Methods and problems in discrete mathematics

WS 2019 / 2020

Goals

- Develop a mathematical toolbox (especially algebraic & analytic) to solve problems in discrete mathematics (especially discrete geometry & graph theory).
- Explain and discuss (open) problems
- Get familiar with contemporary literature in discrete mathematics
- Don't care at all about "purity of methods"

($\rightsquigarrow$ cross-disciplinary approach)

- Presentation will not be "linear" but rather "hilly"

Chapter I Universally optimal distribution of points

(following a paper by Cohn & Kumar)

Potential energy minimisation

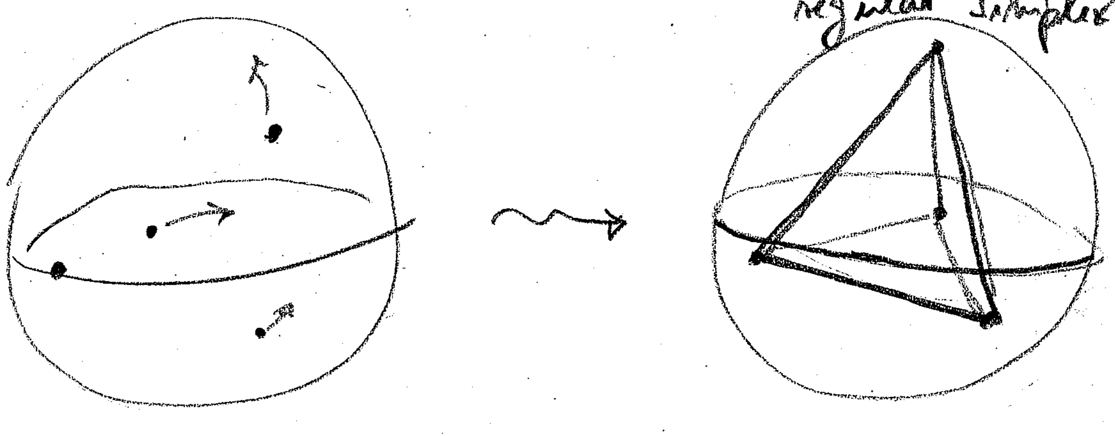
M (compact) Riemannian manifold, for example

$M = S^{n-1} = \{x \in \mathbb{R}^n : \|x\| = 1\}$ the unit sphere.

$\mathcal{C} \subseteq M$ finite point set.

Question Identically charged particles $\mathcal{C}$ move on M according to a potential function. How do they arrange? physics: $\rightsquigarrow$ locally minimise their electrical potential energy

S^2 vertices of regular simplex.



$|\mathcal{C}| = 4$

Here Focus on global minima.

Def. Let $f : (0,4] \to [0,\infty)$ be a decreasing, continuous function (radial potential function).
The f-potential energy of $\mathcal{C}$ is

$$\mathcal{E}_f(\mathcal{C}) = \sum_{\substack{x,y \in \mathcal{C} \\ x \neq y}} f(\|x-y\|^2)$$

Example

$n = 3$ $\quad f(r) = \frac{1}{r^{1/2}}$ electrical (Coulomb) potential

$n \geq 3$ $\quad f(r) = \frac{1}{r^{n/2-1}}$ Riesz potential; inverse power law

Natural class of radial potential functions

Def. $I \subseteq \mathbb{R}$ interval
$f : I \to \mathbb{R}$ $\mathcal{C}^\infty$-function is called completely monotonic if $(-1)^k f^{(k)}(x) \geq 0$ for all $x \in I$, $k \in \mathbb{N}$.

$k=0$: $f(x) \geq 0 \rightarrow f$ nonnegative

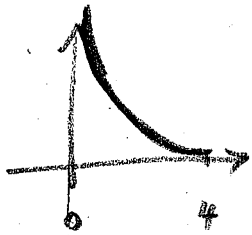
$k=1$: $-f'(x) \geq 0 \rightarrow f$ decreasing

$k=2$: $f''(x) \geq 0 \rightarrow f$ convex

$k=3$: $-f'''(x) \geq 0 \rightarrow f$ has negative jerk
(dt. "Ruck")

$\vdots$ $\leadsto$ causes motion sickness.

Ex



Example

(a) inverse power laws

$$f(r) = \frac{1}{r^s}, \quad s > 0,$$ are (strictly) completely monotonic

$\uparrow$
all ineq. strict in the interior of I

(b) Gaussian potential

$$f(r) = e^{-cr}, \quad c > 0$$

Theorem Completely monotonic functions form a convex cone. This cone is generated by the functions $r \mapsto (4-r)^k$, $k = 0,1,2,\dots$ (if $I = [0,4]$).

Proof see Widder, 1941.

Def. A finite set $\mathcal{C} \subseteq S^{n-1}$ is called a spherical t-design if for every polynomial $p \in \mathbb{R}[x_1, \dots, x_n]$ of degree $\leq t$:

$$\frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} p(x) = \int_{S^{n-1}} p(x) \, d\omega(x),$$

where ω is the unique rotationally invariant probability measure on S^{n-1}.

Def. $\mathcal{C} \subseteq S^{n-1}$ is called a sharp configuration if

(a) there are m inner products between distinct pairs of points:

$$|\{x \cdot y : x, y \in \mathcal{C}, x \neq y\}| = m$$

(b) $\mathcal{C}$ is a spherical $(2m-1)$ design.

Example vertices of regular simplex form a sharp configuration with $m = 1$.

Main Theorem Let $f:(0,4]\to\mathbb{R}$ be completely monotonic and $\mathcal{C}\subseteq S^{n-1}$ be a sharp configuration. Then for all $\mathcal{C}'\subseteq S^{n-1}$ with $|\mathcal{C}|=|\mathcal{C}'|$ we have

$$\mathcal{E}_f(\mathcal{C}) \le \mathcal{E}_f(\mathcal{C}').$$

In this case we say that $\mathcal{C}$ is universally optimal: $\mathcal{C}$ minimises potential energy among all point configuration with $|\mathcal{C}|$ elements and for all completely monotonic potential function.

Applies to:

n	N	M	Inner products	Name
2	N	$N-1$	$\cos(2\pi j/N)$ $(1\le j\le N/2)$	N-gon
n	$N\le n$	1	$-1/(N-1)$	simplex
n	$n+1$	2	$-1/n$	simplex
n	$2n$	3	$-1,0$	cross polytope
3	12	5	$-1,\pm1/\sqrt{5}$	icosahedron
~~4~~	~~120~~	~~11~~	$\cancel{-1,\pm1/2,0,(\pm1\pm\sqrt{5})/4}$	~~600-cell~~
8	240	7	$-1,\pm1/2,0$	E_8 roots
7	56	5	$-1,\pm1/3$	kissing
6	27	4	$-1/2,1/4$	kissing/Schläfli
5	16	3	$-3/5,1/5$	kissing
24	196560	11	$-1,\pm1/2,\pm1/4,0$	Leech lattice
23	4600	7	$-1,\pm1/3,0$	kissing
22	891	5	$-1/2,-1/8,1/4$	kissing
23	552	5	$-1,\pm1/5$	equiangular lines
22	275	4	$-1/4,1/6$	kissing
21	162	3	$-2/7,1/7$	kissing
22	100	3	$-4/11,1/11$	Higman-Sims
$q\frac{q^3+1}{q+1}$	$(q+1)(q^3+1)$	3 (4 if $q=2$)	$-1/q,1/q^2$	isotropic subspaces (q a prime power)

See Cohn & Kumar

It does not apply to the 600-cell but very similar techniques can be used.

More conjectured universal optima:

n	N	t	References
10	40	1/6	Conway, Sloane, and Smith [Sl], Hovinga [H]
14	64	1/7	Nordstrom and Robinson [NR], de Caen and van Dam [dCvD], Ericson and Zinoviev [EZ]

See Ballinger et al

<u>Question</u> Are these all universal optima for S^{n-1}?

<u>Ingredients for proof of main theorem</u>

A) Fourier analysis on the sphere (spherical harmonics)

B) Spherical design strength test

C) Linear programming bound

D) Hermite interpolation

E) Orthogonal polynomials

A) Spherical harmonics

With S^{n-1} one associates the family of orthogonal polynomials $P_k^n(t)$, $k = 0, 1, \ldots$, where P_k^n is a univariate polynomial of degree k normalised by $P_k^n(1) = 1$ and satisfying the orthogonality relation

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

(⇝ p. 99 of CO 2018/19)

⇝ We are going to explain the P_k^n in some detail ⇝ spherical harmonics.

⇝ Co 2018/19 : Schoenberg's theorem.

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

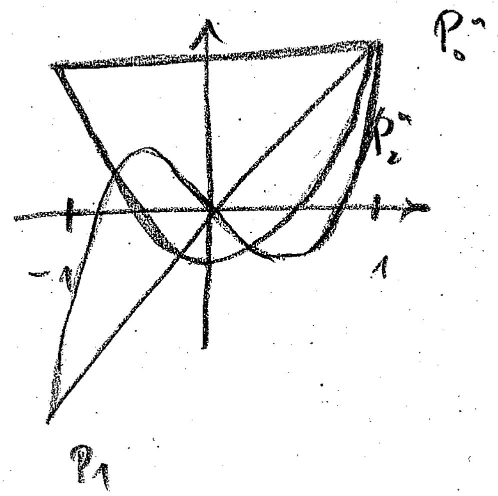
$$(f,g) = \int_{-1}^{1} f(t)\,g(t)\,(1-t^2)^{\frac{n-3}{2}}\,dt.$$

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)

Important property of P_k^n

Positivity property

the map $(x,y) \longmapsto P_k^n(x\cdot y)$ for $x,y \in S^{n-1}$

is a positive kernel, i.e. the infinite matrix

$[P_k(x\cdot y)]_{x,y\in S^{n-1}}$ is positive semidefinite.

In other words,

$\forall N \in \mathbb{N}\ \forall x_1,\dots,x_N \in S^{n-1}$ the finite submatrix

$[P_k(x_i\cdot x_j)]_{i,j=1,\dots,N}$ is pos. semidef.

Proof: $\rightsquigarrow$ spherical harmonics.

B) Spherical design strength test

<u>Lemma</u> $\mathcal{C} \subseteq S^{n-1}$ spherical M-design

$$\Longleftrightarrow \sum_{x,y \in \mathcal{C}} P_k^n(x \cdot y) = 0 \quad \text{for } k = 1, \dots, M.$$

<u>Proof</u> $\rightsquigarrow$ spherical harmonics

C) Linear programming bound

for lower bounding f-potential energy

<u>Theorem</u> (Yudin, 1992)

Let $f : (0,4]$ be any function. Suppose $h : [-1,1] \to \mathbb{R}$ is a polynomial such that

(i) $h(t) \leq f(2-2t)$ for all $t \in [-1,1]$,

(ii) $h(t) = \sum_{k=0}^{d} \alpha_k P_k^n(t)$ with $\alpha_0, \dots, \alpha_d \geq 0$.

Then for every $\mathcal{C} \subseteq S^{n-1}$ with $|\mathcal{C}| = N$ we have

$$\mathcal{E}_f(\mathcal{C}) \geq N^2 \alpha_0 - N h(1).$$

Remarks

- Yudin's bound generalises the LP method of Delsarte, Goethals, Seidel (1977) (see CO 2018/19: page 100) for spherical cap packings.

- Finding an optimal h, giving the best possible lower bound, is an (infinite-dimensional) LP.

- Yudin's bound generalises to unequally charged particles. $\rightsquigarrow$ Exercise.

- Punch line of proof of main theorem: If $\mathcal{C}$ is a sharp configuration, then the LP bound is sharp (lower bound = upper bound) for all completely monotonic function.

Proof (of LP bound)

Observe
$$\|x-y\|^2 = x\cdot x - 2x\cdot y + y\cdot y$$
$$= 2 - 2x\cdot y \quad \text{for } x,y \in S^{n-1}.$$

By assumption (i) and observation

$$\mathcal{E}_f(\mathcal{C}) = \sum_{\substack{x,y\in\mathcal{C}\\ x\neq y}} f(\|x-y\|^2) \geq \sum_{\substack{x,y\in\mathcal{C}\\ x\neq y}} h(x\cdot y)$$

On the other hand, by assumption (ii) and the positivity property

$$\sum_{\substack{x,y\in\mathcal{C}\\ x\neq y}} h(x\cdot y) = -N h(1) + \sum_{x,y\in\mathcal{C}} h(x\cdot y)$$

$$= -N h(1) + \sum_{x,y\in\mathcal{C}} \sum_{k=0}^{d} \alpha_k P_k^n(x\cdot y)$$

$$= -N h(1) + \sum_{k=0}^{d} \underbrace{\alpha_k}_{\geq 0} \underbrace{\sum_{x,y\in\mathcal{C}} P_k^n(x\cdot y)}_{\geq 0}$$

$$\geq -N h(1) + \alpha_0 \underbrace{\sum_{x,y\in\mathcal{C}} \underbrace{P_0^n(x\cdot y)}_{=1}}_{=N^2} = -N h(1) + \alpha_0 N^2.$$

$\boxtimes$

<u>Remark</u> If h proves sharp bound for $\mathcal{E}_f(\mathcal{C})$, then

- $h(x\cdot y) = f(2-2x\cdot y)$ for all $x, y \in \mathcal{C}, x \neq y$.
- if $\alpha_k > 0$, then $\sum_{x,y\in \mathcal{C}} P_k^n(x\cdot y) = 0$

($\leadsto$ spherical design strength test).

D) Hermite interpolation

<u>Idea</u> Given a function f, find a polynomial (of low degree) that matches the values of f and some of its derivatives at some specified points.

<u>Theorem</u> Given $f \in \mathcal{C}^\infty([a,b])$, distinct points $t_1, \dots, t_m \in [a,b]$, positive integers $k_1, \dots, k_m$. Then there is a unique polynomial of degree less than $D = k_1 + k_2 + \dots + k_m$ such that

$$p^{(k)}(t_i) = f^{(k)}(t_i) \quad \text{for all } \begin{array}{l} 1 \le i \le m, \\ 0 \le k < k_i. \end{array}$$

<u>Proof</u> see your favorite numerics class / book.

Usage in the proof of main theorem

Interpolate f at positions $x \cdot y$ for $x, y \in \mathcal{C}$ upto order 2 (i.e. value and 1^{st} derivative) gives polynomial h $\rightsquigarrow$ assumption (i) fullfilled.

E) Orthogonal polynomials

- classical and useful topic in analysis (but not very fashionable ...)
- very good books: for example
  - Szegö - Orthogonal polynomials, 1958
  - Andrews, Askey, Roy - Special functions, 1999
  - ...
- important properties: 3-term recurrence relation, interlacing of roots, ...

Let $w \in C([a,b])$ be a continuous, nonnegative (weight) function, $w \neq 0$.

<u>Def.</u> A sequence of polynomials $(p_n)_{n=0,1,\ldots}$, where $\deg p_n = n$, is <u>orthogonal</u> with respect to w if the following orthogonality relation holds:

$$\int_a^b p_m(x)\, p_n(x)\, w(x)\, dx = h_m \delta_{mn} .$$

<u>Theorem</u> A sequence of orthogonal polynomials $(p_n)_n$ satisfies the <u>3-term recurrence relation</u>

$$p_{n+1}(x) = (A_n x + B_n)\, p_n(x) + C_n p_{n-1}(x), \quad n \geq 0,$$

with $p_{-1}(x) = 0$ and $A_n, B_n, C_n \in \mathbb{R}$.

<u>Proof</u> Determine A_n so that

$$p_{n+1}(x) - A_n x\, p_n(x)$$

has degree n.

Then

$$p_{n+1}(x) - A_n x\, p_n(x) = \sum_{k=0}^{n} \beta_k p_k(x). \qquad (*)$$

for $\beta_k \in \mathbb{R}$. If q is polynomial of degree $m < n$, then by orthogonality

$$\int_a^b p_n(x)\, q(x)\, w(x)\, dx = 0.$$

Hence, $\beta_k = 0$ for $k < n-1$, because

$$\int_a^b \left(p_{n+1}(x) - A_n x\, p_n(x)\right) p_k(x)\, w(x)\, dx$$

$$= \int_a^b p_{n+1}(x)\, p_k(x)\, w(x)\, dx - A_n \int_a^b p_n(x) \left(x\, p_k(x)\right) w(x)\, dx$$

$$= 0.$$

So,

$$p_{n+1}(x) = A_n x\, p_n(x) + \beta_n p_n(x) + \beta_{n-1} p_{n-1}(x)$$

$$= (A_n x + \underbrace{\beta_n}_{B_n})\, p_n(x) + \underbrace{\beta_{n-1}}_{C_n} p_{n-1}(x)$$

$\boxtimes$

Remark

- More can be said about A_n, B_n, C_n.
- 3-term recurrence relations characterise orthogonal polynomials ($\rightsquigarrow$ Favard's theorem).

Example

Chebyshev polynomials of the first kind:

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_{n+1}(x) = 2x\, T_n(x) - T_{n-1}(x).$$

T_n satisfies $T_n(\cos\theta) = \cos n\theta$.

More about: D) Hermite Interpolation

Lemma (Remainder formula)

Given $f \in C^\infty([a,b])$, distinct points $t_1, \dots, t_m \in [a,b]$, positive integers $k_1, \dots, k_m$. Let p the corresponding Hermite interpolation polynomial of f, that is $\deg p < D = k_1 + \dots + k_m$ and $p^{(k)}(t_i) = f^{(k)}(t_i)$ for all $1 \le i \le m$, $0 \le k < k_i$. For every $t \in [a,b]$ there exists $z \in (a,b)$ with

$$\min\{t, t_1, \dots, t_m\} < z < \max\{t, t_1, \dots, t_m\}$$

so that

$$f(t) - p(t) = \frac{f^{(D)}(z)}{D!} (t-t_1)^{k_1} \cdots (t-t_m)^{k_m}.$$

Proof Define

$$g(t) = \frac{f(t) - p(t)}{(t-t_1)^{k_1} \cdots (t-t_m)^{k_m}}.$$

For $t \in [a,b] \setminus \{t_1, \dots, t_m\}$ consider the function

$$h(s) = f(s) - p(s) - g(t)\,(s-t_1)^{k_1} \cdots (s-t_m)^{k_m}.$$

We have $h^{(k_i)}(t_i) = 0$ for $1 \leq i \leq m$, $0 \leq k < k_i$

and $h(t) = 0$. So h has $D+1$ roots (counted with multiplicities) in the interval

$$[\min\{t, t_1, \dots, t_m\}, \max\{t, t_1, \dots, t_m\}].$$

By iterated use of Rolle's theorem ($\rightsquigarrow$ special case of mean value thm), there exists z in this interval so that $h^{(D)}(z) = 0$. Hence,

$$h^{(D)}(z) = f^{(D)}(z) - g(t)\,D! = 0,$$

and the lemma follows. $\boxtimes$

<u>Def</u> $I \subseteq \mathbb{R}$ interval, $f \in C^\infty(I)$ is called <u>absolutely monotonic</u> if $f^{(k)}(x) \geq 0$ for all $x \in I$, $k \in \mathbb{N}$.

[<u>strictly absolutely monotonic</u> if $f^{(k)}(x) > 0$ for all $x \in$ interior of I, $k \in \mathbb{N}$]

Systematic notation for Hermite interpolation

Let $f \in C^\infty$ and let g be a polynomial of $\deg g \geq 1$. By $\underline{H(f,g)}$ denote the polynomial p with $\deg p < \deg g$ such that p agrees with f at each root of g up to the order of that root, i.e.

$$g^{(k_i)}(t_i) = 0 \implies p^{(k_i)}(t_i) = f^{(k_i)}(t_i).$$

Define

$$Q(f,g)(t) = \frac{f(t) - H(f,g)(t)}{g(t)}.$$

Q extends to a C^∞-function at the roots of g.

<u>Lemma</u> Let f be absolutely monotonic in (a,b), let $g(t) = (t-t_1)^{k_1} \cdots (t-t_m)^{k_m}$ with $t_1, \dots, t_m \in [a,b)$. Then $Q(f,g)(t)$ is absolutely monotonic. The same is true for strictly absolutely monotonic.

<u>Proof</u> $\to$ Exercise (see Proposition 2.2 of the paper)

More about: E) Orthogonal polynomials

<u>Def</u> Let $w \in \mathcal{C}([a,b])$ be a continuous weight function. We say w is <u>positive definite up to degree N</u> if for all polynomials f with $\deg f \leq N$ we have

$$\int_a^b f(t)^2 w(t)\, dt \geq 0,$$

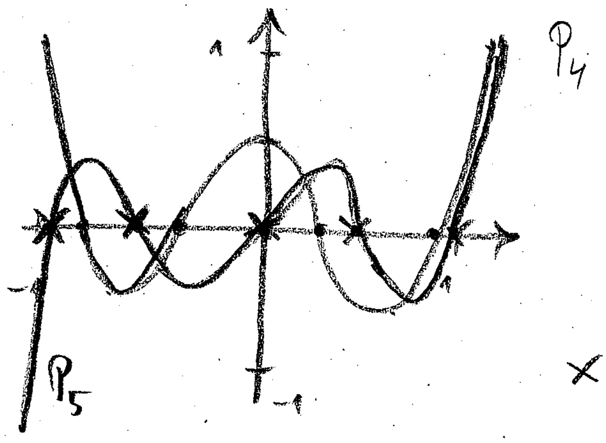
with equality $\Leftrightarrow f = 0$.

<u>Lemma</u> If w is positive definite up to degree N, then there are unique monic poly. $q_0, \dots, q_{N+1}$ such that $\deg(q_i) = i$ and

$$\int_a^b q_i(t)\, q_j(t)\, w(t)\, dt = 0 \quad \text{for } i \neq j.$$

For each i, q_i has i distinct real roots. The root of q_i and q_{i-1} are interlaced.

<u>Example</u> Legendre polynomials P_4, P_5



interlacing roots:

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<u>Proof</u> (of lemma)

- As usual one can determine q_i by applying Gram-Schmidt orthogonalization of $1, t, t^2, \dots, t^{N+1}$:

$$q_i(t) = t^i - \sum_{j=0}^{i-1} q_j(t) \frac{\int_a^b s^i q_j(s)\, w(s)\, ds}{\int_a^b q_j(s)^2 w(s)\, ds},$$

because $\langle p, q \rangle = \int_a^b p(t) q(t) w(t)\, dt$ determines a nondegenerate inner product on the space of polynomials of degree $\leq N$.

Hence, the q_i's are uniquely determined.

- They satisfy a 3-term recurrence relation:

The polynomial $q_i(t) - t q_{i-1}(t)$ has degree $i-1$ and

is orthogonal to all polynomials of degree $< i-2$.
Hence there are constants a_i and b_i with

$$q_i(t) = (t+a_i)\, q_{i-1}(t) + b_i\, q_{i-2}(t).$$

- We have $b_i < 0$ because

$$b_i \int_a^b q_{i-2}(t)^2\, w(t)\, dt$$
$$= \int_a^b \big(q_i(t)\, q_{i-2}(t) - (t+a_i)\, q_{i-1}(t)\, q_{i-2}(t)\big)\, w(t)\, dt$$
$$= \int_a^b -t\, q_{i-1}(t)\, q_{i-2}(t)\, w(t)\, dt$$

and

$$\int_a^b q_{i-1}(t)\, t\, q_{i-2}(t)\, w(t)\, dt = \int_a^b q_{i-1}(t)^2\, w(t)\, dt.$$

- Show by induction that the roots of q_i and q_{i-1} are real and interlaced.

<u>Base case</u>: $i = 1$: clear.

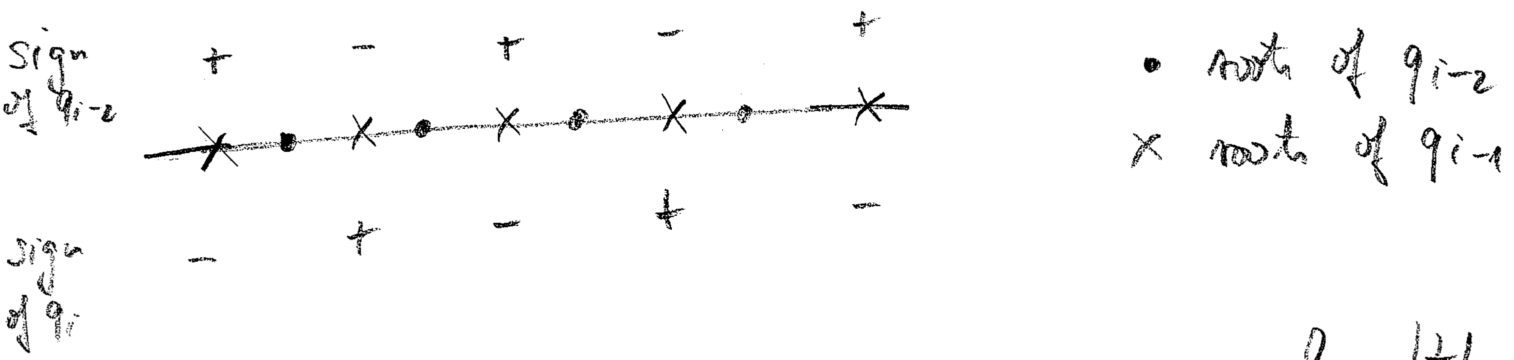
<u>Induction step</u> Suppose roots of q_{i-1} and q_{i-2} are real and interlaced.

Let r be a root of q_{i-1}. By (3TRR)

$$q_i(r) = b_i\, q_{i-2}(r).$$

By induction: q_{i-2} alternates in sign at roots of q_{i-1}. Since $b_i < 0$, q_i and q_{i-2} have opposite signs at roots of q_{i-1}. Hence, q_i has a root between each pair of consecutive roots of q_{i-1}.

Picture of the situation



Because q_i and q_{i-2} have the same sign, when $|t|$ is sufficiently large, q_i must have a root greater than every root of q_{i-1} and a root less than every root of q_{i-1}. This finishes the proof since all i roots of q_i are at the promised position. $\boxtimes$

<u>Lemma</u> (Gauss-Jacobi quadrature)

Let $w \in \mathcal{C}([a,b])$ be positive definite up to every degree $N \in \mathbb{N}$, which defines the monic, orthogonal polynomials $(p_n)_{n\in\mathbb{N}}$. Let $\alpha \in \mathbb{R}$ and let

$$v_1 < v_2 < \dots < v_n$$

be the roots of $p_n + \alpha p_{n-1}$. Then there exist $\lambda_1, \dots, \lambda_n > 0$ so that for every polynomial f, $\deg f \le 2n-2$:

$$\int_a^b f(t)\, w(t)\, dt = \sum_{i=1}^{n} \lambda_i f(v_i). \qquad (GJQ)$$

<u>Proof</u> There exist $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ with

$$\int_a^b f(t)\, w(t)\, dt = \sum_{i=1}^{n} \lambda_i f(v_i) \qquad (*)$$

for all polynomials f, $\deg f < n$.

~~Because~~ Apply Lagrange interpolation with nodes $\tau_1, \dots, \tau_n$. This gives

$$f(t) = \sum_{i=1}^{n} l_i(t) f(\tau_i)$$

with Lagrange polynomials l_i ($l_i(\tau_j) = \delta_{ij}$).

Then

$$\int f(t) w(t)\, dt = \sum f(\tau_i) \underbrace{\int l_i(t) w(t)\, dt}_{= \lambda_i}.$$

Let f be a polynomial with $\deg f \leq 2n-2$. Use polynomial division to find polynomials g, h so that

$$f = (p_n + \alpha p_{n-1}) g + h$$

with $\deg h < n$ and $\deg g \leq n-2$. Then by the orthogonality relation

$$\int f(t) w(t)\, dt = \int h(t) w(t)\, dt$$

and furthermore $f(\tau_i) = h(\tau_i)$.

So $(*)$ extends to all polynomials f with $\deg f \le 2n-2$.

<u>To show</u>: $\lambda_i > 0$

For fixed i specialise f to $f(t) = \prod_{j \neq i} (t - x_j)^2$

Then $\deg f = 2n-2$ and by $(*)$

$$\underbrace{\int f(t)\, w(t)\, dt}_{>0} = \lambda_i f(x_i) = \lambda_i \underbrace{\prod_{j \neq i} (x_i - x_j)^2}_{>0}$$

$\Longrightarrow \lambda_i > 0.$ $\boxtimes$

<u>Again</u>: $w \in \mathcal{C}([a,b])$ positive definite up to every degree $N \in \mathbb{N}$. Defines $(p_n)_{n\in\mathbb{N}}$ orth. poly.

Let $\tau_1 < \dots < \tau_n$ be the roots of $p_n + \alpha p_{n-1}$.

For $j \in \{0, \dots, n\}$ define $w_j \in \mathcal{C}([a,b])$ by

$$w_j(t) = \prod_{i=0}^{j-1} (\tau_{n-i} - t)\, w(t).$$

Clearly, $w_0 = w$.

<u>Lemma</u> For $j \in \{0, \dots, n-1\}$, the weight function w_j is positive definite up to degree $n - j - 1$.

<u>Proof</u> By (GJQ)

$$\int f(t)^2\, w_j(t)\, dt = \int f(t)^2 \prod_{i=0}^{j-1} (\tau_{n-i} - t)\, w(t)\, dt$$

$$= \sum_{i=1}^{n} \underbrace{\lambda_i}_{>0} \underbrace{f(\tau_i)^2}_{\geq 0} \underbrace{\prod_{\ell=0}^{j-1} (\tau_{n-\ell} - \tau_i)}_{\geq 0} \geq 0$$

for all polynomials f with

$2 \cdot \deg f + j \leq 2n - 2 \Rightarrow \deg f \leq n - 1 - j/2.$

We have equality "$=0$" iff

$$f(\tau_1) = f(\tau_2) = \dots = f(\tau_{n-j}) = 0.$$

If $\deg f \leq n-j-1$, then $f = \bar{0}$. $\boxtimes$

* **Theorem** For $k < n$, the polynomial

$$\prod_{i=1}^{k} (t - \tau_i)$$ can be expressed as

$$\prod_{i=1}^{k} (t - \tau_i) = \sum_{n=0}^{k} \alpha_n p_n \quad \text{with } \alpha_0, \dots, \alpha_k \geq 0.$$

Proof Consider weight function

$$w_j(t) = \prod_{i=0}^{j-1} (\tau_{n-i} - t)\, w(t), \quad 0 \leq j \leq n$$

Let $q_{j,i}$ be the monic orthogonal polynomial of deg i for w_j. ($q_{0,i} = p_i$, p_i orth. for w).

We have

$$q_{j,n-j}(t) = (t - \tau_1) \cdots (t - \tau_{n-j})$$

because for a polynomial q with $\deg q < n-j$

$$\int_a^b q(t)\, q_{j,n-j}(t)\, w_j(t)\, dt$$
$$= \int_a^b q(t)\, (t-\tau_1) \cdots (t - \tau_{n-j})\, (t - \tau_{n-j+1}) \cdots (t - \tau_n)\, w(t)\, dt =$$

$$= \int_a^b q(t)\,(p_n + \alpha p_{n-1})(t)\, w(t)\, dt$$

$$= 0.$$

So, for $i < n-j$, the largest root of $q_{j,i}$ is less than τ_{n-j} (by interlacing).

For $i \leq n-j$, the largest root of $q_{j-1,i}$ is less than τ_{n-j+1}, so $q_{j-1,i}(\tau_{n-j+1}) \neq 0$.

Hence for $i \leq n-j$ there are constants $\alpha_{j,i}$ so that

$$q_{j,i}(t) = \frac{q_{j-1,i+1}(t) + \alpha_{j,i}\, q_{j-1,i}(t)}{t - \tau_{n-j+1}}$$

because for $\alpha_{j,i}$ chosen so that

$$q_{j-1,i+1}(\tau_{n-j+1}) + \alpha_{j,i}\, q_{j-1,i}(\tau_{n-j+1}) = 0$$

we have for every polynomial q with $\deg(q) \leq i-1$

$$\int_a^b q \, \frac{q_{j-1,i+1}(t) + \alpha_{ji}\, q_{j-1,i}(t)}{t - \tau_{n-j+1}} \, w_j(t)\, dt$$

$$= \int_a^b q \, \left(q_{j-1,i+1}(t) + \alpha_{ji}\, q_{j-1,i}(t) \right) w_{j-1}(t)\, dt$$

$$= 0$$

Now the theorem follows from the next lemma applied to $q_{k,n-k}$.

<u>Lemma</u> (Lemma 3.8 in Cohn-Kumar paper)

For $1 \leq j \leq n$ and $i \leq n-j$ the polynomial q_{ji} is a positive linear combination of $q_{j-1,0}, \ldots, q_{j-1,i}$.

<u>Proof.</u> $\rightarrow$ Exercise. $\boxtimes$

Choosing h for the LP bound

Let $f : (0,4] \to \mathbb{R}$ be completely monotonic.

Define $a(t) = f(2-2t)$ $\left(\text{because } \|x-y\|^2 = 2 - 2x\cdot y \right)$

Function a is absolutely monotonic on $[-1,1)$.

Three inputs to construct h:

$n \in \mathbb{N}$ (for S^{n-1})

$m \in \mathbb{N}$, $m \geq 1$

$\alpha \in \mathbb{R}$, $\alpha \geq 0$.

Let $t_1 < \dots < t_m$ be the roots of

$P_m^n + \alpha P_{m-1}^n$. We require $t_1 \geq -1$ and then

$\{t_1, \dots, t_m\} \subseteq [-1,+1)$. $\left(\text{Szegö: } \alpha \leq \dfrac{-P_m^n(-1)}{P_{m-1}^n(-1)} \right)$

Let h be the Hermite interpolating polynomial of a of order 2 at each t_i:

$h(t_i) = a(t_i)$ and $h'(t_i) = a'(t_i)$ for $1 \leq i \leq m$.

<u>Lemma</u> $h(t) \leq a(t)$ for all $t \in [-1,1)$.

<u>Proof</u> By the remainder formula (page 19) there is z with

$$\min\{t, t_1, \ldots, t_m\} < z < \max\{t, t_1, \ldots, t_m\}$$

and

$$a(t) - h(t) = \underbrace{\frac{a^{(2m)}(z)}{(2m)!} (t-t_1)^2 \cdots (t-t_m)^2}_{\geq 0}.$$

$\Longrightarrow \quad a(t) \geq h(t).$ $\boxtimes$

Define

$$F(t) = P_m^n(t) + \alpha P_{m-1}^n(t) = \prod_{i=1}^{m} (t-t_i)$$

Then, $h = H(a, F^2)$.

<u>Def.</u> A nonconstant polynomial with all its roots in $[-1,1)$ is called <u>conductive</u> if for every absolutely monotonic function a on $[-1,1)$

$H(a,g)$ lies in the convex cone spanned by P_m^k, $m = 0, 1, \dots$ ($H(a,g)$ positive definite)

g is strictly conductive if it is conductive and for all strictly absolutely monotonic a,

$$H(a,g) = \sum_{m=0}^{\deg g - 1} \alpha_m P_m^k \quad \text{with } \alpha_m > 0.$$

($H(a,g)$ positive definite of degree $\deg g - 1$)

Lemma (a) g_1, g_2 conductive, g_1 positive definite, then $g_1 g_2$ conductive.

(b) g_1 conductive and strictly positive definite and g_2 strictly conductive, then $g_1 g_2$ strictly conductive.

Proof (of a)

$$H(a, g_1 g_2) = \underbrace{H(a, g_1)}_{\text{pos. def}} + \underbrace{g_1}_{\text{po. df.}} \overbrace{H(\underbrace{Q(a, g_1)}_{\substack{\text{absolutely (Prop.}\\ \text{monotonic } 2.2)}}, g_2)}^{\text{po. df.}}$$

(see proof of Proposition 2.2)

Known: The cone of positive definite functions is closed under taking (pointwise) product.

($\leadsto$ Schur-Hadamard product for matrices).

Proof of (b): similar. $\boxtimes$

<u>Lemma</u> $H(a, F^2)$ is conductive

<u>Proof</u>. For $r \in [-1, 1)$, let

$$\ell_r(t) = t - r.$$

We have $H(a, \ell_r) = a(r) \geq 0$, so ℓ_r is conductive (and strictly conductive if $r \neq -1$).

By the previous lemma: g conductive and positive definite

$\Rightarrow g\ell_r$ conductive.

Consider $\prod_{i=1}^{j} (t - t_i)$ for $j \leq m$.

By the * Theorem (p. 31) the product for $j < m$. is positive semidefinite (even strictly). For $j = m$ the product is positive definite because $\alpha \geq 0$. Hence, by the previous lemma, each product is conductive. Hence, F^2 is conductive by the previous lemma. $\boxtimes$

<u>Corollary</u> $h = H(a, F^2)$ is positive definite.

Proof of main theorem

Let $f:(0,4]\to\mathbb{R}$ be completely monotonic, $a(t)=f(2-2t)$ absolutely monotonic, let $\mathcal{C}\subseteq S^{n-1}$ be a sharp configuration with $N=|\mathcal{C}|$. Let

$$-1\le t_1<\dots<t_m<1$$

be the inner products between distinct points in $\mathcal{C}$.

Let $h(t)$ be the Hermite interpolating polynomial that agrees with $a(t)$ to order 2.

- We already proved that $h(t)\le a(t)$ for $t\in[-1,1)$ (Lemma on page 35).

- Write $h(t)=\sum_{k=0}^{d}\alpha_k P_k^n(t)$, with $d=\deg h$.

We have $d=2m-1$. Now all inequalities in the proof of the linear programming bound are equalities in this case since $h(t_i) = a(t_i)$

and since

$$\sum_{x,y \in \mathcal{C}} P_k^n(x \cdot y) = 0 \quad \text{for all} \quad 0 < k \leq 2m-1$$

because $\mathcal{C}$ is a spherical $(2m-1)$-design.

Hence, $\mathcal{E}_f(\mathcal{C}) = N^2 \alpha_0 - N h(1)$

under the condition $\alpha_0, \dots, \alpha_{2m-1} \geq 0$.

- h is positive definite.

Define $F(t) = \prod_{i=1}^{m} (t - t_i)$. Then $h = H(a, F^2)$.

<u>Claim</u> F^2 is conductive.

<u>Lemma</u> F is strictly positive definite.

<u>Proof</u> Set $F(t) = \sum_{k=0}^{m} \beta_k P_k^n(t)$. Then $\beta_m > 0$.

For $0 \leq k < m$ consider

$$\int_{S^{m-1}} F(x\cdot y)\, P_k^n(x\cdot y)\, d\omega(x) = \underbrace{c_k}_{>0} \cdot \beta_k .$$

for $y \in S^{m-1}$. Choose $y \in \mathcal{C}$. We have $\deg(F) + k \le 2\deg(F) - 1$. Because $\mathcal{C}$ is a spherical $(2\deg(F)-1)$-design, it follows that the integral is a positive constant times

$$\sum_{x \in \mathcal{C}} F(x\cdot y)\, P_k^n(x\cdot y).$$

By the definition of $\mathcal{C}$:

$$\sum_{x \in \mathcal{C}} F(x\cdot y)\, P_k^n(x\cdot y) = F(1)\, P_k^n(1) > 0.$$

$\boxtimes$

Let $p_0, p_1, \dots$ be the monic orthogonal polynomials for the weight function $w(t) = (1-t)(1-t^2)^{\frac{n-3}{2}}$. One can show that these polynomials lie in the convex cone generated by $P_0^n, P_1^n, \dots$

Lemma $\exists \alpha : F = p_m + \alpha p_{m-1}$

Proof To show

$$(*) \quad \int_{-1}^{1} (1-t) F(t)\, q(t)\, (1-t^2)^{\frac{n-3}{2}}\, dt = 0$$

for all polynomials q with $\deg q \leq m-2$.

Because $\mathcal{C}$ is a spherical $(2m-1)$-design,

the integral $(*)$ equals a positive linear combination

of

$$(1-t_1) F(t_1) p(t_1), \ldots, (1-t_m) F(t_m) p(t_m),$$

and $(1-1) F(1) p(1)$.

Thus, $(*) = 0$. $\boxtimes$

This lemma combined with the Theorem on page 31 shows that $\prod_{i=1}^{j} (t-t_i)$ for $j < m$ is positive definite. The case $j = m$ is the fact that F is positive definite.

Now the proof that F and F^2 are conductive follows as in the previous paragraph "on choosing h for the LP bound". $\boxtimes$

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