Upper bounds on the kissing number via copositive programming

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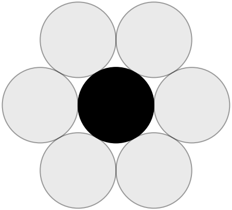
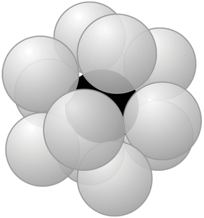
July 2017

Kissing number problem

- **Kissing number $\kappa_\mathbf{n}$** is the maximum number of non-overlapping unit spheres S^{n-1} in $\mathbb{R}^n$ that can touch another unit sphere



$n = 2$



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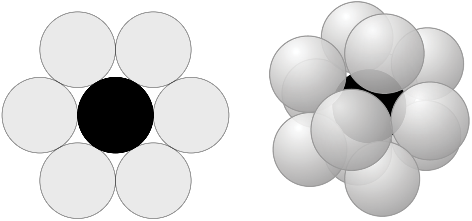

$n = 2$ $n = 3$

- One of the hard fundamental packing problems

Upper bounds on kissing numbers

- Known kissing numbers and bounds on them

dimension n	3	4	5	6	7	8	9	24
upper/lower bound	12	24	44/40	78/72	134/126	240	364/306	196 560
% difference	0	0	10	8.3	6.3	0	19	0

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  $\rightarrow$ all upper bounds in the table above
- **Hierarchies**: f_r [Musin '08]; las_r^* [De Laat and Vallentin '15]
  $\rightarrow$ $r=0$: linear bound, $r=1$: SDP bound, $r>1$: too big to solve

Kissing number and Stability number

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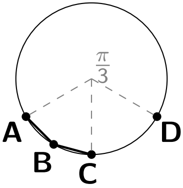

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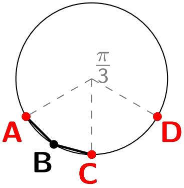

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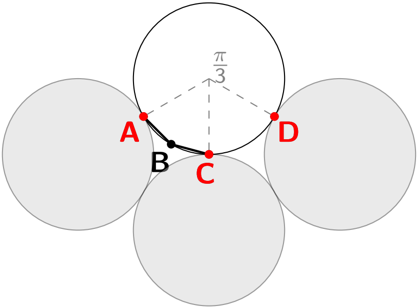

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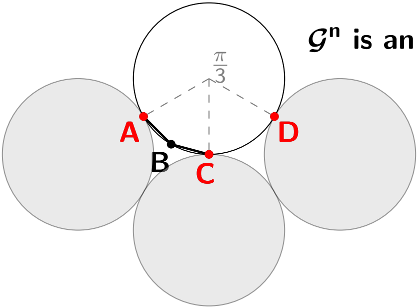

$\mathcal{G}^\mathbf{n}$ is an infinite graph

Copositive programming: introduction

- The cone of copositive matrices:
  $\mathcal{COP}^n = \{K \text{ is } n \times n \text{ symmetric matrix}: \; x^\top K x \geq 0 \text{ for all } x \geq 0\}$

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- Copositive programming $\longleftarrow$ Combinatorial optimization:
  chromatic number, 3-partitioning, stability number

Copositive programming for stability number

Graph $G=(V,E)$, $|V|=n$ [De Klerk and Pasechnik '02]

$$\alpha(G) = \inf_{K\in\mathbb{S}^n,\lambda} \lambda$$

$$\text{s. t.} \quad K(v,v) = \lambda - 1 \quad \text{for all } v \in V$$

$$K(u,v) = -1 \quad \text{for all } (u,v) \notin E$$

$$K \in \mathcal{COP}^n$$

Notation: $\mathbb{S}^n$ are real symmetric matrices,
$\mathcal{COP}^n = \{K\in\mathbb{S}^n : x^\top Kx \geq 0 \text{ for all } x\geq 0\}$ are copositive matrices

Copositive programming for stability number

- $\kappa_n = \alpha(\mathcal{G}^n)$, move from finite to infinite graphs

Graph $\mathcal{G}^n = (S^{n-1}, E)$ [Dobre, Dür, Frerick, Vallentin '16]

$$\alpha(\mathcal{G}^n) = \inf_{K \in \mathcal{K}(S^{n-1}), \lambda} \lambda$$
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$$K \in \mathcal{COP}(S^{n-1})$$

Notation:
$\mathcal{K}(S^{n-1})$ are kernels - real symmetric continuous functions on $S^{n-1} \times S^{n-1}$,
$\mathcal{COP}(S^{n-1})$ are copositive kernels: any finite principal submatrix is copositive

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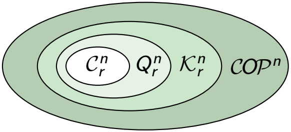

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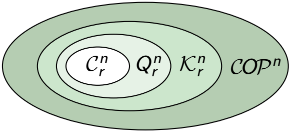

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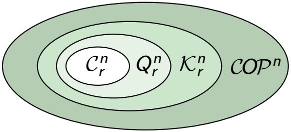

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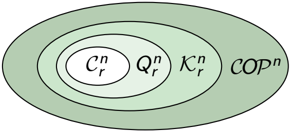

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- **Extend this for kernels to upper bound the kissing number?**

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- Get *tractable* upper bounds on κ_n with the new hierarchies?

  $\rightarrow$ **Yes, using symmetry of the sphere**

Intuition for generalized hierarchies

$$\mathcal{Q}_r^n = \left\{ K \in \mathbb{S}^n : \left[(e^\top x)^r (x^\top K x) - \sum_{|\beta|=r} x^\beta (x^\top S_\beta x) \right] = p(x), \right.$$
$$\left. \text{has nonnegative coefficients}, S_\beta \succeq 0 \text{ for all } \beta \in \mathbb{N}^n, |\beta| = r \right\}$$

- How to construct $p(x)$ for a kernel instead of a matrix?

Notation: $e = (1, \dots, 1)$, $|\beta| := \beta_1 + \ldots + \beta_n$, $x^\beta := x_1^{\beta_1} \cdots x_n^{\beta_n}$

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  $\rightarrow$ do not write $p(x)$, write only its coefficients

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- **Coefficient** of the monomial $(x_{v_1} \cdots x_{v_{r+2}})$ in $(e^\top x)^r (x^\top K x)$ is

$$\sigma\left(K^{\oplus r}\right)(v_1, \ldots, v_{r+2})$$

2-psd functions

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- An $(r+2)$-variate function F is called **2-psd** if for any fixed $u_1, ..., u_r \in S^{n-1}$, the "slice" $F(v_1, v_2, u_1, ..., u_r)$ is PSD

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- A kernel is PSD iff every principal submatrix is PSD

Generalized inner approximations

The initial Q-hierarchy

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The generalized Q-hierarchy for a sphere

$$Q_r^{S^{n-1}} = \left\{ K \in \mathcal{K}(S^{n-1}) : \sigma(K^{\oplus r}) - \sigma(S_r) \geq 0,\ S_r \text{ is 2-psd} \right\}$$

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Analogously, generalize $\mathcal{C}_r^n$ hierarchy into $\mathcal{C}_r^{S^{n-1}}$

Inclusion and convergence

Theorem 1

$\mathcal{C}_r^{S^{n-1}} \subseteq \mathcal{Q}_r^{S^{n-1}} \subseteq \mathcal{COP}(S^{n-1})$ *for any* r*, and subsets grow with* r

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Theorem 2

Replacing $\mathcal{COP}(S^{n-1})$ *by either of* $\mathcal{C}_r^{S^{n-1}}$ *or* $Q_r^{S^{n-1}}$ *gives upper bounds on* $\alpha(\mathcal{G}^n) = \kappa_n$*, converging as* r *grows*

Implementation for the kissing number

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- Use SOS [Lasserre '06], DSOS [Ahmadi and Majumdar '15]
- What are $(r+2)$-variate 2-psd functions on a sphere?
  $\rightarrow$ use invariance of $\mathcal{G}^n$ under orthogonal group O_n

2-psd condition, the case $r = 0$

- Bivariate 2-psd functions are PSD kernels:

Proposition 1 (Schoenberg '42)

A kernel $K : (S^{n-1})^2 \to \mathbb{R}$ *is invariant under* O_n *and PSD iff*

$$\mathbf{K(x, y)} = \sum_{\mathbf{i} \in \mathbb{N}} \mathbf{c_i P_i^{\frac{n-3}{2}}(x^\top y)}, \; \mathbf{c_i} \geq \mathbf{0},$$

where $P_i^{\frac{n-3}{2}}$ *are Jacobi polynomials of order* $\left(\frac{n-3}{2}, \frac{n-3}{2}\right)$*, degree* i

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- $\mathbf{Q_0^{S^{n-1}}}$ **gives the linear bound**

2-psd condition, the case $n \geq r > 0$

- For $x, y, z_1, ..., z_r \in S^{n-1}$ define their inner products Z, χ, υ:

  $\mathbf{Z} = [z_1, ..., z_r]^\top [z_1, ..., z_r],\ \boldsymbol{\chi} = [z_1, ..., z_r]^\top x,\ \boldsymbol{\upsilon} = [z_1, ..., z_r]^\top y$

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Theorem 3

Continuos f-n $F:(S^{n-1})^{r+2} \to \mathbb{R}$ *is invariant under* O_n *and 2-psd iff*

$$\mathbf{F(x, y, z_1, ..., z_r)} = \sum_{\mathbf{i} \in \mathbb{N}} \mathbf{c_i}(\chi, \upsilon, \mathbf{Z}) \mathcal{P}_{\mathbf{i}}^{\frac{\mathbf{n-r-3}}{2}} (\mathbf{Z}, \chi, \upsilon),$$

$\mathcal{P}_i^{\frac{n-r-3}{2}}(Z, \chi, \upsilon)$ *are generalized Jacobi polynomials,* $c_i(\chi, \upsilon, Z)$ *are continuous functions PSD with respect to* χ, υ.

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- $r=1$: [Bachoc and Vallentin '08]; $Z=I$: [Musin '08]

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- **Our bounds for $Q_1^{S^{n-1}}$ are between linear and SDP bounds**

Conclusions and questions for future

- 2 converging inner hierarchies for the set of copositive kernels

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SDP bound, Bachoc and Vallentin	12	24	45	78	135	240	366
$Q_1^{S^{n-1}}$ bound	**12**	**24**	**45**	**80**	**138**	**240**	**377**
linear bound, Delsarte et al.	13	25	46	82	140	240	380
lower bound	12	24	40	72	126	240	306

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- Applications for 2-psd functions?

Thank you for your attention!

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Inner approximations for $\mathcal{COP}^n$

- Parrilo, 2000:

$$\mathcal{K}_r^n = \left\{ K \in \mathbb{S}^n : \left(\sum_{i=1}^n x_i^2 \right)^r \sum_{i=1}^n \sum_{j=1}^n K_{ij} x_i^2 x_j^2 \text{ is a sum of squares} \right\}$$

- De Klerk and Pasechnik, 2002:

$$\mathcal{C}_r^n = \left\{ K \in \mathbb{S}^n : (e^\top x)^r (x^\top K x) \text{ has nonnegative coefficients} \right\}$$

- Peña, Vera, Zuluaga, 2007:

$$Q_r^n = \left\{ K \in \mathbb{S}^n : \left[(e^\top x)^r (x^\top K x) - \sum_{|\beta|=r} x^\beta (x^\top S_\beta x) \right] \right.$$

$$\left. \text{has nonnegative coefficients}, S_\beta \succeq 0 \text{ for all } \beta \in \mathbb{N}^n, |\beta| = r \right\}$$

Notation: $e = (1, \ldots, 1)$, $|\beta| := \beta_1 + \ldots + \beta_n$, $x^\beta := x_1^{\beta_1} \cdots x_n^{\beta_n}$

Write the coefficients explicitely

$$Q_r^n = \Big\{ K \in \mathbb{S}^n : \Big[(e^\top x)^r (x^\top K x) - \sum_{|\beta|=r} x^\beta (x^\top S_\beta x) \Big]$$

has nonnegative coefficients, all $S_\beta \succeq 0 \Big\}$

- **Lifting operator** $^{\oplus \mathbf{r}}$ applied to a kernel K

$$K^{\oplus r}(v_1, v_2, u_1, \dots, u_r) := K(v_1, v_2), \text{ for all } u_1, \dots, u_r \in V$$

- **Symmetrization** $\boldsymbol{\sigma}$ applied to the $(r+2)$-variate function $K^{\oplus r}$

$$\sigma\big(K^{\oplus r}\big)(v_1, \dots, v_{r+2}) := \frac{1}{(r+2)!} \sum_{\pi \in \text{permut.}(1,\dots,r+2)} K^{\oplus r}\big(\pi(v_1, \dots, v_{r+2})\big)$$

- **Coefficient** of the monomial $(x_{v_1} \cdots x_{v_{r+2}})$ in $(e^\top x)^r (x^\top K x)$ is

$$\sigma\big(K^{\oplus r}\big)(v_1, \dots, v_{r+2})$$

2-psd condition, the case $n \geq r > 0$

- For $x, y, z_1, ..., z_r \in S^{n-1}$ define:

$$Z = [z_1, ..., z_r]^\top [z_1, ..., z_r], \; \chi = [z_1, ..., z_r]^\top x, \; \upsilon = [z_1, ..., z_r]^\top y$$

Theorem 4

Let $K : (S^{n-1})^{r+2} \to \mathbb{R}$ be a continuos function invariant under O_n. Define Z, χ, υ as above. Then K is 2-psd iff

$$K(x, y, z_1, ..., z_r) = \sum_{i \in \mathbb{N}} c_i(\chi, \upsilon, Z) Q_i \left(\frac{x^\top y - \chi^\top Z^{-1} \upsilon}{\sqrt{(1 - \chi^\top Z^{-1} \chi)(1 - \upsilon^\top Z^{-1} \upsilon)}} \right),$$

where $Q_i(t) = |Z|^i \big((1 - \chi^\top Z^{-1} \chi)(1 - \upsilon^\top Z^{-1} \upsilon)\big)^{\frac{i}{2}} P_i^{\frac{n-r-3}{2}}(t)$ and $c_i(\chi, \upsilon, Z)$ are continuous functions, PSD w.r.t. χ, υ