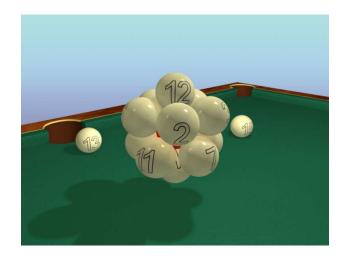
Packing of congruent spheres on a sphere

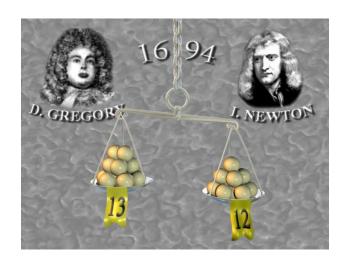
Oleg R. Musin

Fields Institute: November 15, 2011

The thirteen spheres problem



The thirteen spheres problem



The thirteen spheres problem: proofs

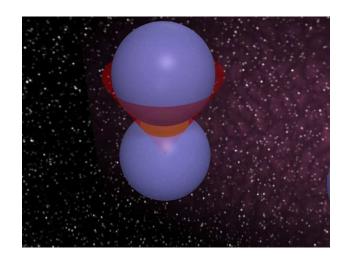
K. Schütte, and B. L. van der Waerden (1953)

John Leech (1956): two-page sketch of a proof

... It also misses one of the old chapters, about the "problem of the thirteen spheres," whose turned out to need details that we couldn't complete in a way that would make it brief and elegant.

Proofs from THE BOOK, M. Aigner, G. Ziegler, 2nd edition.

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W. -Y. Hsiang (2001);H. Maehara (2001, 2007);K. Böröczky (2003);K. Anstreicher (2004);M. (2006)
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How must N congruent non-overlapping spherical caps be packed on the surface of a unit sphere so that the angular diameter of spherical caps will be as great as possible

Tammes PML (1930). "On the origin of number and arrangement of the places of exit on pollen grains". Diss. Groningen.

Let X be a finite subset of \mathbb{S}^2 . Denote

$$\psi(X) := \min_{x,y \in X} \left\{ \mathrm{dist}(x,y) \right\}, \text{ where } x \neq y.$$

Then X is a spherical $\psi(X)$ -code.

Denote by d_N the largest angular separation $\psi(X)$ with |X| = N that can be attained in \mathbb{S}^2 , i.e.

$$d_N := \max_{X \subset \mathbb{S}^2} \{ \psi(X) \}, \text{ where } |X| = N.$$

- L. Fejes Tóth (1943) $N=3,4,6,12,\infty$
- K. Schütte, and B. L. van der Waerden (1951) N=5,7,8,9
- L. Danzer (1963) N = 10, 11
- R. M. Robinson (1961) N = 24
- M. & T. (2010) N = 13

d_N

N	d_N
4	109.4712206
5	90.0000000
6	90.0000000
7	77.8695421
8	74.8584922
9	70.5287794
10	66.1468220
11	63.4349488
12	63.4349488
13	57.1367031
14	55.6705700
15	53.6578501
16	52.2443957
17	51.0903285

Sphere Packing in a Sphere: Methods

- I. Area inequalities. L. Fejes Tóth (1943); for d>3 Coxeter (1963) and Böröczky (1978)
- II. Distance and irreducible graphs. Schütte, and van der Waerden (1951); Danzer (1963); Leech (1956);...
- III. LP and SDP. Delsarte et al (1977); Kabatiansky and Levenshtein (1978);...

Spherical codes

We say that X in \mathbb{S}^{d-1} is a spherical φ -code if for any $x, y \in X$, $x \neq y$, we have $\operatorname{dist}(x, y) \leq \varphi$.

Denote by $A(d,\varphi)$ the maximum cardinality of a φ -code in \mathbb{S}^{d-1} .

In other words, $A(d, \varphi)$ is the maximum cardinality of a sphere of radius $\varphi/2$ packing in \mathbb{S}^{d-1} .

Fejes Tóth's bound

Theorem (L. Fejes Tóth, 1943)

$$A(3,\varphi) \le \frac{2\pi}{\Delta(\varphi)} + 2,$$

where

$$\Delta(\varphi) = 3\arccos\left(\frac{\cos\varphi}{1+\cos\varphi}\right) - \pi,$$

i.e. $\Delta(\varphi)$ is the area of a spherical regular triangle with side length φ .

Fejes Tóth's bound

The Fejes Tóth bound is tight for n = 3, 4, 6 and 12. So for these n it gives a solution of the Tammes problem. This bound is also tight asymptotically.

However, for all other cases the Fejes Tóth upper bound is not tight. For instance, for n=13 this bound is $60.92^{\circ} > 57.14^{\circ}$.

Coxeter's bound

Theorem (Coxeter (1963) and Böröczky (1978))

$$A(d,\varphi) \le 2F_{d-1}(\alpha)/F_d(\alpha),$$

where

$$\sec 2\alpha = \sec \varphi + d - 2,$$

and the function F is defined recursively by

$$F_{d+1}(\alpha) = \frac{2}{\pi} \int_{arcsec(d)/2}^{\alpha} F_{d-1}(\beta) d\theta, \ \sec 2\beta = \sec 2\theta - 2,$$

with the initial conditions $F_0(\alpha) = F_1(\alpha) = 1$.

Coxeter's bound

Coxeter's bounds for kissing numbers $k(d) = A(d, \pi/3)$ with d = 4, 5, 6, 7, and 8 are 26, 48, 85, 146, and 244, respectively.

It also proves that

$$A(4, \pi/5) = 120.$$

Contact graphs

Let X be a finite set in \mathbb{S}^2 . The contact graph CG(X) is the graph with vertices in X and edges $(x, y), x, y \in X$ such that

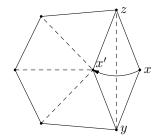
$$dist(x, y) = \psi(X)$$

Shift of a single vertex

Let X be a finite set in \mathbb{S}^2 . Let $x \in X$ be a vertex of CG(X) with deg(x) > 0, i.e. there is $y \in X$ such that $dist(x, y) = \psi(X)$. We say that there exists a shift of x if x can be slightly shifted to x' such that $dist(x', X \setminus \{x\}) > \psi(X)$.

Danzer's flip

Danzer [1963] defined the following flip. Let x, y, z be vertices of CG(X) with $dist(x, y) = dist(x, z) = \psi(X)$. We say that x is flipped over yz if x is replaced by its mirror image x' relative to the great circle yz. We say that this flip is Danzer's flip if $dist(x', X \setminus \{x, y, z\}) > \psi(X)$.



Irreducible contact graph

We say that the graph $\mathrm{CG}(X)$ is irreducible [Schütte - van der Waerden, Fejes Tóth] (or jammed [Connelly]) if there are no shift of vertices.

If there are neither Danzer's flips nor shifts of vertices, then we call CG(X) as a (Danzer's) irreducible graph.

Maximal graphs G_N

Let X be a subset of \mathbb{S}^2 with |X| = N. We say that CG(X) is maximal if $\psi(X) = d_N$ and its number of edges is minimum. We denote this graph by G_N .

Actually, this definition does not assume that G_N is unique. We use this designation for some CG(X) with $\psi(X) = d_N$.

Proposition. Let CG(X) be a maximal graph G_N . Then for $N \geq 6$ the graph CG(X) is irreducible.

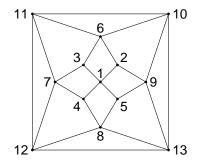
Properties of irreducible graphs

Let the graph CG(X) be irreducible. Then

- \bigcirc CG(X) is a planar graph.
- ② Degrees of CG(X) vertices can take only the values 0 (isolated vertices), 3, 4, or 5.
- **3** All faces of CG(X) in \mathbb{S}^2 are equilateral convex polygons of sides length $\psi(X)$.
- **4** All faces of $\operatorname{CG}(X)$ are polygons with at most $\lfloor 2\pi/\psi(X) \rfloor$ vertices.

N = 13

The contact graph $\Gamma_{13} := CG(P_{13})$ with $\psi(P_{13}) \approx 57.1367^{\circ}$



Tammes' problem for N = 13

The value $d = \psi(P_{13})$ can be found analytically.

$$2\tan\left(\frac{3\pi}{8} - \frac{a}{4}\right) = \frac{1 - 2\cos a}{\cos^2 a}$$

$$d = \cos^{-1}\left(\frac{\cos a}{1 - \cos a}\right).$$

Thus, we have $a \approx 69.4051^{\circ}$ and $d \approx 57.1367^{\circ}$.

Tammes' problem for N = 13

Theorem. The arrangement of 13 points P_{13} in \mathbb{S}^2 is the best possible, the maximal arrangement is unique up to isometry, and $d_{13} = \psi(P_{13})$.

Tammes' problem for N=13: graphs $\Gamma_{13}^{(i)}$

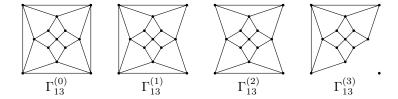


Figure: Graphs $\Gamma_{13}^{(i)}$.

Main lemmas

Lemma 1. G_{13} is isomorphic to $\Gamma_{13}^{(i)}$ with i = 0, 1, 2, or 3.

Lemma 2. G_{13} is isomorphic to $\Gamma_{13}^{(0)}$ and $d_{13} = \psi(P_{13}) \approx 57.1367^{\circ}$.

Properties of G_{13}

- 1 It is a planar graph with 13 vertices.
- 2 The degree of a vertex is 0,3,4, or 5.
- All faces are polygons with m=3,4,5, or 6 vertices.
- If there is an isolated vertex, then it lies in a hexagonal face.
- **3** No more than one vertex can lie in a hexagonal face.

Proof of Lemma 1

The proof consists of two parts:

- (I) Create the list L_{13} of all graphs with 13 vertices that satisfy 1–5;
- (II) Using linear approximations and linear programming remove from the list L_{13} all graphs that do not satisfy the geometric properties of G_{13}

Proof of Lemma 1: The list L_{13}

To create L_{13} we use the program *plantri* (Gunnar Brinkmann and Brendan McKay). This program is the isomorph-free generator of planar graphs, including triangulations, quadrangulations, and convex polytopes.

The program plantri generates 94,754,965 graphs in L_{13} . Namely, L_{13} contains 30,829,972 graphs with triangular and quadrilateral faces; 49,665,852 with at least one pentagonal face and with triangular and quadrilaterals; 13,489,261 with at least one hexagonal face which do not contain isolated vertices; 769,375 graphs with one isolated vertex, 505 with two isolated vertices, and no graphs with three or more isolated vertices.

Proof of Lemma 1

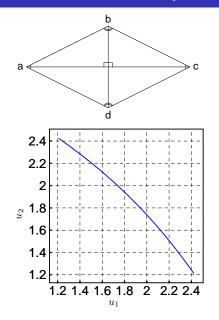
Let G be a graph from the list L_{13} .

Variables: d (the length of edges), angles of faces.

Equations and inequalities:

- $0 d > 57.1367^0$.
- ② For each vertex sum of its angles = 2π .
- **3** For a triangle: $u = \arccos(\cos d/(1 + \cos d))$.
- 4 For a quadrilateral: an explicit equation.
- **o** For a pentagon: an approximation by linear inequalities.
- For an empty hexagon: an approximation by linear inequalities.
- For a hexagon with an isolated vertex: an approximation by linear inequalities.

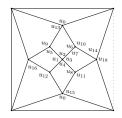
Proof of Lemma 1: Quadrilateral

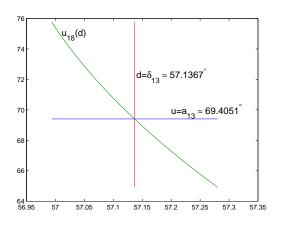


Proof of Lemma 1: Feasible solutions of the system

- Do linear estimations of equations.
- ② Using LP find a convex region containing a possible solution.
- 3 Using a region do more precise linear approximations and go back to steps 1,2.
- **③** If a region becomes empty − system is unfeasible.
- if a region is still not empty split it into two parts, and go back to steps 1–5.
- If all regions (after splitting) become empty system if unfeasible.

Proof of Lemma 2



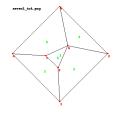


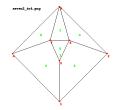
Research directions

- **②** Danzer (1963) considered (Danzer's) irreducible graphs with $N \leq 10$ vertices. We plan to verify and extend Danzer's classification for N up to 13.
- ② We plan to consider maximal and other irreducible graphs for the Tammes problem with N=14 and higher.
- **3** We will also explore the applicability of the methods discussed here to solve the Tammes problem for N=14 and higher.
- We plan to extend the concept of irreducible graphs for packing equal circles into two-dimensional manifolds. In according to Daniel Usikov the case of a flat torus is especially interesting for the problem of "super resolution of images".
- Onnelly considered rigidity of circles packings from the point of view of the theory of tensegrity structures. An interesting follow-up project is extending these ideas to combinatorial structure of irreducible graphs.

Irreducible graphs for N=7

N	d_{min}	d_{max}
1*	1.34978	1.35908
2 * *	1.35908	1.35908

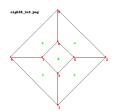


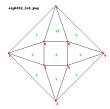


Irreducible graphs for N=8

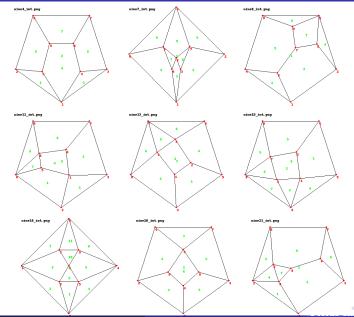
N	d_{min}	d_{max}
1	1.17711	1.18349
6*	1.28619	1.30653
8*	1.23096	1.30653
12 * *	1.30653	1.30653
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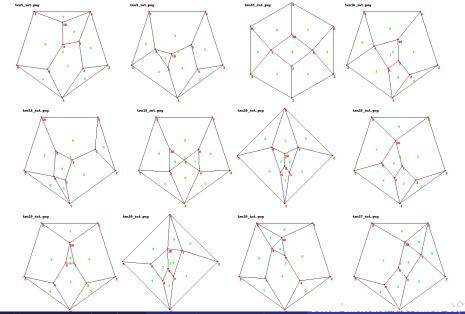


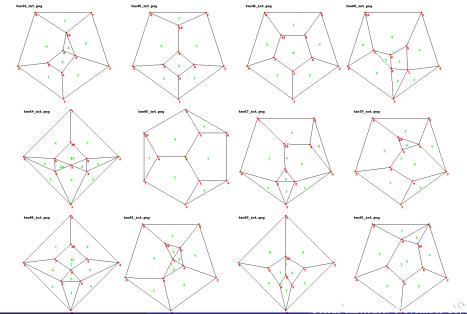


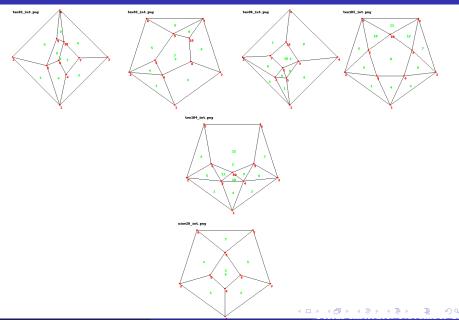


N	d_{min}	d_{max}
4	1.14099	1.14143
7*	1.22308	1.23096
8	1.10525	1.14349
11	1.17906	1.18106
13	1.15448	1.17906
15	1.17906	1.17906
18 * *	1.23096	1.23096
20	1.15032	1.18106
21*	1.10715	1.14342









SDP: Papers

- 1. A. Schrijver, New code upper bounds from the Terwilliger algebra and semidefinite programming, *IEEE Trans. Inform. Theory* 51 (2005), 2859–2866.
- **2.** D. C. Gijswijt, A. Schrijver, and H. Tanaka, New upper bounds for nonbinary codes based on the Terwilliger algebra and semidefinite programming, *JCTA* 113(8), 2006, p.1719–1731.
- **3.** C. Bachoc and F. Vallentin, New upper bounds for kissing numbers from semidefinite programming, *JAMS*. 21 (2008), 909-924.
- 4. C. Bachoc and F. Vallentin, Semidefinite programming, multivariate orthogonal polynomials, and codes in spherical caps, math. MG/0610856.
- **5.** C. Bachoc and F. Vallentin, Optimality and uniqueness of the (4,10,1/6) spherical code, JCTA 116 (2008), 195-204.

SDP: Papers

- **6.** O. R. Musin, Bounds for codes by semidefinite programming, *Proc. Steklov Inst. Math.* 263 (2008), 134-149.
- 7. O. R. Musin, Multivariable positive definite functions on spheres, arXiv:math.MG/0701083.

LP and SDP: History

Laplace and Legendre (1782-1785): n = 3.

Gegenbauer (1880s): all n

Schoenberg (1942); Bochner (1941)

Wang (1952): $\mathbf{M} = \mathbf{S}^n, \mathbf{RP}^n, \mathbf{CP}^n, \mathbf{QP}^n, \mathbf{CayP}^2$

History

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Delsarte (1972); Sidelnikov (1974); Delsarte - Goethals - Seidel (1977); Kabatiansky - Levenshtein (1978)
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Levenshtein (1979); Odlyzko - Sloane (1979): $k(8) = 240; \ k(24) = 196560; \ k(n) \le 25, 46, 82, 140, 240$ for n = 4, 5, 6, 7, 8.

Cohn, Elkies, Kumar (2003, 2004): \mathbf{R}^n

M. (2003):
$$k(4) = 24$$
; Pfender (2005); M. (9/2006): SDP

Schrijver (2005): \mathbf{H}^n ; Gijswijt, Schrijver, and Tanaka (2006); Bachoc and Vallentin (8/2006, 10/2006): \mathbf{S}^n , m=1.

M. (1/2007): \mathbf{S}^{n-1} , $0 \le m \le n-2$.



Zonal spherical functions

With any compact 2-point-homogeneous space \mathbf{M} are associated the zonal spherical functions $\Phi_k(t)$, $k=0,1,2,\ldots$, and the distance function $\tau(x,y)$, where $x,y\in\mathbf{M}$.

For all continuous compact \mathbf{M} and for all currently known finite cases: $\Phi_k(t)$ is a polynomial of degree k.

If M= Hamming space, then $\Phi_k(t)$ is the Krawtchouk polynomial $K_k(t,n)$.

If $M = \text{unit sphere } \mathbf{S}^{n-1} \subset \mathbf{R}^n$, then the corresponding zonal spherical function $\Phi_k(t)$ is the Gegenbauer (or ultraspherical) polynomial $G_k^{(n)}(t)$.

The main property for zonal spherical functions is called "positive-definite degenerate kernels" or p.d.k. This property first was discovered by Bochner (general spaces) and independently for spherical spaces by Schoenberg:

Let **M** be a 2-point-homogeneous space. Then for any integer $k \geq 0$ and for any finite $C = \{x_i\} \subset M$ the matrix $(\Phi_k(\tau(x_i, x_j)))$ is positive semidefinite.

I'm considered two extensions of Delsarte's method via semidefinite programming (SDP).

The first approach shows that using as variables power sums of distances this problem can be considered as a finite semidefinite programming problem. This method allows to improve some upper bounds. (See details: O.R. Musin, Bounds for codes by semidefinite programming, arXiv:math.CO/0609155)

The second approach extends the Bachoc-Vallentin method for spherical codes. In particular, an extension of Schoenberg's theorem for multivariate Gegenbauer polynomials has been proved. (O.R. Musin, Multivariate positive definite functions on spheres, arxiv:math/0701083)

Multivariate Gegenbauer polynomials

Let $0 \le m \le n-2$, $t \in \mathbf{R}$, $\mathbf{u}, \mathbf{v} \in \mathbf{R}^m$ for m > 0, and $\mathbf{u} = \mathbf{v} = 0$ for m = 0. Then the following polynomial in 2m + 1 variables of degree k in t is well defined:

$$\begin{split} G_k^{(n,m)}(t,\mathbf{u},\mathbf{v}) := \\ &= (1 - |\mathbf{u}|^2)^{k/2} (1 - |\mathbf{v}|^2)^{k/2} G_k^{(n-m)} \left(\frac{t - \langle \mathbf{u}, \mathbf{v} \rangle}{\sqrt{(1 - |\mathbf{u}|^2)(1 - |\mathbf{v}|^2)}} \right). \end{split}$$

p.d. functions

We say that $f(\mathbf{u}, \mathbf{v})$ is positive semidefinite and write $f \succeq 0$ if

$$f(\mathbf{u}, \mathbf{v}) = \sum_{i} h_i(\mathbf{u}) h_i(\mathbf{v})$$

p.d. functions on spheres

Theorem. Let $0 \le m \le n-2$. Let $Q = \{q_1, \ldots, q_m\} \subset \mathbf{S}^{n-1}$ with $\operatorname{rank}(Q) = m$. Let e_1, \ldots, e_m be an orthonormal basis of the linear space with the basis q_1, \ldots, q_m , and let L_Q denotes the linear transformation of coordinates.

Then $F \in psd(\mathbf{S}^{n-1}, Q)$ if and only if

$$F(t, \mathbf{u}, \mathbf{v}) = \sum_{k=0}^{\infty} f_k(\mathbf{u}, \mathbf{v}) G_k^{(n,m)}(t, L_Q(\mathbf{u}), L_Q(\mathbf{v})),$$

where $f_k(\mathbf{u}, \mathbf{v}) \succeq 0$ for all $k \geq 0$.

Let $\mathbf{x} = \{x_{ij}\}$, where $1 \le i < j \le m+2$, and $-1 \le x_{ij} \le \cos \theta$.

Let A be a symmetric $m + 2 \times m + 2$ matrix such that all $a_{ii} = 1$, and $a_{ij} = x_{ij}$ for i < j.

Let

$$D_m(\theta) = \{ \mathbf{x} : A \succeq 0 \}.$$

Let C be an (n, M, θ) spherical code.

Split C^{m+2} into subsets $\{C_{\omega}\}$ where C_{ω} with $\omega = (i_1, \ldots, i_k)$ contains all m+2-element sets $(c_1, \ldots, c_1, \ldots, c_k, \ldots, c_k)$, $c_i \in C$ with $|\{c_s\}| = i_s$.

Denote $q(\omega) := |C_{\omega}|/M$.

If
$$(c_1, c_2, ..., c_{m+2}) \in C^{m+2}$$
, then $x_{ij} = \langle c_i, c_j \rangle$.

Theorem. Let $f(\mathbf{x}) - f_0$ be a symmetric m-p.d. function on S^{n-1} , where $f_0 > 0$, $0 \le m \le n-2$. Suppose

$$f(\mathbf{y}) \leq B_{\omega}$$
, for all $\mathbf{y} \in D_{\omega}(\theta)$, $d(\omega) < m + 2$,

and

$$f(\mathbf{x}) \leq 0 \text{ for all } \mathbf{x} \in D_m(\theta).$$

Then an (n, M, θ) spherical code satisfies

$$f_0 M^{m+1} \le \sum_{\omega} q(\omega) B_{\omega} M^{d(\omega)-1}.$$

m = 0 (Delsarte's bound): $f_0 M \leq f(1)$.

m = 1 (the Bachoc-Vallentin bound):

$$f_0 M^2 \le f(1,1,1) + 3(M-1)B_{(2,1)}.$$

m = 2

$$f_0 M^3 \le f(\mathbf{1}) + 4(M-1)B_{(3,1)} + 3(M-1)B_{(2,2)} + 6(M-1)(M-2)B_{(2,1,1)}.$$

p.d. functions on Euclidean spaces

$$H_k^{(n,m)}(t,x,y,{\bf u},{\bf v}):=(xy)^{k/2}\,G_k^{(n,m)}(t',{\bf u}',{\bf v}'),$$

where

$$t' = \frac{t}{\sqrt{xy}}, \quad \mathbf{u}' = \frac{\mathbf{u}}{\sqrt{x}}, \quad \mathbf{v}' = \frac{\mathbf{v}}{\sqrt{y}}$$

Theorem

Let e_1, \ldots, e_n be an orthonormal basis of \mathbf{R}^n , and let p_1, \ldots, p_r be points in \mathbf{R}^n . Then for any $k \geq 0$ and $0 \leq m \leq n-2$ the matrix $\left(H_k^{(n,m)}(\langle p_i, p_j \rangle, |p_i|^2, |p_j|^2, p_i, p_j)\right)$ is positive semidefinite.

$H_k^n(A)$

Let us consider the simplest case m = 0. Let

$$H_k^{(n)}(t, x, y) := H_k^{(n,0)}(t, x, y, 0, 0).$$

Now for any matrix $A = (a_{ij}) \succeq 0$ of size $M \times M$ we introduce a matrix $H_k^n(A)$ of size $M \times M$ by

$$(H_k^n(A))_{ij} = H_k^{(n)}(a_{ij}, a_{ii}, a_{jj}).$$

Note that $(H_k^n(A))_{ij}$ is a polynomial of degree k in a_{ij}, a_{ii}, a_{jj} .

Since $G_1^{(n)}(t) = t$, we have

$$H_1^n(A) = A.$$



$H_2^n(A)$

$$G_2^{(n)}(t) = (nt^2 - 1)/(n - 1)$$
. Therefore,

$$(H_2^n(A))_{ij} = \frac{na_{ij}^2 - a_{ii}a_{jj}}{n-1}.$$

Thus

$$H_2^n(A) = \frac{nA_2 - \mathbf{a}^T \mathbf{a}}{n-1},$$

where

$$(A_2)_{ij} := a_{ij}^2, \quad \mathbf{a} := (a_{11}, a_{22}, \dots, a_{MM}).$$

p.d. constraints

Let $X = [x_1, x_2, ..., x_M]$ be a coordinate matrix in \mathbf{R}^n . Let $Y = X^T X$ be the Gramm matrix of X. It is well known fact: $Y \succeq 0$ and $\operatorname{rank}(Y) \leq n$. Moreover, for any $M \times M$ symmetric matrix Y (we denote it by $Y \in S_M$) with $Y \succeq 0$, $\operatorname{rank}(Y) \leq n$ there exists a coordinate matrix X in \mathbf{R}^n such that $Y = X^T X$.

For k = 1 we have: $H_k^n(Y) = Y \succeq 0$.

Theorem

Let $Y \in S_M$. If $Y \succeq 0$ and $rank(Y) \leq n$, then for all k = 1, 2, ...

$$H_k^n(Y) \succeq 0.$$

It is an interesting question: is converse fact holds? We considered it for n=2. In this case the converse theorem is correct. (However, we are not sure that it holds for all n>1.)

Theorem

Let $Y \in S_M$. Suppose $H_k^2(Y) \succeq 0$ for all $k = 1, 2, \ldots$. Then $rank(Y) \leq 2$, i.e. Y is a Gramm matrix of vectors in \mathbb{R}^2 .

sensor network localization

The Sensor Network Localization (SNL) problem was considered in [P. Biswas, T.-C. Liang, T.-C. Wang, Y. Ye, Semidefinite programming based algorithms for sensor network localization] with great details. Proposition 1 in [Biswas et al] shows that: if 2M + M(M+1)/2 distance pairs each of which has an accurate distance measure, then the SNL problem via SDP has a unique feasible solution.

The SNL problem with measurement noises has no a unique feasible solution. In this case the set of feasible solutions is a set of measure greater than zero. To solve this problem in [Biswas et al] is considered certain SDP relaxations.

For SNL we have $\operatorname{rank}(Y) \leq n$. However, this constraint is not using in current SDP algorithms. Our idea is to add some SDP relaxations of the constraints: $H_k^n(Y) \geq 0$ for $k = 2, \ldots, d$.

sensor network localization

For n=2 (the most interesting dimension for SNL) our theorems show that $\operatorname{rank}(Y) \leq 2$ can be substitute by $H_k^2(Y) \succeq 0$ for all k. So the *first step* of an SDP relaxation (for any dimensions n) is to consider just first d constraints.

The second step is: to find a reasonable SDP relaxation of $H_k^n(Y) \succeq 0$ for a given k.

Research problem: Based on further investigations of Steps 1 and 2 to improve SDP algorithms for SNL.