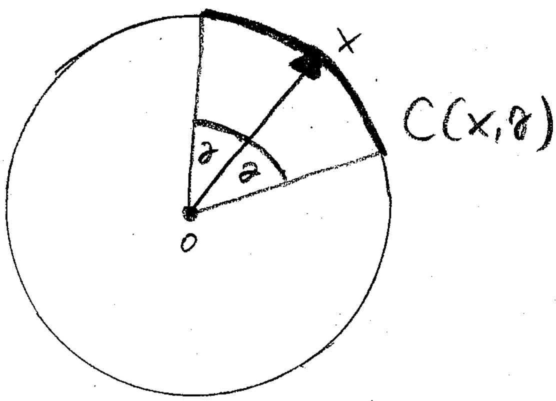
Chapter VII Packings on the (unit) sphere

§1 The unit sphere

Unit sphere $S^{n-1} = \{x \in \mathbb{R}^n : x^T x = 1\}$.

Def. 1 The spherical cap with center $x \in S^{n-1}$ and angle $\gamma \in [0, \pi]$ is

$$C(x, \gamma) = \{y \in S^{n-1} : x^T y \geq \cos \gamma\}.$$



Spherical coordinates in n dimensions

$$x_1 = r \cos \theta_1$$
$$x_2 = r \sin \theta_1 \cos \theta_2$$
$$x_3 = r \sin \theta_1 \sin \theta_2 \cos \theta_3$$
$$\vdots$$
$$x_{n-1} = r \sin \theta_1 \sin \theta_2 \sin \theta_3 \ldots \sin \theta_{n-2} \cos \phi$$
$$x_n = r \sin \theta_1 \sin \theta_2 \sin \theta_3 \ldots \sin \theta_{n-2} \sin \phi,$$

with

$$(r, \theta_1, \dots, \theta_{n-2}, \phi)$$

and

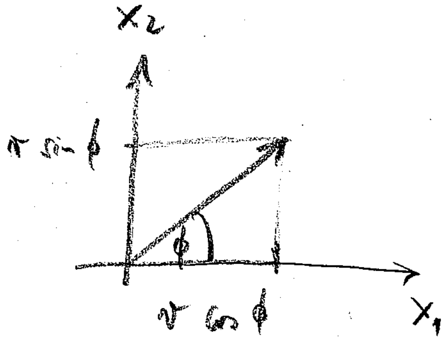
$$r \geq 0, \quad \theta_1, \dots, \theta_{n-2} \in [0, \pi], \quad \phi \in [0, 2\pi].$$

For example

<u>$m = 2$</u>

$$x_1 = r \cos \phi$$

$$x_2 = r \sin \phi$$

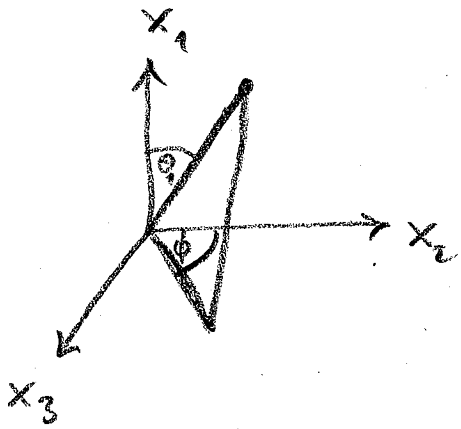


<u>$m = 3$</u>

$$x_1 = r \cos \theta_1$$

$$x_2 = r \sin \theta_1 \cos \phi$$

$$x_3 = r \sin \theta_1 \sin \phi$$



<u>Volume element</u>

$$dV_n = dx_1 \, dx_2 \dots dx_n$$

$$= r^{n-1} \sin^{n-2}\theta_1 \sin^{m-3}\theta_2 \dots \sin^2\theta_{m-3} \sin\theta_{n-2} \cdot$$

$$dr \, d\theta_1 \dots d\theta_{n-2} \, d\phi.$$

Surface element for the unit sphere

$$d\omega_n = \sin^{n-2}\theta_1 \sin^{n-3}\theta_2 \ldots \sin^2\theta_{n-3} \sin\theta_{n-2} \cdot$$
$$\cdot\, d\theta_1 \ldots d\theta_{n-2}\, d\phi$$

$$= \sin^{n-2}\theta_1 \, d\theta_1 \, d\omega_{n-1}$$

$$= (1-t^2)^{\frac{n-3}{2}} \, dt \, d\omega_{n-1}$$

with $t = \cos\theta_1 \quad \left(\frac{dt}{d\theta_1} = \sin\theta_1 \right)$.

Surface area of the sphere

$$\omega_n(S^{n-1}) = \frac{2\pi^{n/2}}{\Gamma(n/2)}$$

Surface area of spherical cap $C(x,\gamma)$

$$\omega_n(C(x,\gamma)) = \omega_{n-1}(S^{n-2}) \int_{\cos\gamma}^{1} (1-t^2)^{\frac{n-3}{2}} \, dt .$$

§ 2 Packings of spherical caps

Def. 1 A packing of spherical caps with angle γ is a set of spherical caps with angle γ having pairwise disjoint interior.

Two spherical caps intersect in their interior

$$\text{int } C(x,\gamma) \cap \text{int } C(y,\gamma) = \emptyset$$

$$\Leftrightarrow \quad -1 \leq x^T y \leq \cos(2\gamma)$$

Def. 2 Given dimension n, angle γ define

$$A(n, 2\gamma) = \max\{N : C(x_1,\gamma), \ldots, C(x_N,\gamma) \text{ is a packing}\}.$$

The kissing number in dimension n is defined as

$$\tau_n = A(n, \tfrac{\pi}{3})$$

Remark τ_n is only known for $n = 1, 2, 3, 4, 8, 24$

$\tau_1 = 2$ $\quad$ $\tau_4 = 24$

$\tau_2 = 6$ $\quad$ $\tau_8 = 240$

$\tau_3 = 12$ $\quad$ $\tau_{24} = 196560.$

Def. 3 **Packing graph.** Given n, γ define

$$G(n, 2\gamma) = (V, E)$$

with $V = S^{n-1}$

$$E = \{ \{x, y\} : x^T y \in (\cos 2\gamma, 1) \}.$$

Then

$$\alpha(G(n, 2\gamma)) = A(n, 2\gamma).$$

Goal: Generalize ϑ to bound $\alpha(G(n, 2\gamma))$.

Def. 4 A continuous function $K : S^{n-1} \times S^{n-1} \to \mathbb{R}$ is called a *positive semidefinite Hilbert-Schmidt kernel* if

(a) $K(x, y) = K(y, x) \quad \forall x, y \in S^{n-1}$

(b) $\forall N \in \mathbb{N}\ \forall x_1, \dots, x_N \in S^{n-1} : \ (K(x_i, x_j))_{1 \le i, j \le N} \in S^N_+$.

Denote the cone of positive semidefinite Hilbert-Schmidt kernels by $C(S^{n-1} \times S^{n-1})_+$.

Def. 5

$$\vartheta'(G(n,2\gamma)) = \inf \lambda$$
$$\lambda \in \mathbb{R},\ K \in C(S^{n-1}\times S^{n-1})_+,$$
$$K(x,x) = \lambda - 1$$
$$K(x,y) \leq -1 \text{ for all } x,y \text{ with } x^T y \in [-1, \cos(2\gamma)].$$

Theorem 6

$$\alpha(G(n,2\gamma)) \leq \vartheta'(G(n,2\gamma)).$$

Proof Let $C \subseteq S^{n-1}$ be independent for $G(n,2\gamma)$. Let K be feasible for $\vartheta'(G(n,2\gamma))$. Then, since K is positive semidefinite

$$0 \leq \sum_{x\in C}\sum_{y\in C} K(x,y) = \sum_{x\in C} K(x,x) + \sum_{x\neq y} K(x,y)$$

$$\leq |C|(\lambda-1) + (-1)(|C|^2 - |C|)$$

$$\Rightarrow |C| \leq \lambda. \quad \boxtimes$$

Remark If $\alpha = \vartheta'$, then "$\leq$" must be "$=$". This means that $K(x,y) = -1$ for $x, y \in C$ with $x \neq y$.

To compute ϑ' apply <u>symmetry reduction</u>.

Let (λ, K) be feasible for ϑ'. Let $A \in O(n)$ be an orthogonal matrix. Then, also (λ, K^A), with

$K^A(x,y) = K(Ax, Ay)$, is feasible for ϑ'.

So we can symmetrize every feasible solution using the Haar measure μ on $O(n)$ and get

$$K'(x,y) = \int_A K^A(x,y)\, d\mu(A),$$

which is $O(n)$-invariant, that is $K(x,y) = K(Ax, Ay)$ for every $A \in O(n)$, $x, y \in S^{n-1}$.

Restrict W.l.o.g. $C(S^{n-1} \times S^{n-1})_+$ to

$$C(S^{n-1} \times S^{n-1})_+^{O(n)} = \{K \in C(S^{n-1} \times S^{n-1}) : K \text{ } O(n)\text{-invariant}\}$$

We get

$$\vartheta'(G(n, 2\vartheta)) = \inf \lambda$$

$$\lambda \in \mathbb{R},\ K \in C(S^{n-1} \times S^{n-1})_+^{O(n)},$$

$$K(x,x) = \lambda - 1 \quad \forall x \in S^{n-1}$$

$$K(x,y) \leq -1 \quad \forall x, y : x^T y \in [-1, \cos(2\vartheta)]$$

§ 3 Schoenberg's theorem

Theorem 1 (Schoenberg, 1941)

$$C(S^{n-1} \times S^{n-1})_+^{O(n)} \tag{$*$}$$
$$= \left\{ \sum_{k=0}^{\infty} f_k E_k^n(x,y) : f_k \geq 0, \sum_{k=0}^{\infty} f_k < \infty \right\},$$

where $E_k^n(x,y) = P_k^n(x^T y)$ and where P_k^n is a polynomial of degree k normalised by $P_k^n(1) = 1$ and satisfying the orthogonality relation

$$\int_{-1}^{1} P_k^n(t) P_l^n(t) (1-t^2)^{\frac{n-3}{2}} dt = 0 \quad \text{if } k \neq l. \tag{$**$}$$

Interpretation of $(*)$:

$K \in C(S^{n-1} \times S^{n-1})_+^{O(n)} \iff \exists f_0, f_1, \ldots \geq 0 : \sum f_k < \infty$

and $K(x,y) = \sum_{k=0}^{\infty} f_k E_k^n(x,y)$. Here convergence is absolute and uniformly over $S^{n-1} \times S^{n-1}$.

About polynomials satisfying (**)

If $n=2$, then P_k^2 are the Chebyshev polynomials T_k with $T_k(\cos\theta) = \cos(k\theta)$

For larger n, P_k^n can be determined by Gram-Schmidt-orthogonalisation using the inner product

$$(f,g) = \int_{-1}^{1} f(t)\, g(t)\, (1-t^2)^{\frac{n-3}{2}}\, dt.$$

Values for small k:

$$P_0^n(t) = 1$$

$$P_1^n(t) = t$$

$$P_2^n(t) = \frac{n}{n-1} t^2 - \frac{1}{n-1}.$$

P_k^n are known by many computer packages:

Jacobi polynomials / Gegenbauer polynomials

(Warning! Be careful with parameters / normalisation)

§4 Delsarte's LP method

- idea goes back to Philippe Delsarte (1973)
- next theorem due to Delsarte, Goethals, Seidel (1977).

Theorem 1 $\alpha(G(n,2\gamma)) \le \vartheta'(G(n,2\gamma)) =$

$$= \inf \lambda$$
$$f_0, f_1, \ldots \ge 0$$
$$\sum_{k=0}^{\infty} f_k = \lambda - 1$$
$$\sum_{k=0}^{\infty} f_k P_k^n(t) \le -1 \quad \text{for } t \in [-1, \cos\gamma].$$

Proof Apply Schoenberg's Theorem to the ϑ' formulation. ☒

Application: $\tau_8 = 240$

$\tau_8 \ge 240$: Define (the E_8-root system)

C = all possible permutations and sign changes of
$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0, 0, 0, 0, 0, 0\right)$
$\cup$ all even sign change of $\frac{1}{\sqrt{8}}(1,1,1,1,1,1,1,1)$

$|C| = \binom{8}{2} 2^2 + 2^7 = 112 + 128 = 240.$

All possible inner products occurring from C are

$\{-1, -\frac{1}{2}, 0, \frac{1}{2}, 1\}.$

$\underline{\tau_8 \leq 240}$: Will show $\vartheta'(G(8, \frac{\pi}{3})) \leq 240.$

$\underline{\text{Recall}}$: If ϑ' proves a tight bound, then

$K(x,y) = -1$ for $x, y \in C$ with

$x^T y = -1, -\frac{1}{2}, 0, \frac{1}{2}.$

$\underline{\text{Ansatz}}$:

$$F(t) = -1 + \beta (t+1)\left(t+\frac{1}{2}\right)^2 t^2 \left(t - \frac{1}{2}\right).$$

Then $F(t) = -1$ for $t = -1, -\frac{1}{2}, 0, \frac{1}{2}$ and $F(t) \leq -1$ for $t \in [-1, \frac{1}{2}]$. Choose β so that $F(1) = 240 - 1$.

Giving $\beta = \frac{320}{3}$. Now verify

$$F(t) = \sum_{k=0}^{6} f_k P_k^8(t) \quad \text{with} \quad f_k \geq 0.$$

$\boxtimes$

§5 Proof of Schoenberg's theorem

Step 1 Orthogonality relation

Let $K, L \in C(S^{n-1} \times S^{n-1})$ be continuous Hilbert-Schmidt kernels. Define their inner product

$$\langle K, L \rangle = \int_{S^{n-1}} \int_{S^{n-1}} K(x,y)\, L(x,y)\, d\omega_n(x)\, d\omega_n(y)$$

Lemma $\langle E_k^n, E_l^n \rangle = 0$ if $k \neq l$.

$\left[E_k^n(x,y) = P_k^n(x^T y) \right.$ and $\int_{-1}^{1} P_k^n(t) P_l^n(t) (1-t^2)^{\frac{n-3}{2}} dt = 0$ if $\left. k \neq l \right]$.

Proof

$$\langle E_k^n, E_l^n \rangle = \int_{S^{n-1}} \int_{S^{n-1}} P_k^n(x^T y)\, P_l^n(x^T y)\, d\omega_n(x)\, d\omega_n(y)$$

$$= \omega_n(S^{n-1}) \int_{S^{n-1}} P_k^n(e_1^T y)\, P_l^n(e_1^T y)\, d\omega_n(y)$$

$$= \omega_n(S^{n-1})\, \omega_{n-1}(S^{n-2}) \int_{-1}^{1} P_k^n(t)\, P_l^n(t)\, (1-t^2)^{\frac{n-3}{2}} dt$$

$$= 0 \quad \text{if } k \neq l.$$

spherical coordinate

$\left(d\omega_n = (1-t^2)^{\frac{n-3}{2}} dt\, d\omega_{n-1} \right)$

$t = \cos\theta_1$

Step 2 Positive semidefiniteness.

Lemma E_k^n is positive semidefinite.

Proof Consider $C(S^{n-1}) = \{ f : S^{n-1} \to \mathbb{R} : f \text{ cont.} \}$

with inner product

$$(f, g) = \int_{S^{n-1}} f(x) g(x) \, d\omega_n(x).$$

Let $V_0 \subseteq C(S^{n-1})$ be the space of constant functions.

Let $V_k \subseteq C(S^{n-1})$ be the space of polynomial functions on S^{n-1} of degree k with $V_k \perp V_0, \dots, V_{k-1}$.

(We identify polynomials which agree on S^{n-1}).

Now: Relate E_k^n to V_k.

Fix $x \in S^{n-1}$ and consider the evaluation map $f \mapsto f(x)$.

This is linear on V_k and so $\exists !\, v_{k,x} \in V_k$ such that

$$(v_{k,x}, f) = f(x), \text{ for all } f \in V_k$$

Claim: $\exists\, \alpha_k > 0 : \alpha_k v_{k,x}(y) = E_k^n(x,y)$

Proof Both sides give polynomial function of the right degree k.

The function $(x,y) \mapsto v_{k,x}(y)$ only depends on $x^T y$:

Let $A \in O(n)$ s.t. $Ax = x$. For $f \in C(S^{n-1})$ set $(Af)(x) = f(A^{-1}x)$. Then,

$$(A v_{k,x})(y) = v_{k,x}(A^{-1}y) = v_{k,x}(y)$$

because

$$\begin{aligned}(Av_{k,x}, f) &= (v_{k,x}, A^{-1}f) \\ &= A^{-1}f(x) \\ &= f(Ax) \\ &= (v_{k,Ax}, f) \\ &= (v_{k,x}, f)\end{aligned}$$

and by the uniqueness of $v_{k,x}$ it follows $Av_{k,x} = v_{k,x}$.

Furthermore: $(v_{k,x}, v_{l,y}) = 0$ if $k \neq l$ since $V_k \perp V_l$.

<u>Hence</u>: $E_k^n(x,y)$ and $v_{k,x}(y)$ are multiple of each other.

Since $E_k^n(x,x) = 1$ and $v_{k,x}(x) = (v_{k,x}, v_{k,x}) > 0$ the claim follows.

Now it is easy to see that E_k^n is positive semidefinite:

For $f \in C(S^{n-1})$ we have

$$\int_{S^{n-1}}\int_{S^{n-1}} E_k^n(x,y)\, f(x)\, f(y)\, d\omega_n(x)\, d\omega_n(y)$$

$$= \alpha_k \int_{S^{n-1}}\int_{S^{n-1}} (v_{k,x}, v_{k,y})\, f(x)\, f(y)\, d\omega_n(x)\, d\omega_n(y)$$

$$= \alpha_k \left(\int_{S^{n-1}} v_{k,x}\, f(x)\, d\omega_n(x), \int_{S^{n-1}} v_{k,y}\, f(y)\, d\omega_n(y) \right)$$

$$\geq 0.$$

Finally, we have to approximate delta function at point $x_1, \dots, x_N \in S^{n-1}$ by f.

<u>Step 3</u> The final.

<u>"$\supseteq$"</u>: Let $f_0, f_1, \dots \geq 0$ with $\sum_{k=0}^{\infty} f_k < \infty$ be given. E_k^n is pos. semidef. So

$$|E_k^n(x,y)| \leq E_k^n(x,x) = P_k^n(1) = 1.$$

Hence, $\sum_{k=0}^{\infty} f_k E_k(x,y)$ converges absolutely.

For all $x,y \in S^{n-1}$:

$$\left| \sum_{k=m}^{\infty} f_k E_k(x,y) \right| \leq \sum_{k=m}^{\infty} f_k ,$$

and so the series converges uniformly.

$\Longrightarrow K(x,y) = \sum_{k=0}^{\infty} f_k E_k^n(x,y)$ continuous (and pos. semidef.)

"$\subseteq$": Let $K \in C(S^{n-1} \times S^{n-1})_+^{O(n)}$ be given. Since K is invariant $\exists\, h : [-1,+1] \to \mathbb{R}$ with $K(x,y) = h(x^T y)$.
Since K is continuous, also h has to be continuous.
The polynomials $P_0^n, P_1^n, P_2^n, \ldots$ form a complete orthogonal system of $L^2([-1,+1], (1-t^2)^{\frac{n-3}{2}} dt)$ (convergence in L^2-norm). So we can write

$$h(t) = \sum_{k=0}^{\infty} f_k P_k^n(t) \qquad (L^2\text{-convergence})$$

for $f_k \in \mathbb{R}$.

<u>Claim</u> $f_k \geq 0$

<u>Proof</u> We have $K(x,y) = \sum_{k=0}^{\infty} f_k E_k^n(x,y)$ and

by psd ness:

$$0 \le \left\langle \sum_{k=0}^{\infty} f_k E_k^n, E_\ell^n \right\rangle$$

$$= f_\ell \underbrace{\langle E_\ell^n, E_\ell^n \rangle}_{>0} \implies f_\ell \ge 0.$$

<u>Claim</u> $\sum_{k=0}^{\infty} f_k < \infty$.

<u>Proof</u> Define $h_m(t) = h(t) - \sum_{k=0}^{m} f_k P_k^n(t)$, $t \in [-1,+1]$

Then

$$h_m(t) = \sum_{k=m+1}^{\infty} f_k P_k^n(t) \qquad (L^2\text{-convergence})$$

and $K_m(x,y) = h_m(x^T y)$ is psd. So $h_m(1) \ge 0$,

and

$$h(1) - \sum_{k=0}^{m} f_k = h(1) - \sum_{k=0}^{m} f_k P_k(1) = h_m(1) \ge 0$$

$$\to h(1) \ge \sum_{k=0}^{m} f_k \quad \text{for every } m.$$

$\boxtimes$