Polynomial optimization methods for extremal problems in discrete geometry on Euclidean sphere

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m — dimension;

$$m \geq 2, \quad \langle q_1, q_2 \rangle = \sum_{k=1}^{m} q_1^{(k)} q_2^{(k)}, \; q_1, q_2 \in \mathbb{R}^m;$$

$$\mathbb{S}^{m-1} = \left\{ q \in \mathbb{R}^m \;\middle|\; \langle q, q \rangle - 1 = 0 \right\}, \; e_m = (0, 0, \ldots, 0, 1) \in \mathbb{S}^{m-1};$$

n — number of points;

$$n \geq 2, \quad (\mathbb{S}^{m-1})^n = \mathbb{S}^{m-1} \times \cdots \times \mathbb{S}^{m-1};$$

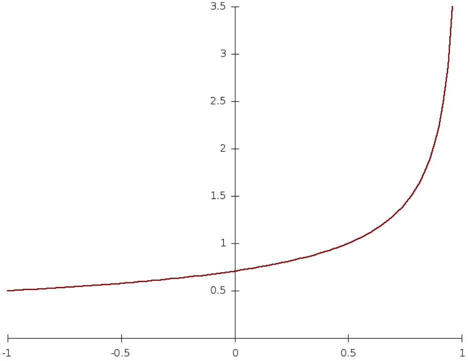
$h \colon [-1, 1] \to (-\infty, \infty]$ — lower semicontinuous function;

$$W_h(q_1, q_2, \ldots, q_n) = \sum_{1 \leq i < j \leq n} h\left(\langle q_i, q_j \rangle\right) \; : \; (\mathbb{S}^{m-1})^n \to (-\infty, \infty].$$

Thomson problem

Posed by J.J. Thomson (1904) for $m = 3$.

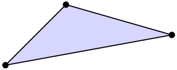
$$\phi(t) = \begin{cases} (2-2t)^{-1/2}, & t \in [-1,1), \\ \infty, & t = 1. \end{cases}$$



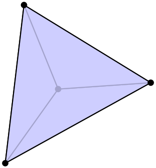
$$\omega_\phi = \min\left\{ W_\phi(q_1, q_2, \ldots, q_n) \mid q_1, q_2, \ldots, q_n \in \mathbb{S}^2 \right\} = ?$$

Thomson problem

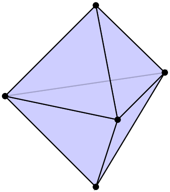
$n = 2$



$n = 3$

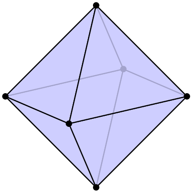


$n = 4$



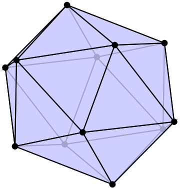
$n = 5$

R.E. Schwartz (2010)



$n = 6$

V.A. Yudin (1993)



$n = 12$

N.N. Andreev (1996)

Hermite interpolation

$T \subset [-1,1)$ — finite set;
h_T — univariate polinomial with:

- $h_T(t) = \phi(t), \quad t \in T;$
- $h'_T(t) = \phi'(t), \quad t \in T \setminus \{-1\};$
- $\deg(h_T) = |T| + |T \setminus \{-1\}| - 1.$

Claim (V.A. Yudin & N.N. Andreev)

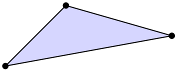
$$h_T(t) \le \phi(t), \quad t \in [-1,1];$$

$$W_{h_T} \le W_\phi \text{ on } (\mathbb{S}^2)^n, \quad \omega_{h_T} \le \omega_\phi;$$

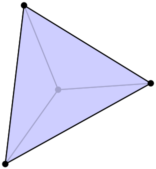
$$\min\left\{W_{h_T}(q_1, q_2, \ldots, q_n) \mid q_1, q_2, \ldots, q_n \in \mathbb{S}^2\right\} = \,?$$

Thomson problem

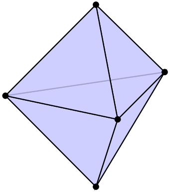
$n = 2$
$T = \{-1\}$
$\deg(h_T) = 0$



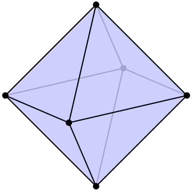
$n = 3$
$T = \{-\frac{1}{2}\}$
$\deg(h_T) = 1$



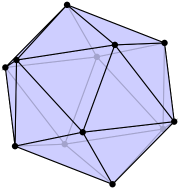
$n = 4$
$T = \{-\frac{1}{3}\}$
$\deg(h_T) = 1$



$n = 5$
$T = \{-1, -\frac{1}{2}, 0\}$
$\deg(h_T) = 4$



$n = 6$
$T = \{-1, 0\}$
$\deg(h_T) = 2$



$n = 12$
$T = \{-1, -\frac{\sqrt{5}}{5}, \frac{\sqrt{5}}{5}\}$
$\deg(h_T) = 4$

Packing problem

$s \in [-1, 1)$;

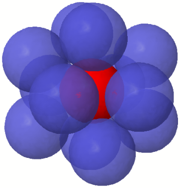
$\tau(m, s) = \max\{n \mid \exists\, q_1, q_2, \ldots, q_n \in \mathbb{S}^{m-1} \colon \langle q_i, q_j \rangle \le s,\ i \ne j\}$.

$$s = 1 - 2\left(\frac{R}{1+R}\right)^2; \quad R = \left(\sqrt{\frac{2}{1-s}} - 1\right)^{-1}.$$

Kissing number problem

$\tau(m) = \tau(m, 1/2)$.

Kissing number problem



$\tau(2) = 6$;

K. Schütte & B.L. van der Waerden (1953): $\tau(3) = 12$;

V.I. Levenshtein; A.M. Odlyzko & N.J.A. Sloane (1978):
$\tau(8) = 240$, $\tau(24) = 196560$;

O.R. Musin (2003): $\tau(4) = 24$;

$40 \leq \tau(5) \leq 44$ (H.D. Mittelman & F. Vallentin, 2009, based on work of C. Bachoc & F. Vallentin, 2006).

Theorem

For $n \geq 3$ the following conditions are equivalent:

- $\tau(m, s) < n$;
- there exists a univariate polynomial h such that
  1. $h(t) \leq 0$, $t \in [-1, s]$;
  2. $W_h > 0$ on $(\mathbb{S}^{m-1})^n$.

Conjecture

The following polynomial is suitable for $m = 3$, $s = 1/2$, $n = 13$:

$$h(t) = (t+1)\left(t+\frac{3}{5}\right)^2\left(t+\frac{1}{5}\right)^2\left(t-\frac{1}{2}\right).$$

Polynomial optimization problem

For given $m \geq 2$, $n \geq 2$ and univariate polynomial h find

$$\omega_h = \min \left\{ W_h(q_1, q_2, \ldots, q_n) \mid q_1, q_2, \ldots, q_n \in \mathbb{S}^{m-1} \right\};$$

$$W_h(q_1, q_2, \ldots, q_n) = \sum_{1 \leq i < j \leq n} h\left(\langle q_i, q_j \rangle\right).$$

Note that W_h is multivariate polynomial of mn variables with $\deg(W_h) = 2\deg(h)$.

Conditions $q_1, q_2, \ldots, q_n \in \mathbb{S}^{m-1}$ are polynomial too: $\langle q_j, q_j \rangle - 1 = 0$, $1 \leq j \leq n$.

We can fix one point:
$\omega_h = \min \left\{ W_h(q_1, q_2, \ldots, q_{n-1}, e_m) \mid q_1, q_2, \ldots, q_{n-1} \in \mathbb{S}^{m-1} \right\}.$

Semidefinite programming (SDP)

$A^0, A^1, \ldots, A^p$ — given symmetric matrices of size $l \times l$;
$c_1, c_2, \ldots, c_p \in \mathbb{R}$;

$$\begin{cases} \max \ X \bullet A^0; \\ X \bullet A^i = c_i, \ 1 \leqslant i \leqslant p; \\ X \succcurlyeq 0; \end{cases}$$

$$X \bullet Y = \sum_{i=1}^{l} \sum_{j=1}^{l} X_{ij} Y_{ij}.$$

Claim

Let $\mathcal{A}$ be a commutative $\mathbb{R}$-algebra, $f \in \mathcal{A}$. For a linear subspace $L = \operatorname{span}\{b_1, \ldots, b_l\} \subset \mathcal{A}$ the following conditions are equivalent:

(1)

$$f = \sum_{k=1}^{r} f_k^2, \quad f_1, \ldots, f_r \in L;$$

(2)

$$f = \sum_{i=1}^{l} \sum_{j=1}^{l} Y_{ij} b_i b_j$$

for some matrix $Y \succcurlyeq 0$ of size $l \times l$.

Convex relaxation

Polynomial optimization problem

$$\omega_h = \min\left\{W_h(q_1, q_2, \ldots, q_{n-1}, e_m) \mid q_1, q_2, \ldots, q_{n-1} \in \mathbb{S}^{m-1}\right\}$$

can be approximated by the following SDP problems $(d \geq \deg(h))$:

$$\begin{cases} \widetilde{\omega}_h(d) = \sup\ \gamma, \quad \gamma \in \mathbb{R}; \\ W_h(q_1, \ldots, q_{n-1}, e_m) - \gamma = Q_0 + \sum_{j=1}^{n-1} (Q_j^+ - Q_j^-) \cdot (\langle q_j, q_j \rangle - 1); \\ Q_j^\pm \text{ is sum of squares of elements of } \mathcal{A}_{\leq d},\ 0 \leq j \leq n-1. \end{cases}$$

$$\mathcal{A} = \mathbb{R}[q_j^{(k)}]_{1 \leq j \leq n-1,\, 1 \leq k \leq m}; \quad \mathcal{A}_{\leq d} = \{f \in \mathcal{A} \mid \deg(f) \leq d\}.$$

$$\widetilde{\omega}_h(d) \leq \omega_h.$$

We can use Gröbner bases (W. Gröbner, B. Buchberger, 1965):

$$\begin{cases} \omega_h(d) = \sup \gamma, \quad \gamma \in \mathbb{R}; \\ W_h(q_1, \ldots, q_{n-1}, e_m) - \gamma = Q_0 \pmod{\mathcal{I}}; \\ Q_0 \text{ is sum of squares of elements of } (\mathcal{A} / \mathcal{I})_{\leq d}; \end{cases}$$

$$\mathcal{I} = \left\{ \sum_{j=1}^{n-1} f_j \cdot (\langle q_j, q_j \rangle - 1) \,\middle|\, f_j \in \mathcal{A} \right\} \subset \mathcal{A},$$

$\mathcal{A} / \mathcal{I}$ is quotient algebra,

$(\mathcal{A} / \mathcal{I})_{\leq d}$ is image of $\mathcal{A}_{\leq d}$ by quotient map.

$$\widetilde{\omega}_h(d) \leq \omega_h(d) \leq \omega_h.$$

Schmüdgen Positivstellensatz (K. Schmüdgen, 1991)

$$\omega_h(d) \nearrow \omega_h, \; d \to \infty.$$

The complexity (size of matrices) of the polynomial optimization problem depends on

$$\dim\left(\mathcal{A}_{\leq d}\right) = \frac{((n-1)m+d)!}{((n-1)m)!\,d!} \asymp d^{(n-1)m},\ d \to \infty;$$

$$\dim\left((\mathcal{A}\,/\,\mathcal{I})_{\leq d}\right) \asymp d^{(n-1)(m-1)},\ d \to \infty.$$

The polynomial

$$W_h(q_1, q_2, \ldots, q_{n-1}, e_m), \quad W_h(q_1, \ldots, q_n) = \sum_{1 \le i < j \le n} h\left(\langle q_i, q_j \rangle\right),$$

is invariant under:

- for $\sigma \in \mathrm{S}(n-1)$ (bijection of the set $\{1, 2, \ldots, n-1\}$):

$$W_h(q_{\sigma(1)}, q_{\sigma(2)}, \ldots, q_{\sigma(n-1)}, e_m) = W_h(q_1, q_2, \ldots, q_{n-1}, e_m);$$

- for $\rho \in \mathrm{O}(m-1)$ (orthogonal matrix) we have

$$W_h(\rho q_1, \rho q_2, \ldots, \rho q_{n-1}, e_m) = W_h(q_1, q_2, \ldots, q_{n-1}, e_m).$$

So the polynomial optimization problem is invariant under the group

$$G = \mathrm{S}(n-1) \times \mathrm{O}(m-1).$$

Irreducible representations

Irreducible representations of groups $\mathrm{S}(n-1)$ and $\mathrm{O}(m-1)$ are absolutely irreducible, so irreducible representations of G are just tensor products of $\mathrm{S}(n-1)$'s and $\mathrm{O}(m-1)$'s ones.

- Irreps of $\mathrm{S}(n-1)$ can be obtained as Specht modules (W. Specht, 1935);
- irreps of $\mathrm{O}(2)$ are sines-cosines + det-representation;
- irreps of $\mathrm{O}(3)$ are spherical harmonics + det-representations;
- $\dots$

Irreducible decomposition

We can obtain irreducible decomposition of $\mathcal{A}/\mathcal{I}$ by using real version of Peter-Weyl theorem (F. Peter & H. Weyl, 1927) for G:

$$\mathcal{A}/\mathcal{I} = \bigoplus_{\nu}^{\infty} \bigoplus_{\lambda}^{N_\nu} V_\nu^\lambda, \; V_\nu^i \cong V_\nu^j.$$

Large dense positive semidefinite matrix becomes block diagonal:

- each ν corresponds to one block;
- the size of ν-th block is $N_\nu \times N_\nu$;
- this process corresponds to selection of symmetry-aware basis of $\mathcal{A}/\mathcal{I}$.

After symmetry reduction the polynomial optimization problem no longer depends on m and n, it depends only on d.

Results

With current mathematical software it is able to solve polynomial optimization problems for $d \leq 3$, i.e. to solve Thomson problem for $n = 2, 3, 4, 6$ and to obtain lower bounds for $n = 5, 7$.

Thank you for your attention!