Sums of Squares, Moments and Applications in Polynomial Optimization

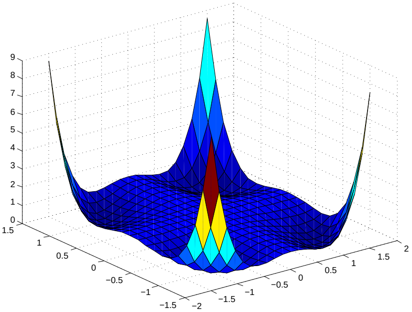
CWI

TILBURG UNIVERSITY

Monique Laurent

Fields Distinguished Lecture Series - May 10, 2021

What is polynomial optimization?



(P)

Minimize a polynomial function f over a region

$$K = \{x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$$

defined by polynomial inequalities (and equations)

Some instances

Testing nonnegativity of polynomials

The unconstrained quadratic case is easy

The quadratic form $x^{\mathsf{T}}Mx$ is nonnegative over $\mathbb{R}^n$ if and only if the matrix M is positive semidefinite ($M \succeq 0$)

This can be tested in **polynomial time**, using Gaussian elimination

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Testing matrix copositivity: co-NP complete [Kabadi-Murty 1987]

A symmetric matrix M is **copositive** if $x^\mathsf{T} M x = \sum_{i,j} M_{ij} x_i x_j \geq 0 \ \ \forall x \geq 0$

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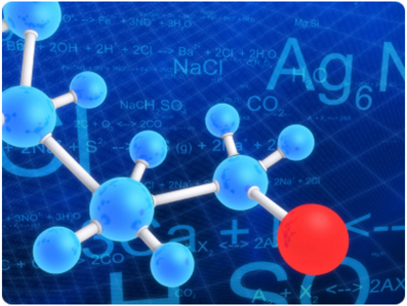
Testing convexity: NP-hard [Ahmadi et al. 2013]

A polynomial $f(x)$ is **convex** if and only if its Hessian matrix $H(f)(x)$ is positive semidefinite

Equivalently, $g(x, y) = y^\top H(f)(x)y$ is nonnegative on $\mathbb{R}^n \times \mathbb{R}^n$

Example from distance geometry



Reconstruct the locations of objects (say) in 3D from partial measurements of mutual distances

Given (partial) pairwise distances $d = (d_{ij})_{ij \in E}$, find (if possible) locations $u_1, \cdots, u_n \in \mathbb{R}^k$ in given dimension k ($k = 1, 2, 3, ..$) such that

$$\|u_i - u_j\|^2 = d_{ij} \qquad \text{for all } \{i, j\} \in E$$

Formulations via SDP and polynomial optimization

Find (if possible) vectors $u_1, \cdots, u_n \in \mathbb{R}^k$ ($k = 1, 2, 3, ..$) such that

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$$\Updownarrow \qquad\qquad X = (\langle u_i, u_j \rangle)$$

Find (if possible) a solution X with rank $\leq k$ to the semidefinite program

$$X \succeq 0, \quad X_{ii} + X_{jj} - 2X_{ij} = d_{ij} \quad (\{i,j\} \in E)$$

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Decide if $p_{\min} = 0$ and find a global minimizer to the quartic polynomial

$$\min_{x \in \mathbb{R}^{kn}} p(x) = \sum_{\{i,j\} \in E} \Big(d_{ij} - \sum_{h=1}^{k} (x_{ih} - x_{jh})^2 \Big)^2$$

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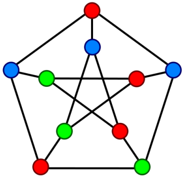
Given $a_1, \ldots, a_n \in \mathbb{N}$, assign distance $d_{i,i+1} = a_i$ to the edges of C_n. Then

$$\exists \text{ locations in } \mathbb{R} \iff \exists \epsilon \in \{\pm 1\}^n \text{ s.t. } \sum_{i=1}^{n} \epsilon_i a_i = 0$$

$\rightsquigarrow$ *hard partition problem*

Examples from combinatorial problems in graphs



$\alpha = 4 \quad \chi = 3$

- **stability number** $\alpha(G)$:

maximum cardinality of a set of pairwise non-adjacent vertices (**stable set**)

- **coloring number** $\chi(G)$:

minimum number of colors needed to properly color the vertices of G

$\alpha(G)$, $\chi(G)$ are NP-complete [Karp 1972]

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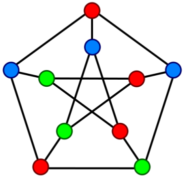

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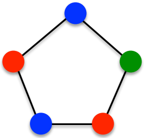
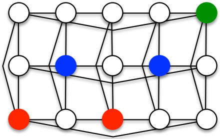
Chvátal's reduction of coloring to the stability number:

$\chi(G)$ is the smallest integer c such that $\alpha(G \square K_c) = \lvert V(G)\rvert$





Polynomial optimization formulations for $\alpha(G)$

- Basic 0/1 formulation:

$$\alpha(G) = \max \sum_{i \in V} x_i \ \text{ s.t. } \ x_i x_j = 0 \ (\{i,j\} \in E), \ x_i^2 = x_i \ (i \in V)$$

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- Motzkin-Straus formulation:

$$\frac{1}{\alpha(G)} = \min \; x^T (I + A_G) x \;\; \text{s.t.} \;\; \sum_{i \in V} x_i = 1, \; x_i \geq 0 \; (i \in V)$$

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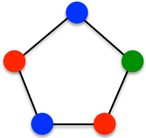
$\rightsquigarrow$ optimization over the **boolean cube** $\{0,1\}^n$, the **standard simplex** Δ_n, the **unit sphere** $\mathbb{S}^{n-1}$, the **copositive cone** COP_n

$\rightsquigarrow$ *More in Lecture 3*

Basic semidefinite bounds for $\alpha(G)$ and $\chi(G)$



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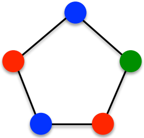

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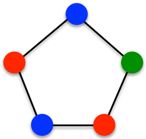

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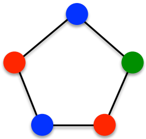

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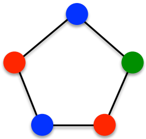

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Strengthen with non-negativity: [McEliece et al. 1978] [Schrijver 1979]

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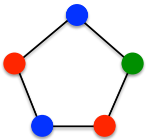

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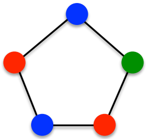

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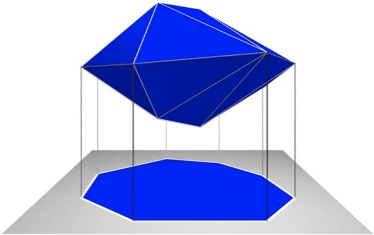
Stronger bounds?

Some key ideas

to get stronger bounds

- **Lift to higher dimensional space:** add new variables modeling products of original variables, such as $x_i x_j, x_i x_j x_k, x_i x_j x_k x_l, \ldots$



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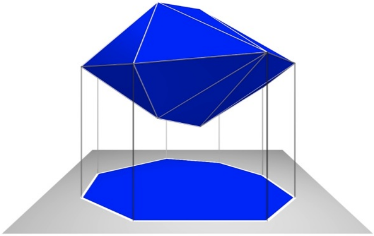

- Use **sums of squares of polynomials** as a 'proxy' for non-negativity of polynomials to get **tractable** relaxations

  Key fact: One can **model sums of squares of polynomials efficiently** using **semidefinite programming (SDP)**

Model sums of squares of polynomials with SDP

$$f(x) = \sum_{|\alpha| \leq 2d} f_\alpha x^\alpha \quad \text{is a } \textbf{sum of squares of polynomials}$$

$f(x) = \sum_i p_i(x)^2$

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$$\Updownarrow$$

$$f(x) = \sum_i [x]_d^T \overline{p_i}\ \overline{p_i}^T [x]_d = [x]_d^T \underbrace{\left(\sum_i \overline{p_i}\ \overline{p_i}^T \right)}_{M \succeq 0} [x]_d = \sum_{\beta,\gamma} M_{\beta,\gamma} x^{\beta+\gamma}$$

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$$\Updownarrow$$

The SDP $\left\{ \begin{array}{l} \displaystyle\sum_{\beta,\gamma|\beta+\gamma=\alpha} M_{\beta,\gamma} = f_\alpha \quad (|\alpha| \le 2d) \\ M \succeq 0 \end{array} \right.$ **is feasible**

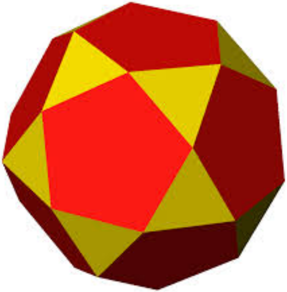
Gram-matrix method [Powers-Wörmann 1998]

Linear Programming vs Semidefinite Programming

Optimize a linear function over

a polyhedron

$a_j^T x = b_j, \; x \geq 0$



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a convex set (spectrahedron)

$\langle A_j, X \rangle = b_j, \; X \succeq 0$

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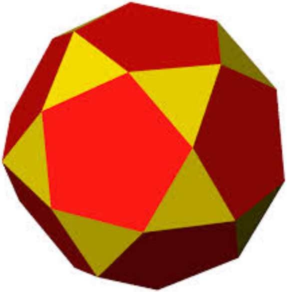

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SDP

There are efficient algorithms to solve LP and SDP (up to any precision)

About the complexity of SDP

- 1980's: There are efficient algorithms to find an **almost optimal** solution, **under some assumptions**

  Roughly: one needs a feasible point, an inscribed ball and a circumscribed ball to the feasible region

  - Grötschel-Lovász-Schrijver: based on Khachiyan *ellipsoid method*

  - Karmarkar, Nesterov-Nemirovski: *interior point algorithms*

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- **Testing feasibility of SDP**: Given rational A_j, b_j, decide

  (F) $\exists X \succeq 0$ s.t. $\langle A_j, X\rangle = b_j \ \ (j \in [m])$?

  - Ramana (1997): (F) $\in$ NP $\Longleftrightarrow$ (F) $\in$ co-NP

About the complexity of SDP

- 1980's: There are efficient algorithms to find an **almost optimal** solution, **under some assumptions**

  Roughly: one needs a feasible point, an inscribed ball and a circumscribed ball to the feasible region

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- Well developed **duality theory** for LP, SDP, conic programs (with no duality gap under some strict feasibility conditions)

General approach to polynomial optimization

Strategy

(P) $$f_{\min} = \min_{x \in K} f(x)$$

Approximate **(P)** by a hierarchy of convex (semidefinite) relaxations

These relaxations can be constructed using

sums of squares of polynomials

and

the dual theory of moments

Shor (1987), Nesterov (2000), **Lasserre, Parrilo** (2000–)

Sums of squares approach

Strategy (use sums of squares)

(P) $$f_{\min} = \min_{x \in K} f(x) = \sup_{\lambda \in \mathbb{R}} \lambda \ \text{ s.t. } \ f(x) - \lambda \geq 0 \ \forall x \in K$$

Testing whether a polynomial f is nonnegative is **hard**

but one can test the *sufficient condition*:

f is a sum of squares of polynomials (SoS)

using semidefinite programming

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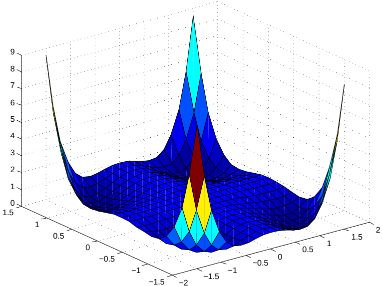

Motzkin [1967]:
$p = x^4y^2 + x^2y^4 + 1 - 3x^2y^2$
is nonnegative,
not a sum of squares,
but $(x^2 + y^2)^2 p$ is SoS

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Observation: If we know a ball of radius R containing K, then just add the (redundant) constraint $R^2 - \sum_i x_i^2 \geq 0$ to the description of K

SoS relaxations for (P)

Truncated quadratic module:

$$Q(g)_t := \{ \underbrace{s_0}_{\deg \leq 2t} + \underbrace{s_1 g_1}_{\deg \leq 2t} + \ldots + \underbrace{s_m g_m}_{\deg \leq 2t} \mid s_j \ \text{ SoS}\}$$

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- Each bound f_t^{sos} can be computed with SDP
- $f_t^{\text{sos}} \leq f_{t+1}^{\text{sos}} \leq f_{\min}$
- **Asymptotic convergence:** $\lim_{t \to \infty} f_t^{\text{sos}} = f_{\min}$ [Lasserre 2001]

Moment approach

$$f_{\min} = \inf_{x \in K} f(x) \quad = \inf_{\mu} \int_K f(x) d\mu \text{ s.t. } \mu \text{ is a probability measure on } K$$

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is the (difficult) **classical moment problem.**

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L is **nonnegative on the quadratic module** $Q(g) = \{s_0 + \sum_j s_j g_j : s_j \text{ SOS}\}$:

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$$L(p^2) \geq 0 \ \ \forall p, \quad \text{i.e.,} \quad M(L) = (L(x^{\alpha+\beta}))_{\alpha,\beta \in \mathbb{N}^n} \succeq 0$$

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$$L(p^2) = L((\textstyle\sum_\alpha p_\alpha x^\alpha)^2) = \sum_{\alpha,\beta} p_\alpha p_\beta L(x^{\alpha+\beta}) = \overline{p}^{\mathsf{T}} M(L) \overline{p}$$

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$M(L)$ is a **moment matrix** and $M(g_j L)$ are **localizing moment matrices**

Moment relaxations for (P)

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$\rightsquigarrow$ dual sdp bounds

Some results on the full/truncated moment problem

Theorem [Putinar 1997]
Assume $L \in \mathbb{R}[x]^*$ is nonnegative on the (archimedean) quadratic module $Q(g)$.

• Then L has a **representing measure** μ supported by K: $L(f) = \int f(x)\mu(dx)$

• [Tchakaloff 1957] For any fixed degree k, the restriction of L to $\mathbb{R}[x]_k$ has a representing measure supported by K, which is **finite atomic**.

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Theorem [Curto-Fialkow 1996 - L 2005: short algebraic proof]

Assume $L \in \mathbb{R}[x]^*_{2t}$ is nonnegative on $Q_t(g)$, i.e., $M_t(L) \succeq 0$,
and $\mathrm{rank}\ M_t(L) = \mathrm{rank}\ M_{t-1}(L)$ [**flatness condition**]

Then L has a **finite atomic representing measure** μ on K.

Main steps of proof:

- Extend L to $L \in \mathbb{R}[x]^*$ with $\mathrm{rank}\ M(L) = \mathrm{rank} M_t(L) =: r$
- $M(L) \succeq 0$ with *finite rank* $r \Longrightarrow L$ has an r-atomic measure μ

Optimality criterion for moment relaxation (MOMt)

$$K = \{x \mid g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$$

$$d_K = \max_j \lceil \deg(g_j)/2 \rceil$$

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Theorem [CF 2000 + Henrion-Lasserre 2005 + Lasserre-L-Rostalski 2008]

Assume L is an optimal solution of (MOMt) such that

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$V(\mathrm{Ker} M_s(L)) \subseteq \{$ global minimizers of f on $K\}$,

with **equality** if $\mathrm{rank}\ M_t(L)$ is **maximum** (rank = # minimizers).

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- Algorithm for computing the (finitely many) **real roots** of polynomial equations (and real radical ideals)

  [Lasserre-L-Rostalski 2008,2009]
  [Lasserre-L-Mourrain-Rostalski-Trebuchet 2013]

$\rightsquigarrow$ large literature, surveys, monographs

Application for bounding matrix factorization ranks

using the moment approach

Matrix factorization ranks

- **Nonnegative factorization** of $A \in \mathbb{R}_+^{m\times n}$:
  $A = \sum_{\ell=1}^{r} a_\ell b_\ell^\mathsf{T}$, where $a_\ell \in \mathbb{R}_+^m$, $b_\ell \in \mathbb{R}_+^n$ [*atomic decomposition*]
  $A = (\langle u_i, v_j \rangle)_{i\in[m], j\in[n]}$, where $u_i, v_j \in \mathbb{R}_+^r$ [*Gram factorization*]
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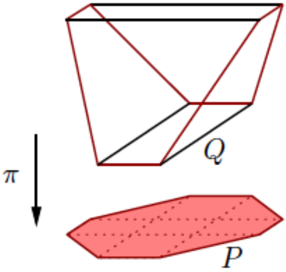
Applications: extended formulations (LP/SDP) of polytopes
(quantum) communication complexity

Nonnegative/psd rank and extended formulations



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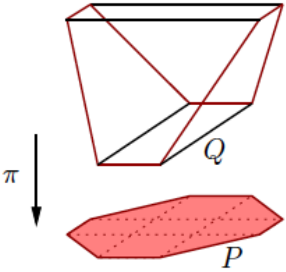

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For a polytope $P = \mathrm{conv}(V) = \{x \in \mathbb{R}^n : a_i^\mathsf{T} x \leq b_i \ \forall i \in [m]\}$

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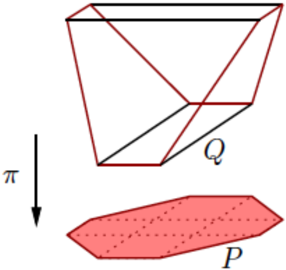

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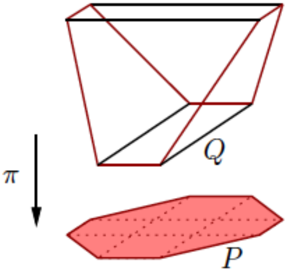

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Extension to other factorization ranks

The moment view point for polynomial optimization offers a systematic, common approach to treat many factorization ranks

- Extension to the **nonnegative rank**, by using two sets of variables x, y; extends also to the more general tensor setting
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Currently working (with Gribling and Steenkamp) on bounds for the **separable rank** of a linear operator ρ acting on $\mathbb{C}^n \otimes \mathbb{C}^n$, asking for the smallest decomposition of the form

$$\rho = \sum_{\ell=1}^{r} a_\ell a_\ell^\mathsf{T} \otimes b_\ell b_\ell^\mathsf{T}$$

Understanding separable states is a fundamental question in quantum information

Concluding remarks

- The two (dual) approaches via moments and sums-of-squares provide **interesting complementary information**
- This extends to the **problem of moments** (*optimize over measures*) and to polynomial optimization in **noncommutative variables** (*optimize over matrix-valued variables*), with *many applications*
- What about the quality of the relaxations? (see Lecture 2)
- Approximation hierarchies for graph problems (see Lecture 3)

THANK YOU !

Some references

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