(Hidden) Symmetries of Computational Problems

Michael Walter (Ruhr-Uni Bochum)

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joint works with P. Bürgisser, L. Dogan, C. Franks, A. Garg, V. Makam, H. Nieuwboer, R. Oliveira, A. Ramachandran, F. Witteveen, A. Wigderson, . . .

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Prelude: Matrix scaling

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

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

It is called *doubly stochastic* if row & column sums are 1.

Matrix scaling problem: Given X, find approx. doubly stochastic scalings.

Sinkhorn algorithm: Alternatingly normalize rows & columns:

$$\begin{pmatrix} 1 & 2 \\ 4 & 0 \end{pmatrix} \xrightarrow{\text{rows}} \begin{pmatrix} 1/3 & 2/3 \\ 1 & 0 \end{pmatrix} \xrightarrow{\text{cols}} \begin{pmatrix} 1/4 & 1 \\ 3/4 & 0 \end{pmatrix} \longrightarrow \ldots \longrightarrow \begin{pmatrix} \varepsilon & 1 \\ 1-\varepsilon & 0 \end{pmatrix}$$

- This converges whenever possible, and in polynomial time! [LSW]
- Possible iff bipartite perfect matching in support of X.

Applications to statistics, combinatorics, numerics, complexity, machine learning, ...

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Sinkhorn algorithm: Alternatingly normalize rows & columns:

- Why does such a simple "greedy" algorithm work?
- What's the deal with perfect matchings?
- Answer to both: **Hidden symmetry** – the permanent of X. *And this is not an accident...*

Applications to statistics, combinatorics, numerics, complexity, machine learning, ...

Overview

There are geometric and algebraic problems, arising from group actions, that are amenable to convex optimization on symmetric spaces.

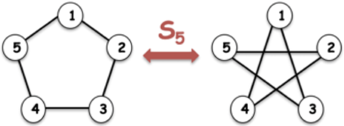
Scaling & marginal problems	$\longleftrightarrow$	Norm minimization

These are connected to a wide range of problems in mathematics and computer science that at first glance might appear unrelated.

Plan for today:

1. Introduction to the setting
2. Applications and connections
3. Algorithmic solutions

Symmetries and group actions



Problem: How can we algorithmically and efficiently check equivalence?

Interesting (and often difficult) problems with many applications:

- no polynomial-time algorithm known for graph isomorphism
- matrices equivalent iff equal rank, but how about tensors?
- given an arithmetic formula, does it always compute zero? finding a deterministic algorithm is famous open problem in computer science
- computing *normal forms*, describing *moduli spaces* and *invariants*...

In many applications, *equivalence* can be modeled by *group action*...

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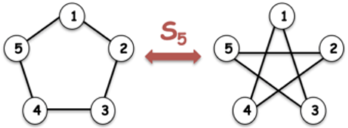

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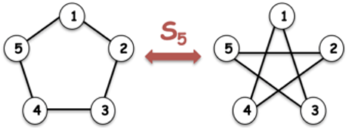

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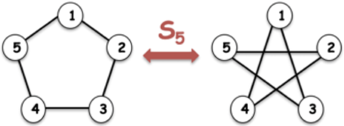

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Examples: Group actions and symmetries

- Matrices and want to ignore basis: GL(n) by conjugation

$$g \cdot M := gMg^{-1}$$

- Tensor networks: simultaneous conjugation on matrix tuples

$$g \cdot (M_j) := (gM_jg^{-1})$$

- Quantum channels: left-right action on matrix tuples

$$(g,h) \cdot (M_j) := (gM_jh^T) \qquad \Phi(X) = \sum_j M_jXM_j^*$$

- The above are also examples of quiver representations.
- Quantum states, but also bilinear problems: tensor action

$$(A,B,C) \cdot T := (A \otimes B \otimes C)T$$

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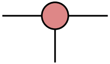

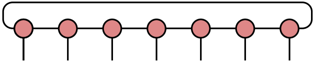

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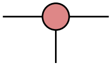

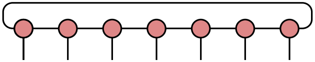

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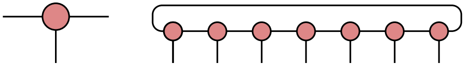

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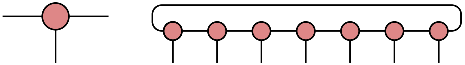

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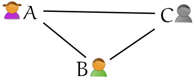
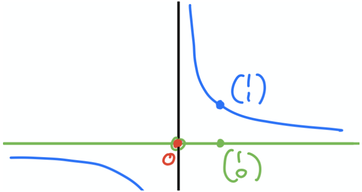


Formalizing equivalence: Orbit problems

Group $G \subseteq \mathrm{GL}_n(\mathbb{C})$ complex reductive, such as GL_n, SL_n, or $\mathrm{T}_n = \left(\begin{smallmatrix} \cdot & \\ & \cdot \end{smallmatrix}\right)$

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: Is $w \in \overline{Gv}$? Is $\overline{Gv} \cap \overline{Gw} \neq \emptyset$?
- **Null cone problem:** $0 \in \overline{Gv}$?

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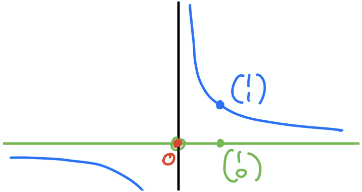

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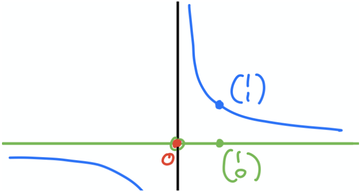

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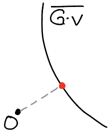
Big picture: Orbits, optimization, and scaling

For concreteness, focus on **null cone problem**:

Is $0 \in \overline{Gv}$?



Big picture: Orbits, optimization, and scaling

Is $P(v) = P(0)$ for every *invariant* polynomial P? Algebra

$\Updownarrow$

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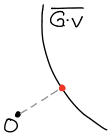

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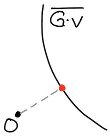
Optimization



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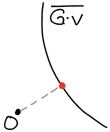

$\Nearrow$

Minimize $\|g \cdot v\|$ over $g \in G$. $\Longrightarrow$ Find $g \in G$ s.th. $\nabla_g \|g \cdot v\| \approx 0$.

Optimization

"Scaling Problem"

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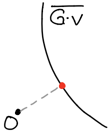

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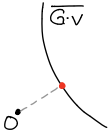

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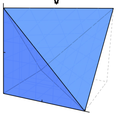
Optimization (which $\Rightarrow$ Is $0 \in \overline{Gv}$?)

$\Downarrow$

Natural normal forms to tackle other orbit problems.

"Scaling Problem"

symplectic $\Updownarrow$ geometry



Polytopes

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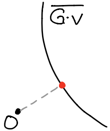

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Optimization — "Scaling Problem"

$\Downarrow$ — symplectic $\Updownarrow$ geometry

Na…

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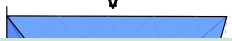
Why care? Surprisingly many problems fit this picture. Make it *quantitative* to obtain new insights and efficient algorithms.



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Example: Matrix scaling revisited

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Norm minimization:

$$\inf_{g,h} \|(g,h) \cdot M\|^2 = \inf_{g,h} \sum_{i,j} |g_i M_{ij} h_j|^2 = \inf_{x,y \in \mathbb{R}^n} \sum_{i,j} |M_{ij}|^2 e^{x_i + y_j}$$

- log-convex in x and y

Gradient:

$$\nabla_{x=y=0}(\ldots) = \big(\mathbf{r}(M), \mathbf{c}(M)\big)$$

where $\mathbf{r}(M)$, $\mathbf{c}(M)$ row and column sums of matrix with entries $|M_{ij}|^2$.

Matrix scaling and norm minimization are equivalent by convexity! ☺
Explains Sinkhorn & permanent. Starting point for cutting-edge algos.

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Let $G = \mathrm{ST}_n \times \mathrm{ST}_n$ act on $V = \mathrm{Mat}_n(\mathbb{C})$:

$$(g,h) \cdot M = \begin{pmatrix} g_1 & & \\ & \ddots & \\ & & g_n \end{pmatrix} M \begin{pmatrix} h_1 & & \\ & \ddots & \\ & & h_n \end{pmatrix}$$

Norm minimization:

$$\inf_{g,h} \|(g,h) \cdot M\|^2 = \inf_{g,h} \sum_{i,j} |g_i M_{ij} h_j|^2 = \inf_{x,y \in \mathbb{R}^n_{\sum=0}} \sum_{i,j} |M_{ij}|^2 e^{x_i + y_j}$$

- log-convex in x and y

Gradient:

$$\nabla_{x=y=0}(\ldots) = \big(\mathbf{r}(M), \mathbf{c}(M)\big) - \|M\|^2 (\mathbf{1}, \mathbf{1})$$

where $\mathbf{r}(M)$, $\mathbf{c}(M)$ row and column sums of matrix with entries $|M_{ij}|^2$.

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GIT vs symplectic quotient: Given semistable M, Sinkhorn algorithm approximates $M' \in \overline{G\cdot M}$ with zero moment map...

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In general, torus actions capture linear programming – one of the most widely used paradigms in convex optimization (and more)!

Example: Horn problem

Let $\alpha_1 \geqslant \ldots \geqslant \alpha_n$, $\beta_1 \geqslant \ldots \geqslant \beta_n$, $\gamma_1 \geqslant \ldots \geqslant \gamma_n$ be integers.

> Horn problem: When $\exists$ Hermitian $n \times n$ matrices A, B, C with spectrum α, β, γ such that $A + B = C$?

- Horn conjectured exponentially many linear inequalities on α, β, γ
- e.g., $\alpha_1 + \beta_1 \geqslant \gamma_1$
- proved in late 90s. by now, very precise mathematical understanding.
  [Klyachko, Knutson-Tao, Belkale, Ressayre, Paradan, . . .]

Knutson-Tao: . . . iff *Littlewood-Richardson coefficient* $c^{\gamma}_{\alpha,\beta} > 0$

- counts multiplicities in representation theory, combinatorial gadgets, integer points in polytopes, . . .
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> Yet, no known efficient algorithms to **find** such A, B, C (if α, β, γ are compatible), or to find a violated inequality (if they are not).

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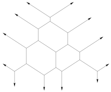

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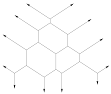

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Example: Operator scaling and polynomial identity testing

Any matrix tuple $X = (X_k)$ defines map $\Phi(A) = \sum_k X_k A X_k^*$. *Scaling:*

$$(g, h) \cdot (X_k) = (g X_k h^T) \qquad (g, h \in \mathrm{GL}_n)$$

Doubly stochastic if $\Phi(I) = I$ and $\Phi^*(I) = I$.

Operator scaling problem: Given X, find approx. doubly stochastic scaling.

Possible iff $\det \sum_k \alpha_k \otimes X_k \neq 0$ for some matrices α_k (semi-invariants!).

- equivalent: is arithmetic formula in *non-commuting variables* nonzero?
- a simple algo solves this in deterministic poly-time! [Garg et al, Ivanyos et al]

When α_k restricted to scalars: major open problem in computer science!

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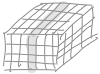
Example: Tensor scaling



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What other interesting polytopes are hidden in this way?

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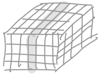

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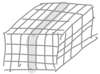

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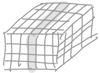

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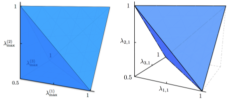

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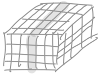

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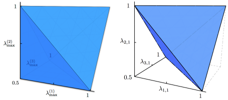

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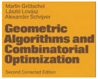

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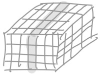

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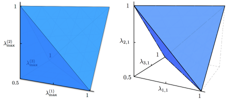

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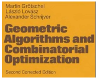


Connections and applications

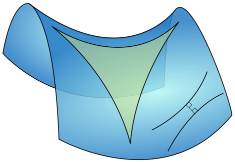
Scaling problems capture and connect many other applications (thanks to often hidden symmetries):

- theoretical: program testing, VP vs VNP
- algebraic: representation theory, moduli spaces
- quantum: quantum entanglement, tensor networks
- classical: derandomization
- continuous: optimal transport
- applied: maximum likelihood
- · · ·

This was discovered in a series of works, by many authors, over the past years. It has already proved key to faster algorithms and structural insight.

> General picture? How to find algorithms beyond Sinkhorn & friends?

Symmetry and Optimization



Norm minimization and gradient

In general, we want to minimize the Kempf-Ness function:

$$F\colon G \to \mathbb{R}, \quad F(g) := \log \|g \cdot v\|$$

For concreteness, $G = \mathrm{GL}_n$. By the polar decomposition, can restrict to:

$$\mathrm{PD}_n = \{p = e^X \;:\; X \in \mathrm{Herm}_n\} \cong K \backslash G$$

This is a Hadamard symmetric space. It has nonpositive curvature:

Gradient $\nabla F(I)$ is *moment map* in the sense of symplectic geometry.
As discussed $\nabla F = 0$ captures natural "scaling" problems!

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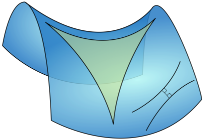

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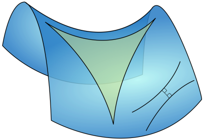

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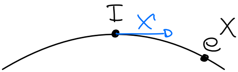
is convex along the geodesics of PD_n, i.e., $\partial_t^2 F(e^{Xt}) \geq 0$. [Kempf-Ness]



This implies critical points are global minima (like in the Euclidean case).

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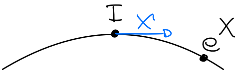

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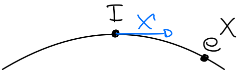

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How convex for given action? Necessary for algorithms!

Geodesic convexity made quantitative

Easy: The objective $F(p) = \log \|p \cdot v\|$ is "smooth", meaning

$$\partial_t^2 F(e^{Xt}) \leqslant L\|X\|_2^2.$$

Not so easy: Quantitative Kempf-Ness theorem. For $F_* = \inf_p F(p)$,

$$1 - \frac{\|\nabla F\|_2}{\gamma} \leqslant e^{F_* - F} \leqslant 1 - \frac{\|\nabla F\|_2^2}{2L}$$

- ☺ relates norm minimization ⇔ scaling in a quantitative way
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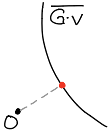
Action of complex reductive $G \subseteq \mathrm{GL}_n$ on $V \cong \mathbb{C}^m$.



Is $0 \in \overline{Gv}$?

Minimize $\|g \cdot v\|$ over $g \in G$. $\overset{\text{convexity}}{\underset{\text{quantitative}}{\Longleftrightarrow}}$ Find $g \in G$ s.th. $\nabla \|g \cdot v\| \approx 0$.

Norm Minimization — Scaling Problem

- All examples mentioned earlier fall into this framework.
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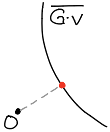

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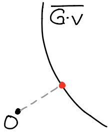

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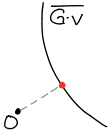

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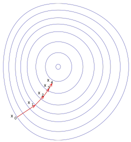
Algorithmic appetizer

Simplest approach: Repeatedly perform geodesic gradient steps



$$g \leftarrow e^{-\frac{1}{L}\nabla F(g)} g.$$

Theorem

If F bounded from below, algorithm finds $g \in G$ such that $\|\nabla F(g)\| \leqslant \varepsilon$ within $T = \text{poly}(\frac{1}{\varepsilon}, \text{input size})$ steps.

Analysis: Smoothness implies F decreases in each step. Combine with a priori lower bound obtained using constructive invariant theory.

Corollary

Same algorithm solves null cone problem in time $\text{poly}(\frac{1}{\gamma}, \text{input size})$.

Much faster (in theory and practice) than algebraic methods (e.g., via Gröbner bases).

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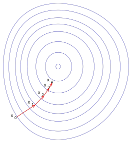

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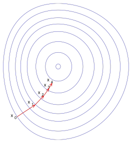

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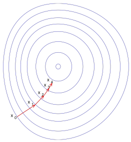

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These minimize local quadratic approximations

$$F(e^H g) \approx Q(H) = F(g) + \nabla F(g)[H] + \frac{1}{2}\nabla^2 F(g)[H, H]$$

on small neighborhoods. Need F "robust" or "self-concordant".

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Algorithms for moment polytopes

$F(g) = \log \|g \cdot v\|$

Recall scaling problem: Find $g \in G$ such that $\nabla F(g) \approx 0$. Depending on action, this can mean *doubly stochastic* matrix, ... $\rightsquigarrow$ uniform marginals.

More generally, we can ask nonuniform scaling problem:

Given $\mathbf{p}$, find $g \in G$ s.th. $\nabla F(g) \approx \mathbf{p}$.

In other words, want to prescribe an arbitrary value for the moment map.

Moment polytope captures possible values if restrict to Weyl chamber:

State of the art: Algorithms discussed above can also solve nonuniform scaling problem and membership in moment polytopes. Polynomial in most parameters for many interesting actions – but not in the bitsize of $\mathbf{p}$!

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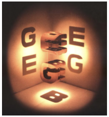
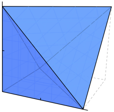
Summary and outlook

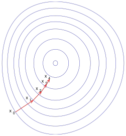
Symmetries lie behind many natural computational problems from algebra and analysis to classical and quantum CS.



Polytopes encode answers & clues to many of these problems. Often exp. vertices & facets, yet can admit efficient algos.



Symmetries are key to tackling these problems by optimization. Enabled by geodesic convexity and invariant theory.



Many open questions: Polynomial time algorithms for all actions? Complexity of algebraic problems? Structured or typical data? Other problems with natural symmetries? . . . **Happy birthday, Michèle!**