $X = \frac{1}{t} S^{-1}$  then the following hold:

$$\begin{cases} X \succeq 0, \operatorname{tr}(A_i X) = b_i \quad (i = 1, \dots, m) \\ S \succeq 0, S = C - \sum_{i=1}^m z_i A_i \\ XS = \frac{1}{t} I \end{cases}$$

Modified KKT system!

# Discussion

- Complexity of solving SDP is  $\approx \sqrt{n}(n^4 + m^2n^2 + m^3)$  floating-point operations
- Well-implemented interior-point method reliable and can give high accurate solutions. Solvers include Mosek, SeDuMi, SDPT3, SDPA, CSDP, ...
- Recently, research focus on simpler (first-order) methods that scale to large problems, e.g., ADMM.
- Good implementation of ADMM: SCS (Splitting Conic Solver) [O'Donoghue]
- Main drawback of first-order methods is **accuracy**. Slow convergence/stall at low-medium accuracy.



# Polynomial optimization, sums of squares

# Polynomial optimization

Let  $p \in \mathbb{R}[x_1, \dots, x_n]$  be a polynomial.

- Decision question:

$$\text{is } p(x) \geq 0 \quad \forall x \in \mathbb{R}^n?$$

- NP-hard (but decidable, by Tarski's theorem)
- Sufficient condition for nonnegativity of  $p$  is that  $p$  is a sum-of-squares:

$$p(x) = \sum_i q_i(x)^2$$

for some polynomials  $q_i(x)$ .

- If  $\deg p = 2d$  then the  $q_i$  are necessarily of degree  $\leq d$
- If  $p$  is sos, then it is a sum of squares of finitely many polynomials ( $\leq \binom{n+d}{d}$ ).

# Sums of squares and semidefinite programming

Deciding if  $p$  is a sum-of-squares is a semidefinite feasibility problem



# Hilbert's question

- Are all nonnegative polynomials sums of squares? No! Hilbert (1888) showed that nonnegative polynomials are sos only in the following cases:
  - $n = 1$  (one variable)
  - $2d = 2$  (quadratics)
  - $n = 2, 2d = 4$

In all the other cases, there are nonnegative polynomials that are not sums of squares

- Motzkin's polynomial ( $n = 2, 2d = 6$ ) is one such example

$$M(x, y) = x^4y^2 + x^2y^4 + 1 - 3x^2y^2.$$

- Hilbert's 17th problem: are all nonnegative polynomials sums of squares of **rational functions**? Question answered positively by Artin (1927)

# Optimization

$$\min_{x \in \mathbb{R}^n} p(x) = \max \gamma \quad \text{s.t.} \quad p - \gamma \geq 0.$$

Sum-of-squares relaxation:

$$\max \gamma \quad \text{s.t.} \quad p - \gamma \text{ sum-of-squares}$$

This is an SDP.

# Constrained polynomial optimization: the case of the sphere

Let  $p(x)$  be a (homogeneous) polynomial of degree  $2d$ .

$$p_{\min} := \min p(x) \text{ s.t. } \sum_{i=1}^n x_i^2 = 1.$$

Define

$$p_\ell = \max_{\gamma, s(x), g(x)} \gamma$$

s.t.

$$p(x) - \gamma = s(x) + g(x)(|x|^2 - 1) \quad \text{Equality of polynomials}$$
$$s(x) \text{ is a sum-of-squares, } \deg s \leq 2\ell \quad \text{Semidefinite constraint}$$
$$g(x) \in \mathbb{R}[x], \deg g \leq 2\ell - 2$$

- Each  $p_\ell$  is a lower bound on  $p_{\min}$

$$\cdots \leq p_{\ell-1} \leq p_\ell \leq p_{\min}$$

- Note that  $\deg s$  can be larger than  $\deg p$ ! (Cancellation)

# Relaxations based on linear programming

- Any *certificates of nonnegativity* give us a way to construct a relaxation
- Example (positivity on  $\mathbb{R}_+^n$ ): Given  $p \in \mathbb{R}[x]$

$$\text{is } p(x) \geq 0 \quad \forall x = (x_1, \dots, x_n) > 0 ?$$

- Sufficient condition 1: coefficients of  $p$  are  $\geq 0$
- Sufficient condition 2: there is  $N \in \mathbb{N}$  such that

$$\left( \sum_{i=1}^N x_i \right)^n p(x) \text{ has nonnegative coefficients.}$$

- Polya's theorem: if  $p > 0$  on  $\mathbb{R}_+^n$  then sufficient condition 2 is also necessary.



# Linear programming hierarchy

Polya's theorem suggests a hierarchy of linear programs to compute

$$p_{\min} = \min p(x) \text{ s.t. } x \geq 0, \sum_{i=1}^n x_i = 1.$$

If  $p$  is homogeneous of degree  $d$ , consider

$$p_N = \max \gamma$$

s.t.  $(\sum_{i=1}^n x_i)^N (p(x) - \gamma (\sum_{i=1}^n x_i)^d)$  has nonnegative coefficients

- For each  $N$ ,  $p_N \leq p_{\min}$ , and Polya's theorem guarantees that  $p_N \rightarrow p_{\min}$ .
- Computing  $p_N$  is a linear program, with a number of inequalities equal to  $\binom{n+N+d}{n} =$  dimension of space of polynomials of degree at most  $N+d$  in  $n$  variables.

# Quantum information

- Entropies
- The set of separable states

# Entropies

- Relative entropy, jointly convex in  $(\rho, \sigma)$  [Lieb-Ruskai]

$$D(\rho||\sigma) = \text{tr}[\rho(\log \rho - \log \sigma)]$$

- Petz Rényi divergence, concave for  $\alpha \in [0, 1]$  and convex for  $\alpha \in [1, 2]$  [Lieb]

$$Q_\alpha(\rho||\sigma) = \text{tr}[\rho^\alpha \sigma^{1-\alpha}]$$

- Geometric Rényi divergence [Matsumoto]

$$\hat{Q}_\alpha(\rho||\sigma) = \text{tr}[\sigma(\sigma^{-1/2}\rho\sigma^{-1/2})^\alpha].$$

# Optimizing entropies

Optimization problems with Rényi divergences are very common in QI

To solve such optimization problems, either:

- 1 Implement your own optimization algorithm, using expression for the gradient (and Hessian) of these functions.

Pros: can exploit problem structure with custom algorithm

Cons: have to implement your algorithm (deal with choices of step sizes, scaling, ...), time-consuming

- 2 Or, try to formulate such problems as *semidefinite programs*, and rely on existing solvers for SDPs.

Pros: very easy to use/compose with other constraints via interfaces such as CVX, Yalmip

Cons: restriction to SDPs means we have to do approximations (more on this later)

We'll focus on semidefinite representations

# Interfaces to convex solvers

Example: distance to PPT in the relative entropy sense

$$\min D(\rho \parallel \tau) \text{ s.t. } \tau \in \text{PPT}$$

```
cvx_begin sdp
    variable tau(na*nb,na*nb) hermitian;
    minimize    (quantum_rel_entr(rho,tau));
    subject to  tau >= 0; trace(tau) == 1;
               Tx(tau,2,[na nb]) >= 0; % Positive partial transpose
cvx_end
```

# Semidefinite representations

- Concave function  $f$  has a *semidefinite representation* if:

$$f(x) \geq t \quad \iff \quad \mathcal{S}(x, t) \succeq 0$$

for some affine function  $\mathcal{S} : \mathbb{R}^{n+1} \rightarrow \mathbf{H}^d$

- **Key fact:** if  $f$  has a semidefinite representation then can solve optimisation problems involving  $f$  using semidefinite solvers.

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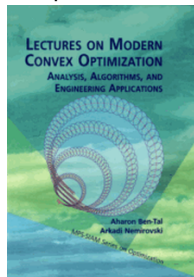
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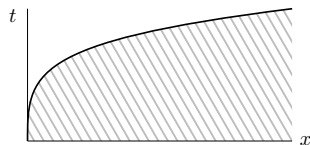
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- **Key fact:** if  $f$  has a semidefinite representation then can solve optimisation problems involving  $f$  using semidefinite solvers.
- Book by Ben-Tal and Nemirovski gives semidefinite representations of many convex/concave functions.



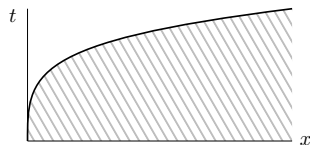
## Examples of semidefinite formulation

$$\sqrt{x} \geq t \iff \begin{bmatrix} x & t \\ t & 1 \end{bmatrix} \succeq 0$$

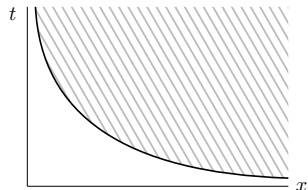


## Examples of semidefinite formulation

$$\sqrt{x} \geq t \iff \begin{bmatrix} x & t \\ t & 1 \end{bmatrix} \succeq 0$$



$$\frac{1}{x} \leq t \iff \begin{bmatrix} x & 1 \\ 1 & t \end{bmatrix} \succeq 0$$



# Matrix geometric mean

Geometric mean of  $A, B \succ 0$  is

[Kubo-Ando]

$$A\#B = A^{1/2} \left( A^{-1/2} B A^{-1/2} \right)^{1/2} A^{1/2}$$

- Homogeneous,  $(rA)\#(rB) = r(A\#B)$
- Jointly operator concave in  $(A, B)$

$$(A_1 + A_2)\#(B_1 + B_2) \succeq A_1\#B_1 + A_2\#B_2$$

- Symmetric:  $A\#B = B\#A$ .

## SDP representation of geometric mean

$$A\#B = \max_{X \succeq 0} \left\{ X : \begin{bmatrix} A & X \\ X & B \end{bmatrix} \succeq 0 \right\}$$

Proof

## SDP representation of geometric mean (2)

$$A \# B \preceq T \iff \exists X \text{ s.t. } \begin{bmatrix} A & X \\ X & B \end{bmatrix} \preceq 0 \text{ and } X \preceq T.$$

# SDP representation of geometric means

The  $t$ -geometric mean of  $(A, B)$  is

[Kubo-Ando]

$$A\#_t B = A^{1/2} \left( A^{-1/2} B A^{-1/2} \right)^t A^{1/2}$$

Jointly concave in  $(A, B)$  for  $t \in [0, 1]$  / convex for  $t \in [-1, 0] \cup [1, 2]$ .

Semidefinite representation:

- Use composition property

$$A\#_{1/4} B = A\#(A\#B)$$

+ monotonicity of  $\#$  in 2nd argument, to get:

$$A\#_{1/4} B \succeq T \iff \exists Z : \begin{cases} A\#B \succeq Z \\ A\#Z \succeq T. \end{cases}$$

- Can get  $A\#_{3/4} B$  using  $A\#_{3/4} B = B\#_{1/4} A$ .
- $\Rightarrow$  SDP representation of  $A\#_t B$  for all dyadic numbers  $t \in [0, 1]$ .

## SDP representation of geometric mean for $t \in [-1, 0]$

For  $t \in [-1, 0]$  we use  $A\#_{-t}B = A\#_{-1}(A\#_tB)$  to get

$$A\#_{-t}B \preceq T \iff \exists Z : \begin{cases} A\#_tB \succeq Z \\ A\#_{-1}Z \preceq T \end{cases}$$

and

$$A\#_{-1}Z \preceq T \iff \begin{bmatrix} T & A \\ A & Z \end{bmatrix} \succeq 0.$$

(Schur complement)



## Petz divergence

$$Q_\alpha(\rho||\sigma) = \text{tr}[\rho^\alpha \sigma^{1-\alpha}].$$

Concave for  $\alpha \in [0, 1]$  and convex for  $\alpha \in [1, 2]$  [Lieb].

# Petz divergence

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*Proof:* [Ando]

1  $Q_\alpha(\rho\|\sigma) = \langle \Phi, (\rho^\alpha \otimes \bar{\sigma}^{1-\alpha}) \Phi \rangle$  where  $\Phi = \sum_{i=1}^d e_i \otimes e_i \in \mathbb{C}^{d^2}$ .

More generally:  $\langle \Phi, (M \otimes N) \Phi \rangle = \text{tr}[M\bar{N}]$

## Petz divergence

$$Q_\alpha(\rho\|\sigma) \geq t \iff \exists T \in \mathbf{Herm}(d^2) : \begin{cases} (\rho \otimes I) \#_{1-\alpha} (I \otimes \bar{\sigma}) \succeq T \\ \langle \Phi, T\Phi \rangle \geq t. \end{cases}$$

# Relative entropy

$$D(\rho\|\sigma) = \text{tr}[\rho(\log \rho - \log \sigma)]$$

- We know that

$$D(\rho\|\sigma) = \lim_{h \rightarrow 0} (Q_{1+h}(\rho\|\sigma) - \text{tr}[\rho])/h$$

Follows from  $\log(x) = \lim_{h \rightarrow 0} (x^h - 1)/h$

- Yields SDP approximations of  $D(\rho\|\sigma)$  with approximation quality  $O(h)$ .
- To follow: a different approach to get more accurate approximation, namely in  $O(h^m)$  for any choice of  $m$ .

# Better approximation of log

Approximation

$$\log(x) \approx \frac{x^h - 1}{h}$$

is a composition of two things:

- 1  $\log(x) \approx x - 1$
- 2  $\log(x) = \frac{1}{h} \log(x^h)$

Goal: use a rational approximation  $\log(x) \approx r(x)$  instead of  $\log(x) \approx x - 1$ .  
Then use second point to improve it

$$\log(x) \approx \frac{1}{h} r(x^h).$$

# Matrix logarithm

- Integral representation of log:

$$\log(\mathbf{X}) = \int_0^1 (\mathbf{X} - I)(I + s(\mathbf{X} - I))^{-1} ds$$

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$$(X - I)(I + s(X - I))^{-1} \succeq T \quad \Leftrightarrow \quad \begin{bmatrix} I + s(X - I) & I \\ I & I - sT \end{bmatrix} \succeq 0$$

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- Get semidefinite approximation of matrix log using quadrature:

$$\log(\mathbf{X}) \approx \sum_{j=1}^m w_j \frac{\mathbf{X} - I}{I + s_j(\mathbf{X} - I)}$$

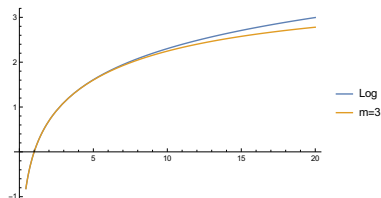
Right-hand side is semidefinite representable



# Rational approximation

$$\log(x) \approx \underbrace{\sum_{j=1}^m w_j \frac{x-1}{1+s_j(x-1)}}_{r_m(x)}$$

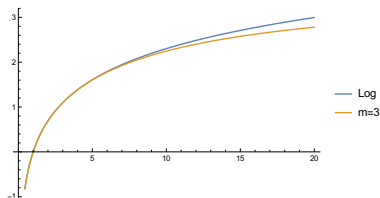
$r_m$  =  $m$ 'th diagonal Padé approximant of  $\log$  at  $x = 1$  (matches the first  $2m$  Taylor coefficients).



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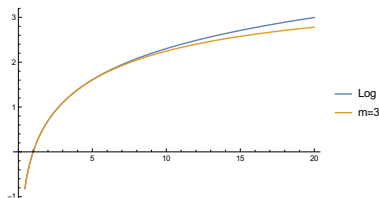
- Improve approximation by bringing  $x$  closer to 1 and using  $\log(x) = \frac{1}{h} \log(x^h)$  ( $0 < h < 1$ ):

$$r_{m,h}(x) := \frac{1}{h} r_m(x^h)$$

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$$r_{m,h}(x) := \frac{1}{h} r_m(x^h)$$

- $r_{m,h}$  is still concave and semidefinite representable!

## From (matrix) logarithm to (matrix) relative entropy

$$\log(X) \approx r_{m,h}(X)$$

- This allows us to approximate the *operator relative entropy*, which is the operator perspective of  $-\log$ .

$$D_{op}(A\|B) = A^{1/2} \log(A^{1/2} B^{-1} A^{1/2}) A^{1/2}$$

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- Finally we use the fact that

$$D(\rho\|\sigma) = \langle \Phi, D_{op}(\rho \otimes I \| I \otimes \bar{\sigma}) \Phi \rangle$$

where  $\Phi = \sum_{i=1}^d e_i \otimes e_i$ .

# Implementation

- These formulations are implemented in the Matlab package CVXQUAD  
`https://www.github.com/hfawzi/cvxquad/`
- Augments Matlab's CVX [Grant, Boyd] with functions  
`quantum_rel_entr`, `lieb_ando`, `quantum_cond_entr`, ...
- Please let me know if there are bugs :)

## Separable states and semidefinite hierarchies

## Separable states

$$\text{Sep}(n, m) = \text{conv} \left\{ (x \otimes y)(\bar{x} \otimes \bar{y})^T : x \in \mathbb{C}^n, y \in \mathbb{C}^m \quad |x| = |y| = 1 \right\}.$$

- Convex set living in  $\{\rho \in \mathbf{Herm}(nm) : \text{Tr}[\rho] = 1\} \simeq \mathbb{C}^{n^2 m^2 - 1}$
- Sep = set of *non-entangled* bipartite states on  $\mathbb{C}^n \otimes \mathbb{C}^m$



# Linear optimization on Sep

$$\text{Sep}(n, m) = \text{conv} \left\{ (x \otimes y)(\bar{x} \otimes \bar{y})^T : x \in \mathbb{C}^n, y \in \mathbb{C}^m \quad |x| = |y| = 1 \right\}.$$

Cost vector  $M \in \mathbf{Herm}(nm)$ :

$$\max_{\rho \in \text{Sep}(n, m)} \text{tr}[M\rho]$$

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Linear optimization on  $\text{Sep}(n, m) \leftrightarrow$  Optimizing a (Hermitian) polynomial on a product of two spheres ( $\mathcal{S}_{\mathbb{C}^n} \times \mathcal{S}_{\mathbb{C}^m}$ ).

# Optimization on the sphere

Polynomial optimization on the sphere:

$$\max p(x_1, \dots, x_n) \quad : \quad \sum_{i=1}^n x_i^2 = 1.$$

Hard in general (Nesterov).

- Stable set problem on a graph can be written as a maximizing a degree-4 polynomial on the sphere (Motzkin formulation of the stable set problem)

$$1 - \frac{1}{\alpha(G)} = \max_{x \in S^{n-1}} 2 \sum_{ij \notin E} x_i^2 x_j^2$$

- $2 \rightarrow 4$  norm of a matrix  $A$

$$\max \|Ax\|_4^4 \quad \text{s.t.} \quad \|x\|_2^2 = 1.$$

# Hardness of Sep

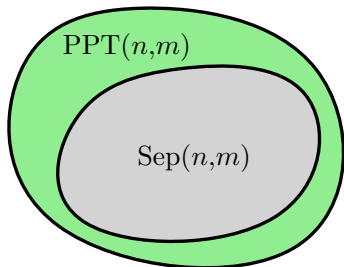
- Deciding membership in  $\text{Sep}(n, m)$  is NP-hard in general [Gurvits]
- Semidefinite relaxations

## PPT relaxation (positive partial transpose)

With  $T : \mathbb{C}^{m \times m} \rightarrow \mathbb{C}^{m \times m}$  = transpose map, let

$$\text{PPT}(n, m) = \{\rho \in \mathbf{Herm}(nm) : \rho \succeq 0, \text{tr}[\rho] = 1, \text{ and } (I \otimes T)(\rho) \succeq 0\}$$

(Check that  $\text{Sep} \subset \text{PPT}$ :  $(I \otimes T)(xx^\dagger \otimes yy^\dagger) = xx^\dagger \otimes \bar{y}y^\dagger \succeq 0$ )



Størmer–Woronowicz [60/70's]:  $\text{Sep}(n, m) = \text{PPT}(n, m)$  iff  $n + m \leq 5$

$$\mathbf{Sep}(n, m) = \text{conv} \left\{ (x \otimes y)(\bar{x} \otimes \bar{y})^T : x \in \mathbb{C}^n, y \in \mathbb{C}^m \right\}.$$

- Dual of  $\mathbf{Sep}$ :

$$\mathbf{Sep}^* \stackrel{\text{def}}{=} \{M \in \mathbf{Herm}(nm) : \text{tr}[M\rho] \geq 0 \forall \rho \in \mathbf{Sep}\}$$



# Duality

$$\mathbf{Sep}(n, m) = \text{conv} \left\{ (x \otimes y)(\bar{x} \otimes \bar{y})^T : x \in \mathbb{C}^n, y \in \mathbb{C}^m \right\}.$$

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where

$$p_M(x, y) = \sum_{ijkl} M_{ij,kl} x_i \bar{x}_k y_j \bar{y}_l.$$

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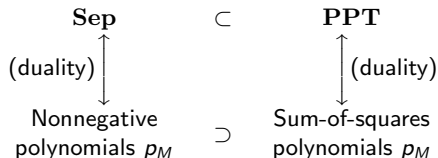
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- $\mathbf{PPT}^* = \{M \in \mathbf{Herm}(nm) : p_M \text{ is sum-of-squares}\}$

# Duality

$$p_M(x, \bar{x}, y, \bar{y}) = \sum_{ijkl} M_{ijkl} x_i \bar{x}_k y_j \bar{y}_l$$



# Sums of squares

- A polynomial  $f(z, \bar{z})$  in  $z \in \mathbb{C}^d$  is Hermitian if it is real-valued.
- Hermitian polynomial  $f(z, \bar{z})$  is a **sum of squares** if

$$f(z, \bar{z}) = \sum_i g_i(z, \bar{z})^2$$

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- $f(z, \bar{z})$  is a (complex) sum of squares if

$$f(z, \bar{z}) = \sum_i |h_i(z)|^2$$

for some polynomials  $h_i(z) \in \mathbb{C}[z]$

The two notions are different:  $f(z, \bar{z}) = (z + \bar{z})^2$  is real sos but not complex sos.

# Proof $\mathbf{PPT}^* \leftrightarrow \text{sos}$

# Outline

- Sum-of-squares hierarchy for the set of separable states
  
  
  
  
  
  
  
  
  
  
- Semidefinite lifts of  $\text{Sep}(n, m)$ ?

# SDP hierarchy

We have seen

- $\mathbf{Sep}^* = \{M \in \mathbf{Herm}(nm) : p_M \text{ is nonnegative}\}$ .
- $\mathbf{PPT}^* = \{M \in \mathbf{Herm}(nm) : p_M \text{ is sos}\}$

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The *Doherty-Parrilo-Spedalieri* hierarchy is (from the dual point of view):

$$\mathbf{DPS}_\ell^* = \left\{ M \in \mathbf{Herm}(nm) : |y|^{2(\ell-1)} p_M \text{ is sos} \right\}.$$

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We have

$$\mathbf{Sep} \subset \mathbf{PPT} = \mathbf{DPS}_1 \subset \mathbf{DPS}_2 \subset \cdots \subset \mathbf{DPS}_\ell$$

Convergence of the hierarchy? (Note:  $\mathbf{DPS}_\ell$  has an SDP representation of size  $\approx d^\ell$ )

# Convergence

We prove a general convergence result for the sum-of-squares hierarchy on the sphere

## Theorem (Fang-Fawzi)

Let  $p(x_1, \dots, x_d)$  homogeneous polynomial such that

$$\epsilon \leq p(x) \leq 1 \quad \forall x \in S^{d-1}$$

Then  $p$  is  $\ell$ -sos with  $\ell \gtrsim d/\sqrt{\epsilon}$ .

- Best previous result gives convergence in  $d/\epsilon$  instead of  $d/\sqrt{\epsilon}$  [Reznick 95, Doherty-Wehner 12]

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- Best previous result gives convergence in  $d/\epsilon$  instead of  $d/\sqrt{\epsilon}$  [Reznick 95, Doherty-Wehner 12]
- Applied to the DPS hierarchy we get that, for  $M \succeq 0$

$$h_{\text{Sep}}(M) \leq h_{\text{DPS}_\ell}(M) \leq \left(1 + c \left(\frac{d}{\ell}\right)^2\right) h_{\text{Sep}}(M)$$

where  $h_C(M) = \max_{\rho \in C} \text{tr}[M\rho]$ . Recovers result of Navascués-Owari-Plenio [2009] based on quantum information tools.

# Overview of proof

- Let  $p(x)$  real polynomial such that  $0 < \epsilon \leq p \leq 1$  on  $S^{n-1}$ .

Goal: write  $p$  as a sum of squares

- Define integral transform

$$(Kp)(x) = \int_{y \in S^{d-1}} \phi(x^T y) p(y) d\sigma(y)$$

where  $\phi : [-1, 1] \rightarrow \mathbb{R}$  is a univariate function.

- Observations:

- If  $\phi(t) = \delta(t - 1)$  [Dirac delta] then  $Kp = p$ .
- If  $\phi(t) = h(t)^2$  where  $\deg h \leq \ell$  then  $Kp$  is an (integral) sum of squares of degree  $\ell$  polynomials.

- Strategy of proof: we write  $p = K(K^{-1}p)$ . If  $p \geq \epsilon > 0$ , and if  $K \approx$  identity then we hope that  $K^{-1}p \geq 0$ . In this case  $p = K(K^{-1}p)$  is a sum of squares.

# Fourier analysis

$$(Kp)(x) = \int_{y \in S^{d-1}} \phi(x^T y) p(y) d\sigma(y)$$

- Need to understand how close  $K$  is to the identity operator
- Fourier analysis: there is a decomposition  $\mathbb{R}[x] = H_0 \oplus H_1 \oplus H_2 \oplus \dots$  (*harmonic spaces*) such that if  $p = p_0 + p_1 + \dots$  then

$$Kp = \lambda_0 p_0 + \lambda_1 p_1 + \dots$$

where  $(\lambda_i)$  are coefficients of  $\phi$  in a basis of Gegenbauer polynomials.

$$\|K^{-1}p - p\|_\infty = \left\| \sum_i (\lambda_i^{-1} - 1)p_i \right\|_\infty \leq \|p\|_\infty C \sum_i |\lambda_i^{-1} - 1|.$$

## Continued

**To recap:** if we can find  $\phi(t) = h(t)^2$  with  $\deg h \leq \ell$  such that  $C \sum_i |\lambda_i^{-1} - 1| \leq \epsilon$ , then  $K^{-1}p \geq 0$ , and thus  $p = K(K^{-1}p)$  is  $\ell$ -sos on the sphere.

- Some analysis with orthogonal polynomials tells us that we can find such a  $\phi(t) = h(t)^2$  with  $\ell \approx d/\sqrt{\epsilon}$ .
- Idea not new, rediscovered many times: Reznick, Doherty-Wehner, Parrilo. Main difference is choice of kernel/Fourier analysis part

Semidefinite representations of Sep?



# Semidefinite programming lifts

**Spectrahedra** A *spectrahedron* is a convex set of the form

$$S = \{w \in \mathbb{R}^d : \mathcal{A}(w) \succeq 0\}$$

where  $\mathcal{A} : \mathbb{R}^d \rightarrow \mathbf{Herm}(N)$  is a linear map.

PPT( $n, m$ ) is a spectrahedron where  $\mathcal{A}(\rho) = \begin{bmatrix} \rho & 0 \\ 0 & (I \otimes \mathbb{T})(\rho) \end{bmatrix}$

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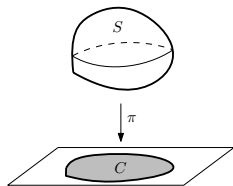
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**Projection** We say that  $C$  has an *SDP lift* of size  $N$  if

$$C = \pi(S)$$

where  $S$  is a spectrahedron as above, and  $\pi$  is a linear map.  
More expressive!



- Can show that

$$C = \{(x, y) : x^4 + y^4 \leq 1\}$$

has a SDP representation, but is *not* a spectrahedron.

# Lifting

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- If  $C$  has a SDP representation, then optimizing a linear function on  $C$  is a semidefinite program:

$$\min_{x \in C} \ell(x) = \min_{\mathcal{A}(y) \succeq 0} \ell \circ \pi(y).$$

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- Lifting can be very helpful from a complexity point of view

## Other lifting examples

- Permutahedron

$$\text{conv} \{(\sigma(1), \dots, \sigma(n)) : \sigma \in \mathcal{S}_n\}$$

has  $n!$  vertices and  $\sim 2^n$  facets. Can express it as the projection of the convex polytope of doubly stochastic matrices

$$DS_n = \{M \in \mathbb{R}^{n \times n} : M_{ij} \geq 0 \forall ij \text{ and } M\mathbf{1} = \mathbf{1}^T M = \mathbf{1}\}$$

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- For perfect graphs Lovász showed

$$STAB(G) = \left\{x \in \mathbb{R}^n : \exists X \text{ s.t. } \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \geq 0, X_{ii} = x_i, X_{ij} = 0 \forall ij \in E \right\}.$$

# SDP lifts

Which convex sets  $C$  have an SDP lift? A necessary condition is that  $C$  is *semialgebraic* (Tarski)

## Semialgebraic geometry

- A set is *semialgebraic* if it is a boolean combination (union, intersection, complement) of sets defined using polynomials equalities and inequalities
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- Scheiderer (2012): convex semialgebraic sets in the **plane** have SDP lift

# SDP lifts

Which convex sets  $C$  have an SDP lift? A necessary condition is that  $C$  is *semialgebraic* (Tarski)

## Semialgebraic geometry

- A set is *semialgebraic* if it is a boolean combination (union, intersection, complement) of sets defined using polynomials equalities and inequalities
- Tarski's quantifier elimination (1940s): the projection of any semialgebraic set is semialgebraic
- Nemirovski (ICM 2006): does any convex *semialgebraic* set  $C$  have a semidefinite lift?
- Helton-Nie (2009): if boundary of  $C$  is **smooth** with positive curvature then it has SDP lift. They conjectured a positive answer to Nemirovski.
- Scheiderer (2012): convex semialgebraic sets in the **plane** have SDP lift
- Scheiderer (2016): there are (many) convex semialgebraic sets that **do not** have an SDP representation

# No exact SDP representations exist for Sep in general

## Theorem (Fawzi)

*If  $\text{Sep}(n, m) \neq \text{PPT}(n, m)$  then  $\text{Sep}(n, m)$  has no SDP lift. In other words,  $\text{Sep}(3, 3)$  and  $\text{Sep}(4, 2)$  have no SDP lift.*

- Horodecki's formulation of  $\text{Sep}(n, m)$ :

$$\text{Sep}(n, m) = \{ \rho \in \mathbf{Herm}(nm) : (I \otimes \Phi)(\rho) \geq 0 \ \forall \Phi : M_m \rightarrow M_n \text{ positive} \}.$$

Skowronek (2016) showed that for  $\text{Sep}(3, 3)$  it is not possible to reduce the quantifier  $\forall \Phi$  to a finite number of maps  $\Phi_1, \dots, \Phi_k$ .

- Result also includes as a special case that the DPS (Doherty-Parrilo-Spedalieri) hierarchy does not converge in a finite number of levels when  $n + m > 5$ .

# Conclusion

- Use tools from semidefinite programming, polynomial optimization and sums of squares to study problems in quantum information.
- Things I did not talk about: noncommutative polynomial optimization (NPA hierarchy), tomography problems and compressed sensing, ...

Thank you!



Proof Sep has no semidefinite lift

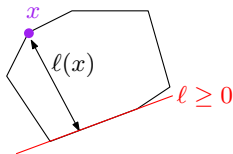


# Semidefinite lifts

- Definition of SDP lift is hard to work with. Need a more algebraic way of thinking about it
- Given convex cone  $C = \text{conv}(X)$ , we associate a *slack matrix*  $\mathbf{S}$  (potentially infinite) defined as follows:

$$\mathbf{S}(x, \ell) = \ell(x) \geq 0 \quad \forall x \in X, \ell \in C^*$$

- If  $C$  polytope, then slack matrix  $\mathbf{S}$  has size  $\#vertices \times \#facets$



# Factorization theorem

SDP lift of  $C$   $\Leftrightarrow$  Factorization of  $\mathbf{S}$

# Factorization theorem

SDP lift of  $C \iff$  Factorization of  $\mathbf{S}$

## Theorem (Gouveia, Parrilo, Thomas)

$C = \text{conv}(X)$  has an SDP lift of size  $N$  iff one can find maps  $A : X \rightarrow \mathbf{Herm}_+^N$  and  $B : C^* \rightarrow \mathbf{Herm}_+^N$  such that we have the factorization

$$\mathbf{S}(x, \ell) = \text{Tr}[A(x)B(\ell)] \quad \forall x \in X, \ell \in C^*$$

Generalizes a result of Yannakakis 1991 (LPs) to SDPs

# SDP lifts and sums of squares

A corollary of the previous theorem is

## Theorem

*Assume  $C = \text{conv}(X)$  has an SDP lift of size  $N$ . Then there is a subspace  $\mathcal{V}$  of functions on  $X$  of dimension at most  $N^2$  s.t. for any  $\ell \in C^*$*

$$\ell|_X = \sum_k h_k^2 \quad \text{where} \quad h_k \in \mathcal{V}.$$

Proof: write

$$\ell(x) = \text{tr}[A(x)B(\ell)] = \text{tr}[F(x)F(x)^T G(\ell)G(\ell)^T] = \|F(x)^T G(\ell)\|_F^2 = \sum_k h_k(x)^2$$

## General result in the real case

### Theorem (Main, real case)

Let  $p \in \mathbb{R}[\mathbf{x}]$  be a nonnegative polynomial that is not sos. Let

$$A = \{\alpha \in \mathbb{N}^n : \alpha \leq \beta \text{ for some } \beta \in \text{supp}(p)\}$$

be the “staircase” under  $\text{supp}(p)$ . Then

$$C_A = \text{conv} \{(\mathbf{x}^\alpha)_{\alpha \in A} : \mathbf{x} \in \mathbb{R}^n\}$$

has no semidefinite representation.

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- Linear functions nonnegative on  $C_A \leftrightarrow$  nonnegative polynomials supported on  $A$

Characterization of SDP lifts using sum-of-squares:

## Theorem

*$C_A$  has an SDP representation iff there are functions  $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$  ( $i = 1, \dots, k$ ) such that any nonnegative polynomial supported on  $A$  can be written as a sum of squares of functions from  $\text{span}(f_1, \dots, f_k)$ .*

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$C_A$  has an SDP representation iff there are *semialgebraic* functions  $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$  ( $i = 1, \dots, k$ ) such that any nonnegative polynomial supported on  $A$  can be written as a sum of squares of functions from  $\text{span}(f_1, \dots, f_k)$ .

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- $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is *semialgebraic* if its graph  $\{(x, f(x)) : x \in \mathbb{R}^n\}$  is a semialgebraic subset of  $\mathbb{R}^{n+1}$



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- **Semialgebraic functions are tame:** They are smooth ( $C^\infty$ ) almost everywhere (except on a set of measure 0)

# Proof of main theorem

$p$  nonnegative polynomial not sos,  $A = \text{staircase under } \text{supp}(p)$

$$C_A = \text{conv} \{(x^\alpha)_{\alpha \in A} : x \in \mathbb{R}^n\}.$$

- Assume  $C_A$  has an SDP representation, and let  $f_1, \dots, f_k : \mathbb{R}^n \rightarrow \mathbb{R}$  be the semialgebraic functions associated to this representation
- Since the  $(f_i)_{i=1, \dots, k}$  are smooth almost everywhere, there is a point  $a \in \mathbb{R}^n$  such that the  $f_i$  are all smooth at  $a$
- Since  $A$  is the staircase under  $\text{support}(p)$ , the polynomial  $p(x + a)$  is supported on  $A$ , and since it is nonnegative, it must be a sum-of-squares from  $\text{span}(f_1, \dots, f_k)$ . Shifting by  $a$ , this means that  $p$  is a sum of squares from  $\text{span}(\tilde{f}_1, \dots, \tilde{f}_k)$  where  $\tilde{f}_i(x) = f_i(x - a)$

# Smooth sums of squares

## Proposition

Assume  $p$  is a homogeneous polynomial such that  $p = \sum_j f_j^2$  for some arbitrary functions  $f_j$  that are  $C^\infty$  at the origin. Then  $p$  is a sum of squares of *polynomials*.

Proof: Taylor expansion

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Proof: Taylor expansion

- Proves theorem when  $p$  is homogeneous
- Additional technical argument based on Puiseux expansions is needed for general  $p$

## Main result, complex case

### Theorem (Main, complex case)

Let  $p$  be a nonnegative Hermitian polynomial that is not sos. Let

$$A = \{(\alpha, \alpha') \in \mathbb{N}^n \times \mathbb{N}^n : (\alpha, \alpha') \leq (\beta, \beta'), \text{ for some } (\beta, \beta') \in \text{supp}(p)\}$$

be the “staircase” under  $\text{supp}(p)$ . Then

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has no semidefinite representation.

- If  $\text{Sep}(n, m) \neq \text{PPT}(n, m)$ , apply theorem above with  $p =$  (dehomogenized) nonnegative Hermitian biquadratic on  $(n, m)$  variables that is not sos
- For  $\text{Sep}(3, 3)$  use the Choi polynomial. For  $\text{Sep}(4, 2)$  use a polynomial exhibited by Woronowicz and further studied by Ha and Kye.