Orbitopes and Theta bodies

Raman Sanyal (UC Berkeley)

based on joint work with
Bernd Sturmfels and Frank Sottile
and ongoing work with
Philipp Rostalski

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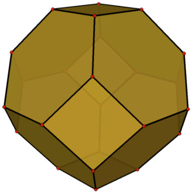
$$\mathrm{conv}(G \cdot v) = \mathrm{conv}\{g \cdot A : g \in G\} \subset V.$$



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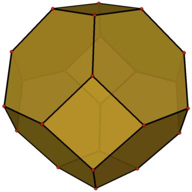

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here: G linear algebraic group, V rational representation

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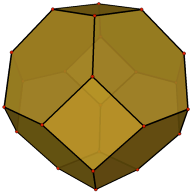

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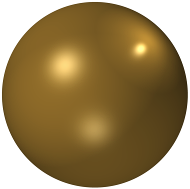

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Perspectives of Convex Algebraic Geometry

Convex geometry: faces, face lattices, dual bodies

Algebraic geometry: algebraic boundary, its equation, Whitney stratification

Optimization: How to optimize over an orbitope?

Why do we care?

finite groups

- classic geometry
  platonic solids, Permutahedra, Birkhoff polytopes, ...
- combinatorial optimization (see [Onn'93])
  matching polytope, traveling salesman polytope, graph isomorphism, ...

compact groups

- protein structure prediction [Longinetti-Sgheri-Sottile'08]
  magnetic susceptibility of folding proteins $\rightarrow$ $SO(3)$-orbitopes
- Calibrated geometries à la [Harvey-Lawson'82]
  'local geometry' of area-minimizing smooth manifolds
  faces of Grassmann orbitopes: convex hull of Grassmann manifold
- norm balls with transitive G-action
  balls, ellipses, operator norms, nuclear norms,...
- non-negative trigonometric polyn. are dual to *Carathéodory* orbitopes
- non-negative k-forms are dual to *Veronese orbitopes*

fascinating objects – plenty in supply!

How to compute with orbitopes? How to represent them?

Basic question: What is the dimension of a face of $\mathcal{O}_v$ in a given direction?

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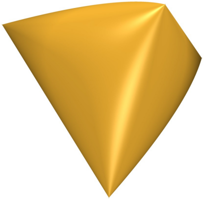

Easy, if orbitope can be represented as spectrahedron, i.e. feasible region of semidefinite program:

$S = \{ \ y \ : \ A_0 + y_1 A_1 + \cdots + y_d A_d \succeq 0 \ \}$ (positive semidefinite)

$A_0, \ldots, A_d$ symmetric $n \times n$-matrices.

S is a polyhedron if the A_i are commuting.

Example: Set of symmetric matrices A with eigenvalues at most λ

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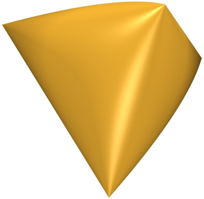

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Further Benefits

- information about facial structure; e.g. all faces exposed!
- readily available presentation for algebraic boundary

Caveat: Class of spectrahedra not closed under projection!

Alternatives: spectrahedral shadows such as Theta bodies

60 second commercial: Project proposals (with Philipp)

When is a spectrahedron a polytope?

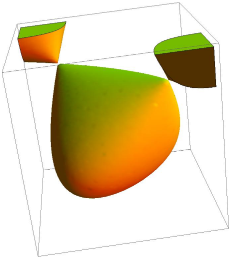
$$S = \{\ y\ :\ A_0 + y_1 A_1 + \cdots + y_d A_d \succeq 0\ \}$$

If the A_i do not commute, it might still be a polytope.

How do you check that algorithmically?

How do you prove that theoretically?

Is there such a 3-dim'l spectrahedron?



I.e. smooth boundary except for a single edge?
If No then this has intersting consequences for hyperbolic polynomials...

Degtyarev and Itenberg construct interesting/extremal 3-spectrahedra with 10 singular points in the boundary. Maybe degenerations thereof?

Kind of a sub-project to Anand Kulkarni projects regarding the combinatorial types of 3-spectrahedra.

In this talk

Tautological orbitopes for $O(n)$ and $SO(n)$

$$\mathcal{O} = \text{conv}\{ \text{ (special) orthogonal matrices } \} \subset \mathbb{R}^{n\times n}$$

(Tautological orbitope is convex hull over the representation $G \subset \mathrm{End}(V)$)
$\mathcal{O}$ is the norm ball in the operator norm for $\mathbb{R}^{n\times n}$

Grassmann orbitopes

$$\mathcal{G}(k,n) = \text{conv}\{ \text{ oriented } k\text{-dim subspaces of } \mathbb{R}^n \} \subset \wedge_k \mathbb{R}^n$$

Known as the mass ball in differential geometry

Tautological orbitope for the orthogonal group

$$\mathcal{O}_n = \operatorname{conv}(O(n)) \;=\; \operatorname{conv}\{\, g \in \mathbb{R}^{n\times n} : g \cdot g^T = \mathrm{Id} \,\}$$

- $\mathcal{O}_n$ convex body of dimension n^2
- all faces are exposed and isomorphic to $\mathcal{O}_k$ for $k \leq n$
- equation algebraic boundary is $f(A) = \det(A \cdot A^T - \mathrm{Id})$
- $\mathcal{O}_n$ is the spectrahedron

$$A : \begin{pmatrix} \mathrm{Id} & A \\ A^T & \mathrm{Id} \end{pmatrix} \succeq 0$$

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Key observation

T^n diagonal matrices, $\mathrm{Pr}_{T^n} : \mathbb{R}^{n\times n} \to T^n$ orthogonal projection

$$\mathcal{O}_n \cap T^n \; = \; \mathrm{Pr}_{T^n}(\mathcal{O}_n) \; = \; [-1, +1]^n \text{ (n-cube)}$$

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- $\mathcal{O}_n$ is the unit ball for the operator norm (=max singular value ≤ 1)
  $\rightarrow$ projects to unit ball for ℓ_∞-norm
- dual body $\mathcal{O}_n^\circ$ is the unit ball for the nuclear norm (=sum of sing. vals ≤ 1)
  $\rightarrow$ projects to unit ball for ℓ_1-norm

Tautological orbitope for the special orthogonal group

$$\mathcal{SO}_n = \text{conv}(SO(n)) \ = \ \text{conv}\{ \, g \in \mathbb{R}^{n\times n} : g \cdot g^T = \mathrm{Id}, \det(g) = 1 \, \}$$

- $\mathcal{SO}_n$ convex body of dimension n^2, for $n \geq 3$
- faces are linearly isomorphic to $\mathcal{SO}_k$ for $k \leq n$ or free spectrahedra

$$\mathcal{F}_k = \text{conv}\{uu^T : \|u\| = 1\} = \mathrm{PSD}_k \cap \{ \, \mathrm{trace} = 1 \, \} \subset \mathbb{R}^{k\times k}$$

- equation of the algebraic boundary is not known
- is $\mathcal{SO}_n$ a spectrahedron???

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n-Halfcube

$$H_n = \text{conv}\big\{x \in \{-1,+1\}^n : \text{ even number of } x_i = -1\big\}$$

for $n = 1, 2, 3, 4$ the halfcubes are: point, segment, tetrahedron, octahedron

Grassmann orbitopes

Exterior algebra $\wedge_k \mathbb{R}^n = \mathbb{R}\{e_J : J \subseteq [n], |J| = k\} \cong \mathbb{R}^{\binom{n}{k}}$

$$\mathbb{R}^{k\times n} \ni (v_1, \ldots, v_k) \;\mapsto\; v_1 \wedge \cdots \wedge v_k \;=\; \sum_J p_J \, e_J$$

$SO(n)$ acts on $\wedge_k \mathbb{R}^n$ by $g \cdot v_1 \wedge \cdots \wedge v_k = gv_1 \wedge \cdots \wedge gv_k$

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Grassmannian of oriented k-planes

$$G(k, n) := SO(n) \cdot e_1 \wedge e_2 \wedge \cdots \wedge e_k$$

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$v_1 \wedge \cdots \wedge v_k$ decomposable and $p = (p_J)_J$ decomposable iff p satisfies the Plücker relations $\mathrm{I}_{k,n} \subset \mathbb{R}[x_J : |J| = k]$

$$\left\{ \begin{array}{c} L \subset \mathbb{R}^n \\ \text{oriented} \\ \text{k}-\text{plane} \end{array} \right\} \overset{1:1}{\longleftrightarrow} \left\{ \begin{array}{c} v_1 \wedge \cdots \wedge v_k \\ \text{decomposable} \\ \text{unit length} \end{array} \right\} \overset{1:1}{\longleftrightarrow} \left\{ \begin{array}{c} p = (p_J)_J \in \mathbb{R}^{\binom{n}{k}} \\ \text{Plücker relations} \\ \sum_J p_J^2 = 1 \end{array} \right\}$$

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Grassmannian $G(k,n) = V(\mathrm{I}_{k,n}) \cap \{\text{unit sphere}\}$ is a compact real variety

The Grassmannian $G(2,4)$ of 2-planes in 4-space

$\wedge_2\mathbb{R}^4 = \mathbb{R}\{e_i \wedge e_j : 1 \le i < j \le 4\} = \mathbb{R}\{p_{12}, p_{13}, p_{14}, p_{23}, p_{24}, p_{34}\}$ 6-dim'l vector space

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for $u, v \in \mathbb{R}^4$

$$u \wedge v \ = \ p_{12}\, e_{12} + \cdots + p_{34}\, e_{34} \quad \text{with} \quad p_{ij} = \det \begin{pmatrix} u_i & v_i \\ u_j & v_j \end{pmatrix}$$

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Plücker relations + unit sphere determine unit decomposable vectors

$$\langle p_{12}p_{34} - p_{13}p_{24} + p_{14}p_{23},\; p_{12}^2 + p_{13}^2 + p_{14}^2 + p_{23}^2 + p_{24}^2 + p_{34}^2 - 1 \rangle$$

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A linear change of coordinates

$$u = \tfrac{1}{\sqrt{2}}(p_{12} + p_{34}), \quad v = \tfrac{1}{\sqrt{2}}(p_{13} - p_{24}), \quad w = \tfrac{1}{\sqrt{2}}(p_{14} + p_{23}),$$
$$x = \tfrac{1}{\sqrt{2}}(p_{12} - p_{34}), \quad y = \tfrac{1}{\sqrt{2}}(p_{13} + p_{24}), \quad z = \tfrac{1}{\sqrt{2}}(p_{14} - p_{23}).$$

yields

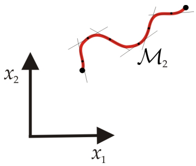
$$\left\langle\, u^2 + v^2 + w^2 - \tfrac{1}{2}\,,\ x^2 + y^2 + z^2 - \tfrac{1}{2}\, \right\rangle \subset \mathbb{R}[x, y, z, u, v, w]$$

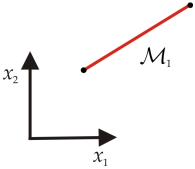
So, $G(2,4) = S^2 \times S^2$ is the Cartesian product of two 2-spheres.

$\mathcal{G}(2,4) = \operatorname{conv} G(2,4)$ is the Cartesian product of two 3-balls.

Area-minimizing manifolds and Grassmann orbitopes

Audience participation: Which 1-manifold is area-minimizing?





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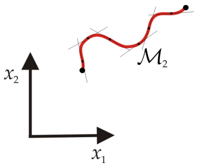

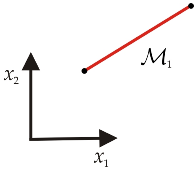

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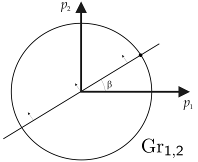

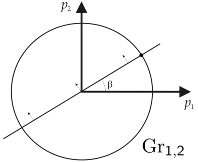

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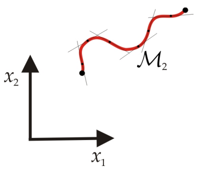

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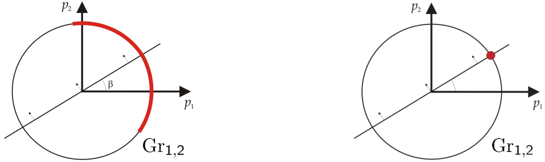

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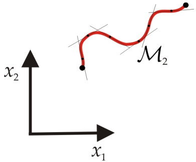

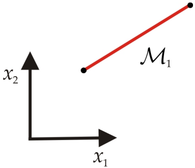

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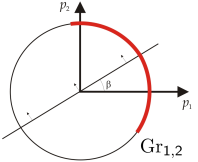

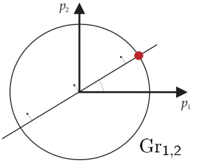

The collection of extreme points $F \cap G(k,n)$ is called a calibrated geometry. Elements of the dual face $F^\diamond$ are calibrations.

What we know about Grassmann orbitopes

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What about computer experimentation?

Back to the Basic Question

Basic question: What is the dimension of a face of $\mathcal{O}_v$ in direction $\ell(\mathbf{x})$?

The orbit is a real variety $G \cdot v = V_{\mathbb{R}}(\mathrm{I})$ for $\mathrm{I} \subseteq \mathbb{R}[\mathbf{x}]$

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Rephrased: What is the affine dimension of set of solutions to the optimization problem max $\ell(x)$ subject to $x \in V_{\mathbb{R}}(\mathrm{I})$?

- Polynomial optimization is hard **but** powerful relaxations (SOS, moment) are available [Parrilo, Lasserre, Laurent...]!
- The geometry behind (particular) relaxations are called Theta bodies [Gouveia, Parrilo, Thomas'08].
- In particular, Theta bodies are projected spectrahedra.

If the relaxation is exact, then local information about $\mathcal{O}_v$ are computable!

SOS relaxations and Theta bodies

Sum-of-Squares relaxation of degree k for $\ell(\mathbf{x})$ and $\mathrm{I} \subset \mathbb{R}[\mathbf{x}]$

$$\min \delta$$

$$s.t.\ \delta - \ell(\mathbf{x}) = \sum_{i=1}^{m} h_i(\mathbf{x})^2 \mod \mathrm{I}$$

for $h_1, \ldots, h_m \in \mathbb{R}[\mathbf{x}]$ polynomials of degree $\leq k$. $\delta - \ell(\mathbf{x})$ is called k-SOS mod I

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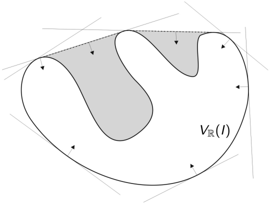

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Chain of convex bodies

$$\mathrm{TH}_1(\mathrm{I}) \ \supseteq \ \mathrm{TH}_2(\mathrm{I}) \ \supseteq \ \cdots \ \supseteq \ \overline{\text{conv } V_{\mathbb{R}}(\mathrm{I})}$$

I is TH_k-exact if $\mathrm{TH}_k(\mathrm{I}) = \overline{\text{conv } V_{\mathbb{R}}(\mathrm{I})}$

The Theta rank TH-rank(I) is the least k for which I is TH_k-exact

Theta ranks

Let $V \subset \mathbb{R}^n$ be a finite set and $\mathrm{I} = \mathrm{I}(V) \subset \mathbb{R}[\mathbf{x}]$ its ideal.
A linear function $\ell(\mathbf{x})$ has *m*-levels with respect to V if $\ell(\mathbf{x})$ takes m distinct values on V. V is *m*-level if every facet direction is.

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Proposition. If every facet direction of $\mathrm{conv}(V)$ has $\leq m$ levels, then I has Theta rank $\leq m - 1$. In particular, if V is 2-level, then V is TH_1-exact.

- actual Theta rank might be much smaller!
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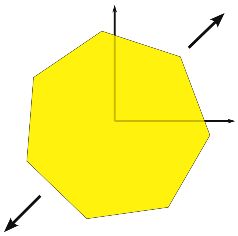
Example. TH-rank of the regular heptagon. For what k is $\delta \pm \ell(x)$ k-SOS?



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Theorem.[Gouveia,Parrilo,Thomas'08] If I is TH_1-exact, then

$$\mathrm{conv}(V) = \{x \in \mathbb{R}^n : q(x) \leq 0 \text{ for all } q \in \mathrm{I} \text{ convex quadric}\}$$

A useful tool for bounding Theta rank is

Lemma. If $L \subset \mathbb{R}^n$ is a linear space such that

$$\mathrm{conv}(V \cap L) \; = \; \mathrm{conv}(V) \cap L$$

then $\text{TH-rank}(\mathrm{I}) \geq \text{TH-rank}(\mathrm{I} + \mathrm{I}(L))$.

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- Both $O(n)$ and $SO(n)$ have such special cross-sections
- $G(3,6)$ has such a special cross section, the Segre orbitope

Theta ranks for some Orbitopes

Theta rank for $O(n)$

- cross-section with diagonal matrices $L = T^n$

$$\mathrm{conv}(O(n)) \cap L \;=\; [-1,+1]^n \;=\; \mathrm{conv}\{-1,+1\}^n \;=\; \mathrm{conv}(O(n) \cap L)$$

  the n-cube is 2-level $\rightarrow$ TH-rank$(O(n)) \geq 2$ (ok, trivial)

- up to symmetry only one facet direction: $\ell(X) = X_{11}$

$$1 - X_{11} \;\equiv\; \tfrac{1}{2}(X_{11} - 1)^2 \;+\; \tfrac{1}{2}X_{21}^2 \;+\; \cdots \;+\; \tfrac{1}{2}X_{n1}^2 \text{ on } O(n)$$

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Proposition. The n-dim'l halfcube H_n is has Theta rank $\lceil \frac{n}{2} \rceil$. In particular, H_n and $SO(n)$ have the same Theta rank.

Slightly simpler yoga as in the case for the heptagon...

Theta rank of Grassmann orbitopes

Theorem. The Grassmann orbitopes $\mathcal{G}(2, n)$ and $\mathcal{G}(n-2, n)$ are TH_1-exact.

- there is only one inclusion maximal face up to symmetry
  $\rightarrow$ show that facet direction is 1-SOS for $G(k, n)$

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based on computer experiments we

Conjecture. All Grassmann orbitopes $\mathcal{G}(k, n)$ are TH_1-exact.

For $\mathcal{G}(3, 6)$ there are up to symmetry only finitely many special Lagrangian faces but infinitely many doubletons (edges).
$\rightarrow$ show that the family doubleton directions is 1-SOS.

For $\mathcal{G}(3, 7)$ and $\mathcal{G}(4, 8)$ we recover 'all' known faces.

Experimentation is fast: For $\mathcal{G}(3, 9)$ the ideal has $1050 + 1$ generators on 84 variables. Computations in < 10min on laptop

Conjecture of Harvey-Lawson

In their 1982 paper we found that Harvey and Lawson conjecture that if

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Theorem. H-L conjecture is equivalent to $G(n,k)$ being TH_1-exact.

Take home messages

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Theta bodies of Orbitopes

- $O(n)$ is TH_1-exact, $SO(n)$ is $TH_{\lceil \frac{n}{2} \rceil}$-exact
- $\mathcal{G}(2, n)$ and $\mathcal{G}(n-2, n)$ are TH_1-exact
- strong computational evidence that $\mathcal{G}(3, 6)$ is TH_1-exact, but no proof yet...
- we conjecture that all Grassmann orbitopes are TH_1-exact
- Do orbitopes have finite Theta rank? 'small' Theta rank?