Exact semidefinite programming bounds for packing problems

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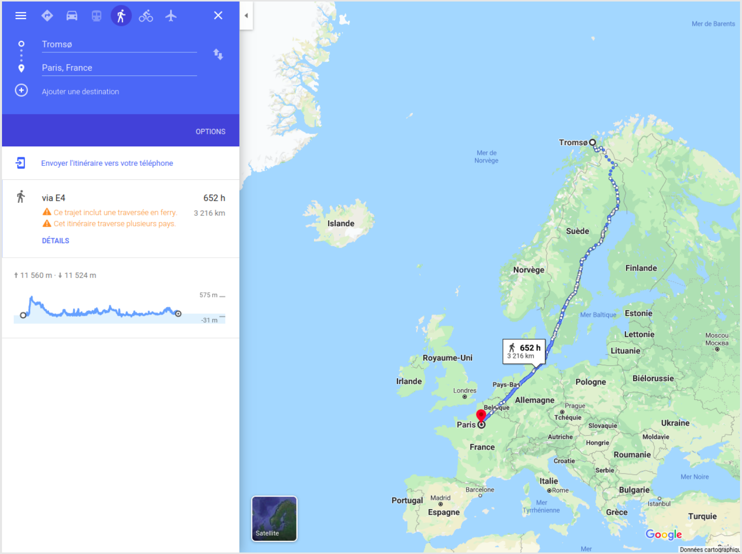
Joint work with M. Dostert (EPFL) and D. de Laat (TU Delft).

Point Distribution Webinar - June 24, 2020

Tromsø: the Paris of the North



Tromsø: the Paris of the North

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Problem:

Usually semidefinite programming provides approximate numerical bounds.

How can we turn these bounds into exact bounds?

Motivation: the kissing number problem

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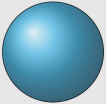

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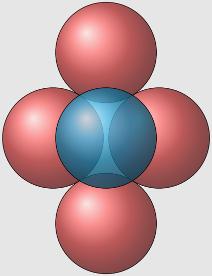

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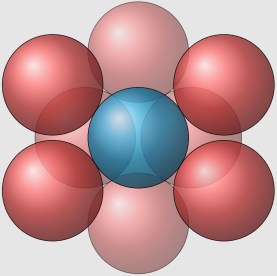

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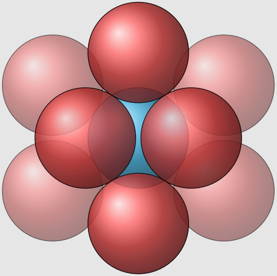

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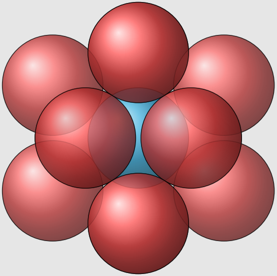

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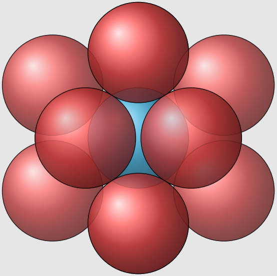
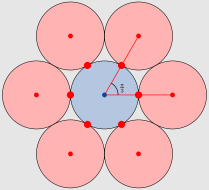


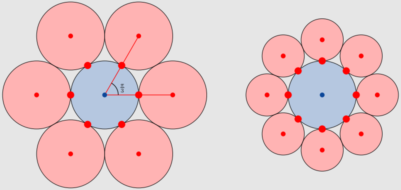
Known for $n \in \{1, 2, 3, 4, 8, 24\}$.



Kissing number:

$$\max\{|C|, \quad C \subset S^{n-1}, \quad x \cdot y \leq 1/2 \text{ for all } x \neq y \in C\}$$

Formulation and generalizations



Spherical codes:

$$\max\{|C|, \quad C \subset S^{n-1}, \quad x \cdot y \leq \cos\theta \text{ for all } x \neq y \in C\}$$

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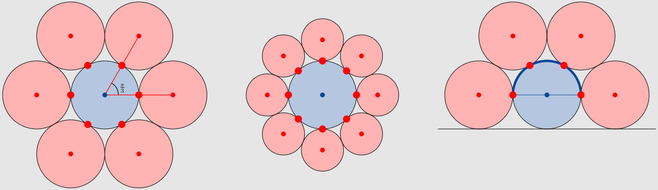

Kissing number of the hemisphere:

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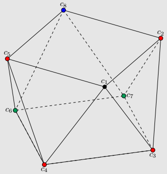
- The square antiprism, the unique optimal θ-spherical code in dimension 3 with $\cos\theta = (2\sqrt{2}-1)/7$ (Schütte-van der Waerden 1951, Danzer 1986).



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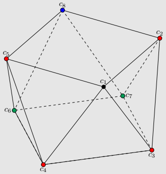
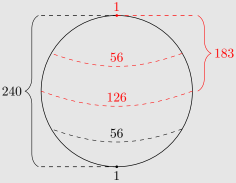


- For the Hemisphere in dimension 8: the E_8 lattice provides an optimal configuration (Bachoc-Vallentin, 2008). What about uniqueness?



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  - For finite graphs: hierarchies of semidefinite upper bounds. (Lovász-Schrijver 1991, Lasserre 2001, Laurent 2007)

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  - For finite graphs: hierarchies of semidefinite upper bounds. (Lovász-Schrijver 1991, Lasserre 2001, Laurent 2007)
  - For infinite graphs: Generalization of Lasserre's hierarchy (de Laat-Vallentin 2015), related to the previous 2-point (Delsarte-Goethals-Seidel 1977) and 3-point bounds (Bachoc-Vallentin 2008).

2-point bound for spherical codes (Delsarte-Goethals-Seidel 1977)

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- Up to symmetry, a couple x, y of points in a θ-spherical code is uniquely determined by

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- The normalized Gegenbauer polynomials $P_k^n(u)$ (with $P_k^n(1) = 1$), satisfying:

$$\text{For every } X \subset S^{n-1} \text{ finite, } \sum_{x,y \in X} P_k^n(x \cdot y) \geq 0.$$

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- there exists coefficients $\alpha_0, \ldots, \alpha_d \geq 0$ such that

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So

$$|C| \leq f(1) + 1$$

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So for every $d \geq 0$, the size of a θ-spherical code is at most

$$\begin{aligned} \min\{M \in \mathbb{R} : \alpha_0, \ldots, \alpha_d &\geq 0, \\ f(1) &\leq M - 1, \\ f(u) &\leq -1 \text{ for all } u \in [-1, \cos\theta]\} \end{aligned}$$

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This is a linear programming bound.

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  with (u, v, t) in

$$\begin{cases} \{(1,1,1)\} & x = y = z \\ \Delta_0 = \{(u,u,1) : u \in [-1, \cos\theta]\} & x \neq y = z \\ \Delta & x, y, z \text{ distinct} \end{cases}$$

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- Matrix polynomials $S_k^n(u, v, t)$ satisfying:

  For every $X \subset S^{n-1}$ finite, $\sum_{x,y,z \in X} S_k^n(x \cdot y, x \cdot z, y \cdot t) \succeq 0$.

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So for every $d \geq 0$, the size of a θ-spherical code is at most

$$\min\{M \in \mathbb{R} : \alpha_k \geq 0, F_k \succeq 0$$

$$\sum_{k=0}^{d} \alpha_k + F(1,1,1) \leq M - 1,$$

$$\sum_{k=0}^{d} \alpha_k P_k^n(u) + 3F(u,u,1) \leq -1 \text{ for all } u \in [-1, \cos\theta],$$

$$F(u,v,t) \leq 0 \text{ for all } (u,v,t) \in \Delta\}$$

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This leads to semidefinite upper bounds using sums of squares.

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So why do we want an exact sharp bound?

- Optimization: When does a bound give the independence number?
- Geometry: Sharp bounds provide additional information on optimal configurations, leading to uniqueness proofs.

Example: Kissing number in dimension 8 (Bannai-Sloane 1981)

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$$\Rightarrow \text{for all } x, y \in C, x \cdot y \in \{0, \pm 1/2, \pm 1\}$$

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$$\Rightarrow \text{for all } x, y \in C, x \cdot y \in \{0, \pm 1/2, \pm 1\} \quad \Rightarrow C = C_0$$

Recap

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- For spherical codes in spherical caps:
  - Delsarte bound does not apply anymore due to the lack of symmetry.
  - The 3-point bound can be adapted to a 2-point semidefinite programming bound (Bachoc-Vallentin 2009).

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- Numerically sharp for the square antiprism (Bachoc-Vallentin 2009)
  $\rightarrow$ Rigorous proof (Dostert-de Laat-M 2020)
- E_8 gives an optimal configuration on the hemisphere in dimension 8 (Bachoc-Vallentin 2009)
  $\rightarrow$ Uniqueness (Dostert-de Laat-M 2020)

Solving an SDP: Rage against the machine precision

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A semidefinite program:

$$\inf\{ \underbrace{c^t x}_{\text{objective}} : \underbrace{Ax = b}_{\text{linear constraints}} , \underbrace{\mathcal{B}_i(x) \succeq 0}_{\text{PSD constraints}} \}$$

with x the vector of unknowns, and $\mathcal{B}_i(x)$ the blocks of x.

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- Even if the SDP is defined over $\mathbb{Q}$, optimal solutions can require high algebraic degree (Nie-Ranestad-Sturmfels 2008).
- Our context: The problems provide a candidate field to round over, either $\mathbb{Q}$ or $\mathbb{Q}(\sqrt{d})$.

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The linear system is then satisfied... But what about the PSD conditions?

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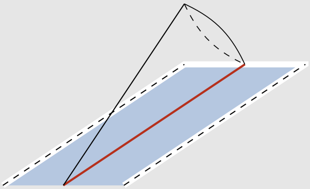

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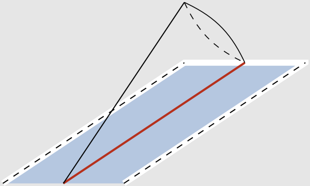

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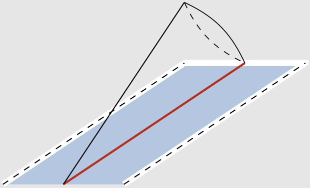

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- Sometimes not. How to force all these constraints?

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- Then $\mathcal{B}_i(x)v = 0$ provides new linear constraints on x!

Rounding over $\mathbb{Q}$: detecting kernel vectors (general case)

This is not enough in general. How to extract a nice basis from the numerical values?

$$\ker(\mathcal{B}_i(x^*)) \approx \left\langle \begin{pmatrix} 0.19550004741012542 \\ -0.10616756374846323 \\ -0.25700180101766007 \\ -0.33241916014721035 \end{pmatrix}, \begin{pmatrix} -0.8676883652023846 \\ -0.4321427618192919 \\ -0.2143699892153049 \\ -0.1054836185183479 \end{pmatrix} \right\rangle$$

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Key idea: use the LLL algorithm to detect an integer linear equation almost sastisfied by the kernel vectors...

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$$\left\{ -u_1 + 3u_2 - 2u_3 = 0 \right.$$

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...and another one...

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$$\begin{cases} -u_1 + 3u_2 - 2u_3 = 0 \\ u_2 - 3u_3 + 2u_4 = 0 \end{cases}$$

Rounding over $\mathbb{Q}$: detecting kernel vectors (general case)

With enough equations, we can compute the expected kernel basis.

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$$\ker(\mathcal{B}_i(x)) = \langle \begin{pmatrix} 7 \\ 3 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -6 \\ -2 \\ 0 \\ 1 \end{pmatrix} \rangle$$

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- If needed compute the possible 3-point distance distribution of an optimal code.
- Use this information and a bit of geometry to prove that the candidate optimal configuration is unique!

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- What about other applications?

Thank you!

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- We also expect a solution over $\mathbb{Q}(\sqrt{d})$, so write

$$x = x_1 + \sqrt{d}x_2$$

  and work over $\mathbb{Q}$:

$$\begin{pmatrix} A_1 & dA_2 \\ A_2 & A_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

Bonus: extension to quadratic fields (finding good x_1^*, x_2^*)

- From the numerical x^* satisfying $Ax^* \approx b$ we need to find x_1^* and x_2^* such that $x^* \approx x_1^* + \sqrt{d}x_2^*$ and

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- To do so, solve (in floating point) the linear system:

$$\begin{pmatrix} A_1 & dA_2 \\ A_2 & A_1 \end{pmatrix} \begin{pmatrix} y \\ \frac{1}{\sqrt{d}}(x^* - y) \end{pmatrix} \approx \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

Encore: extension to quadratic fields (kernel detection)

- Compute the approximate kernel of $\mathcal{B}_i(x^*)$

$$\ker(\mathcal{B}_i(x^*)) \approx \langle \begin{pmatrix} u_1^1 \\ \vdots \\ u_l^1 \end{pmatrix}, \dots, \begin{pmatrix} u_1^r \\ \vdots \\ u_l^r \end{pmatrix} \rangle$$

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Encore: extension to quadratic fields (kernel detection)

- Compute the approximate kernel of $\mathcal{B}_i(x^*)$

$$\ker(\mathcal{B}_i(x^*)) \approx \langle \begin{pmatrix} u_1^1 \\ \vdots \\ u_l^1 \end{pmatrix}, \dots, \begin{pmatrix} u_1^r \\ \vdots \\ u_l^r \end{pmatrix} \rangle$$

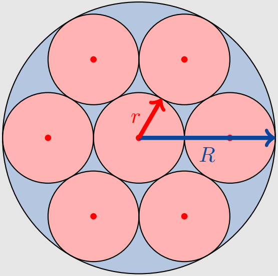
- Look for integer relations in

$$\begin{pmatrix} u_1^1 \\ \vdots \\ u_l^1 \\ \sqrt{d}u_1^1 \\ \vdots \\ \sqrt{d}u_l^1 \end{pmatrix}, \dots, \begin{pmatrix} u_1^r \\ \vdots \\ u_l^r \\ \sqrt{d}u_1^r \\ \vdots \\ \sqrt{d}u_l^r \end{pmatrix} \begin{matrix} \lambda_1 \\ \vdots \\ \lambda_l \\ \mu_1 \\ \vdots \\ \mu_l^r \end{matrix} \rightarrow \sum_{i=1}^{l} (\lambda_i + \sqrt{d}\mu_i) u_i = 0$$

- Compute the expected kernel over $\mathbb{Q}$ and add the corresponding constraints on x_1 and x_2.

Bonus 2: packing spheres in spheres (formulation)

How many spheres of radius r can be packed into a sphere of radius R?



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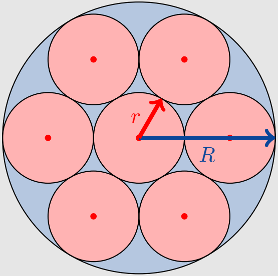

$$\max\{|C| : C \subset B(0, R-r), \|x-y\| \geq 2r \text{ for all } x \neq y \in C\}$$

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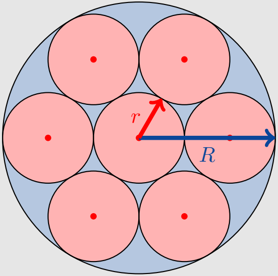

$$\max\{|C| : C \subset B(0, R-r), \|x-y\| \geq 2r \text{ for all } x \neq y \in C\}$$

Again, we can turn the 3-point bound into a 2-point bound with

$$u = \|x\|, \quad v = \|y\|, \quad t = x \cdot y.$$

Bonus 2: packing spheres into spheres (results)

The Lovász ϑ-number gives a sharp bound on the largest number M of n-dimensional unit spheres that can be packed into a sphere of radius R, for

(i) $n \geq 2$ with $R = 2$ and $M = 2$;

(ii) $n \geq 2$ with $R = 2/\sqrt{3} + 1$ and $M = 3$;

(iii) $n \geq 2$ with $R = \sqrt{2n/(n+1)} + 1$ and $M = n + 1$;

(iv) $n \geq 2$ with $R = \sqrt{2} + 1$ and $M = 2n$;

(v) $n = 2$ with $R = 1 + \sqrt{2\left(1 + 1/\sqrt{5}\right)}$ and $M = 5$;

(vi) $n = 2$ with $R = 3$ and $M = 7$.