## Tensors, invariants, and optimization

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based on joint works with Peter Bürgisser, Cole Franks, Ankit Garg, Rafael Oliveira, Avi Wigderson (ITCS'18, FOCS'18, FOCS'19)

## Overview

There are geometric and algebraic problems, originating in invariant theory, that are amenable to numerical optimization algorithms over groups.

Marginal & scaling problems

 $\longleftrightarrow$  Null cone problems

These capture a wide range of surprising applications – from algebra and analysis to computer science and quantum information.

Plan for today:

- Introduction to the framework
- Panorama of applications
- Algorithmic solution

Optimization algorithms for problems with natural symmetries!

Group actions mathematically model symmetries and equivalence.



Problem: How can we algorithmically and efficiently check equivalence?

Interesting (and often difficult) problems with many applications:

- no polynomial-time algorithms are known for graph isomorphism
- matrices equivalent under row and column operations iff equal rank; but tensor rank is NP-hard
- derandomizing PIT implies circuit lower bounds
- computing normal forms, describing moduli spaces and invariants...

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**Group**  $G \subseteq GL_n(\mathbb{C})$ , such as  $GL_n$ ,  $SL_n$ , or  $T_n = (\mathbb{C}^*)^n$ **Action** on  $V = \mathbb{C}^m$  by linear transformations **Orbits**  $Gv = \{g \cdot v : g \in G\}$  and their closures  $\overline{Gv}$ 



Orbit problems:

- Given v and w, are they in the same orbit? That is, is Gv = Gw?
- Robust versions:  $v \in \overline{Gw}$ ?  $\overline{Gv} \cap \overline{Gw} \neq \emptyset$ ?
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# Example: Conjugation

$$G = GL_n$$
,  $V = Mat_n$ ,  $g \cdot X = gXg^{-1}$ 

$$\begin{pmatrix} \lambda_1 & 1 & & \\ & \lambda_1 & 1 & \\ & & \lambda_1 & \\ & & & \ddots \end{pmatrix}$$

- ► X, Y are in same orbit iff same Jordan normal form
- ► X, Y have intersecting orbit closures iff same eigenvalues
- ► X is in *null cone* iff nilpotent

NB: The last two problems have a meaningful approximate version!

# Orbit problems and optimization

For concreteness, focus on the null cone problem: Is  $0 \in \overline{Gv}$ ?

We can translate this into an optimization problem on the group G:

$$\inf_{g \in G} \|g \cdot v\| = ?$$

*First-order condition*? Clearly, the gradient at any minimizer g is zero. Remarkably, this is also sufficient! [Kempf-Ness

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# Summary so far

 $G \subseteq \operatorname{GL}_n$  acting linearly on  $V = \mathbb{C}^m$ 

Null cone problem: Given v, is  $0 \in \overline{Gv}$ ?

... and its relaxations:

Norm minimization problem: Given v, find  $g \in G$  s.th.  $||g \cdot v|| \approx \inf$ .

Scaling problem: Given  $v \in V$ , find  $g \in G$  s.th.  $\nabla ||g \cdot v|| \approx 0$ .

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But they also provide path to other orbit problems.

Useful *model problems*. Plausibly solvable in polynomial time, but rich enough to have interesting applications. Let us look at some...

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A panorama of applications



# Example: Matrix scaling (raking, IPFP, ...)

Let X be matrix with nonnegative entries. A scaling of X is a matrix

$$Y = \begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix} X \begin{pmatrix} b_1 & & \\ & \ddots & \\ & & & b_n \end{pmatrix} \qquad (a_1, \dots, b_n > 0).$$

A matrix is called *doubly stochastic* (*d.s.*) if row & column sums are 1.

#### Matrix scaling (Geometry): Given X, $\exists$ (approximately) d.s. scalings?

Permanent (Algebra): ... iff per(X) > 0!

- ► ... iff ∃ bipartite perfect matching in support of X
- can be decided in polynomial time
- find scalings by alternatingly fixing rows & columns ③

[Sinkhorn]

Connections to statistics, complexity, combinatorics, geometry, numerics, ....

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$$\begin{array}{c} \mathsf{Pe} \\ V = \mathsf{Mat}_n, \quad G = \mathsf{T}_n \times \mathsf{T}_n, \quad (g_1, g_2)v = g_1vg_2. \\ \\ \mathsf{Then}, \quad \nabla ||g \cdot v||^2 = (\mathsf{row sums, column sums}) \text{ of } X_{ij} = |v_{ij}|^2. \\ \end{array}$$

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## Example: Sinkhorn algorithm

$$\begin{pmatrix} 1 & 2 \\ 4 & 0 \end{pmatrix} \stackrel{\text{fix rows}}{\longrightarrow} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ 1 & 0 \end{pmatrix} \stackrel{\text{fix cols}}{\longrightarrow} \begin{pmatrix} \frac{1}{4} & 1 \\ \frac{3}{4} & 0 \end{pmatrix} \longrightarrow \ldots \longrightarrow \begin{pmatrix} \frac{1}{2t} & 1 \\ \frac{2t-1}{2t} & 0 \end{pmatrix}$$

after *t* steps. Why does it work? Permanent increases monotonically – can be used to control convergence:

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distance to doubly stochastic

State-of-the-art algorithms directly optimize the norm square (in disguise).

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#### Example: Operator scaling and non-commutative PIT

Let  $T(\rho) = \sum_{i} X_{i} \rho X_{i}^{\dagger}$  be a CP map. A *scaling* of T is of the form  $S(\rho) = AT(B\rho B^{\dagger})A^{\dagger}$   $(A, B \in GL_{n})$ 

Say *T* is quantum doubly stochastic if  $T(I) = T^{\dagger}(I) = I$ .

**Operator scaling**: Given T,  $\exists$  approximately quantum d.s. scalings?

Polynomial identity testing: ... iff  $\exists$  matrices  $Y_k$  s.th. det  $\sum_k Y_k \otimes X_k \neq 0$ .

- natural iterative algorithm: alternatingly make unital and trace-preserving
- can solve in deterministic polynomial time

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[Gurvits]

# Applications and connections

Invariant theory: Null cone & orbit closure intersection, moment polytopes

Analysis: Brascamp-Lieb inequalities, solution of Paulsen's problem

Symplectic geometry: Horn's problem $\exists A + B = C$  with spectrum  $\alpha$ ,  $\beta$ ,  $\gamma$ ?Combinatorics: Positivity of Littlewood-Richardson coefficients

Statistics: MLE in Gaussian models, Tyler's M-approximation Optimization: Efficient algorithms for classes of quadratic equations

Computational complexity: Polynomial identity testing, tensor ranks Quantum information: Marginal problems, entanglement transformations

All these are special cases of a general class of problems! We now focus on one scenario that is in many ways 'representative'.

#### Quantum states and marginals

Pure quantum state of d particles is described by unit-norm tensor:

$$X \in V = \mathbb{C}^{n_1} \otimes \cdots \otimes \mathbb{C}^{n_d}$$

$$\times$$
  $\bigcirc$   $\bigcirc$   $\bigcirc$   $\bigcirc$   $\bigcirc$   $\bigcirc$   $\bigcirc$ 

State of individual particles described by density matrices  $\rho_1, \ldots, \rho_d$ :

$$\mathsf{tr}[\mathbf{\rho}_1 H_1] = \langle X | H_1 \otimes I \otimes \ldots \otimes I | X \rangle \quad \forall H_1$$

Quantum marginal problem: Which  $\rho_1, \ldots, \rho_d$  are consistent with a global pure state X?

Answer only depends on the eigenvalues  $\lambda_i$  of  $\rho_i$ !



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# Examples

Two particles:  $\rho_A$  and  $\rho_B$  compatible with global pure state iff same nonzero eigenvalues (Schmidt decomposition)

Three particles:

$$egin{aligned} \lambda_{\mathcal{A},\max} + \lambda_{\mathcal{B},\max} \leqslant \lambda_{\mathcal{C},\max} + 1 \ \lambda_{\mathcal{A},\max} + \lambda_{\mathcal{C},\max} \leqslant \lambda_{\mathcal{B},\max} + 1 \ \lambda_{\mathcal{B},\max} + \lambda_{\mathcal{C},\max} \leqslant \lambda_{\mathcal{A},\max} + 1 \end{aligned}$$



necessary and sufficient for qubits

[Higuchi, Sudbery, Szulc]

► follows from variational principle:  $\lambda_{A,max} = \max_{\varphi_A} \langle \varphi_A | \varphi_A | \varphi_A \rangle$  etc.

# Tensor scaling and SLOCC

A scaling of X is a tensor of the form

 $Y = (A_1 \otimes \ldots \otimes A_d) X \quad (A_i \in \mathsf{GL}_{n_i})$ 



- state that can be obtained by SLOCC (postselected local operations & classical communication)
- ► X constrains the entanglement class

#### Tensor scaling problem: Which $\rho_1, \ldots, \rho_d$ arise from scaling of given X?

- e.g. for ρ<sub>i</sub> ∝ l, each system maximally entangled with rest
  (= locally maximally mixed = quantum version of stochastic tensor)
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Thus, answer to tensor scaling problem is encoded by:

 $\Delta(X) = \left\{ (\lambda_1, \dots, \lambda_d) \text{ for scalings of } X \text{ (and limits)} \right\} \subseteq \mathbb{R}^{dn}$ 

e.g., for three qubits, GHZ =  $|000\rangle+|111\rangle$  and W =  $|100\rangle+|010\rangle+|001\rangle$ :

In general, always convex polytopes:

- encode local info about entanglement
- encode recent notions of tensor ranks

However, explicit description intractable. Exponential number of vertices and facets

We provide algorithmic solution!



[Kirwan, Mumford]

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## Geodesic optimization algorithms



# The Algorithm

Given state X, want to find scaling Y with desired marginals – whenever possible. For simplicity, uniform marginals ( $\rho_i \propto I$ ,  $\lambda_i \propto 1$ ) and d = 3.

**Algorithm:** Start with Y = X. For t = 1, ..., T: Compute marginals  $\rho_1$ ,  $\rho_2$ ,  $\rho_3$  of Y. If  $\varepsilon$ -close to uniform, stop. Otherwise, replace Y by  $(e^{-\eta \rho_1^o} \otimes e^{-\eta \rho_2^o} \otimes e^{-\eta \rho_3^o})Y$ .  $X^o = traceless part$ 

 $\eta = suitable step size$ 

#### Theorem

Algorithm finds  $Y = (A_1 \otimes A_2 \otimes A_3)X$  with marginals  $\varepsilon$ -close to uniform within  $T = \text{poly}(\frac{1}{\varepsilon}, \text{input size})$  steps.

- generalizes to arbitrary  $\lambda_i$ , d > 3, (anti)symmetric tensors, MPS, ...
- ► can run on quantum computer (but how well? ©)
- ► solve quantum marginal problem by using random X

cf. algorithm by Verstraete et al which we analyzed in prior work

# Why does it work?

"Otherwise, replace Y by  $(e^{-\eta \rho_1^o} \otimes e^{-\eta \rho_2^o} \otimes e^{-\eta \rho_3^o}) Y$ ."

#### Consider the problem of minimizing the norm

 $N(A_1, A_2, A_3) = \|(A_1 \otimes A_2 \otimes A_3)X\| \qquad (A_i \in SL_{n_i})$ 

Its derivative in direction given by *traceless*  $H_1$ ,  $H_2$ ,  $H_3$  is

 $\partial_{t=0} N(e^{tH_1}, e^{tH_2}, e^{tH_3}) = tr[\rho_1^{o}H_1] + tr[\rho_2^{o}H_2] + tr[\rho_C^{o}H_3].$ 

Therefore, the gradient can be identified with  $\nabla N = (\rho_1^o, \rho_2^o, \rho_3^o)$ .

- Algorithm implements geodesic gradient descent...
- ... and minimizing the gradient makes the marginals uniform! ③

How to make quantitative? What is the big picture?

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## Non-commutative optimization

In general, consider  $N(g) = \|g \cdot X\|$ .

We discussed that the following optimization problems are equivalent:

$$\inf_{g \in G} N(g) \iff \inf_{g \in G} \|\nabla N(g)\|$$
 [Kempf-Ness]

- primal: norm minimization, dual: scaling problem
- non-commutative version of linear programming duality

We develop quantitative duality theory and 1st & 2nd order methods.

All examples from introduction fall into this framework. Numerical algorithms that solve algebraic problems!

Everything works for general actions of reductive G. Norm is log-convex along geodesics.

# Geodesic convexity

Why does the duality hold? Consider geodesics  $g_t = e^{tH}g$  in the group G.



**Proposition:**  $N(g) = ||g \cdot v||$  satisfies along these geodesics:

• convexity: 
$$\partial_{t=0}^2 N(g_t) \ge 0$$

**2** smoothness: 
$$\partial_{t=0}^2 N(g_t) \leq 2C^2 \|H\|_F^2$$

C is typically small, upper-bounded by degree of action.

Smoothness implies that

$$N(e^Hg) \leq N(g) + \nabla N(g) \cdot H + C^2 ||H||_F^2.$$

Thus, gradient descent makes progress if steps not too large!

# Analysis of Algorithm

"Unless  $\varepsilon$ -close to uniform, replace Y by  $(e^{-\eta\rho_1^o} \otimes e^{-\eta\rho_2^o} \otimes e^{-\eta\rho_3^o})$ Y."

To obtain rigorous algorithm, show:

- progress in each step:  $||Y_{\text{new}}|| \leq (1 c_1 \varepsilon) ||Y||$
- ► a priori lower bound:  $\inf_{det=1} || (A_1 \otimes A_2 \otimes A_3) X || \ge c_2$

Then,  $(1 - c_1 \varepsilon)^T \ge c_2$  bounds the number of steps T.

The first point follows from smoothness, as just discussed.

For the second, construct 'explicit' invariants with 'small' coefficients, so that  $P(X) \neq 0$  implies bound in terms of bitsize of X.

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For the second, construct 'explicit' invariants with 'small' coefficients, so that  $P(X) \neq 0$  implies bound in terms of bitsize of X.

# Summary and outlook



Effective algorithms for large class of optimization problems over groups, incl. quantum marginal and tensor scaling problems. Based on geodesic convex optimization and geometric invariant theory.

Many exciting directions:

- Polynomial-time algorithms in all cases?
- ► Better tools for geodesic optimization? Quantum algorithms?
- ► Tensors in quantum information are often special. Implications?
- Can we tackle other problems with natural symmetries?

Thank you for your attention!

# A general equivalence

 $\mathcal{V}\subseteq \mathbb{P}(V)$ 

All points in  $\Delta(\mathcal{V})$  can be described via invariant theory:

$$V_\lambda \subseteq \mathbb{C}[\mathcal{V}]_{(k)} \quad \Rightarrow \quad rac{\lambda}{k} \in \Delta(\mathcal{V})$$

( $\lambda$  highest weight, k degree)

• Can also study multiplicities  $g(\lambda, k) := \# V_{\lambda} \subseteq \mathbb{C}[\mathcal{V}]_{(k)}$ .

This leads to interesting computational problems:

$$g = ?$$
 $g > 0 ?$  $\exists s > 0 : g(s\lambda, sk) > 0 ?$  $(\#-hard)$ (NP-hard)(our problem!)

Completely unlike Horn's problem: *Knutson-Tao saturation property does not hold, and hence we can hope for efficient algorithms!*