Real varieties of spherical designs

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Outline

Notation

- k — either $\mathbb{R}$ or $\mathbb{C}$
- $\Omega_d(k)$ — unit sphere in k^d
- $\mathrm{Hom}_t(k^d)$ — homogeneous polynomials of degree t in k^d
- $\mathrm{Hom}_{t,t}(k^d)$ — homogeneous polynomials over k of degree t in d variables and of degree t in the conjugates of the variables, more precisely

$$\mathrm{Hom}_{t,t}(k^d) = \mathrm{span}_k\{z^\alpha \bar{z}^\beta : z = z_1 \cdots z_n, |\alpha| = |\beta| = t\}$$

(where we used multinomial notation).

Examples of spherical designs

Spherical t-designs

Let $t \in \mathbb{N}$. A **spherical half-design** of order t in $\mathbb{R}^d$ is a set $X \subseteq \Omega_d(\mathbb{R})$ of n vectors such that

$$\forall_{f \in \mathrm{Hom}_t(\mathbb{R}^d)} \qquad \int_{\Omega_d(\mathbb{R})} f \, d\omega = \frac{1}{n} \sum_{x \in X} f(x)$$

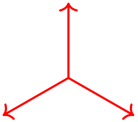
(where $d\omega$ is the normalised surface measure on the sphere).
A finite set $X \subseteq \Omega_d(\mathbb{R})$ is a **spherical t-design** if it is a spherical half-design of order s for all $s \leq t$.

Spherical t-designs

Theorem (Seymour-Zaslavsky, 1984)

For all t and all d, there exists some n such that there is a spherical t-design of n vectors in $\mathbb{R}^d$.

Examples of spherical t-designs

- The **Mercedez-Benz frame** is a 2-design in $\mathbb{R}^2$: 
- More generally, for any t the vertices of the regular $(t+1)$-gon are a t-design in $\mathbb{R}^2$.
- The vertices of the icosahedron are a 5-design in $\mathbb{R}^3$.

General framework for t-design-like objects

Theorem (Waldron, 2016)

Let $X = \{x_1, ..., x_n\} \subseteq k^d$ be a set of n distinct vectors, not all zero. Then

$$\sum_{i=1}^{n} \sum_{j=1}^{n} | \left\langle x_i \middle| x_j \right\rangle |^{2t} \geq c_{t,d}(k) \left(\sum_{i=1}^{n} \|x_i\|^{2t} \right)^2$$

(where $c_{t,d}(k)$ is some fixed known constant) and equality holds iff

$$\forall_{f \in \mathrm{Hom}_{t,t}(k^d)} \qquad \int_{\Omega_d(k)} f \, d\omega = \frac{1}{\sum_{i=1}^{n} \|x_i\|^{2t}} \sum_{x \in X} f(x).$$

A set where equality holds in the above is a **spherical** (t, t)**-design** of n vectors in k^d.

General framework for t-design-like objects

Theorem (Waldron, 2016)

Let $X = \{x_1, \ldots, x_n\} \subseteq k^d$ be a set of n distinct vectors, not all zero. Then

$$\sum_{i=1}^{n} \sum_{j=1}^{n} |\langle x_i, x_j \rangle|^{2t} \geq c_{t,d}(k) \left(\sum_{i=1}^{n} \|x_i\|^{2t} \right)^2$$

and equality holds iff

$$\forall_{f \in \mathrm{Hom}_{t,t}(k^d)} \qquad \int_{\Omega_d(k)} f \, d\omega = \frac{1}{\sum_{i=1}^{n} \|x_i\|^{2t}} \sum_{x \in X} f(x).$$

Since conjugation in $\mathbb{R}$ is trivial, the unit norm spherical (t,t)-designs for $\mathbb{R}^d$ are precisely the spherical half-designs of order $2t$ (compare the expressions in red above with the definition of a spherical half-design.)

Spherical (t,t)-designs

Every spherical (t,t)-design is a (s,s)-design for $s \leq t$. For fixed d,t there is always some n (in general large) such that there is a spherical (t,t)-design of n vectors for $\mathbb{R}^d$.

Of interest is the construction of designs of *minimal* n for fixed d,t.

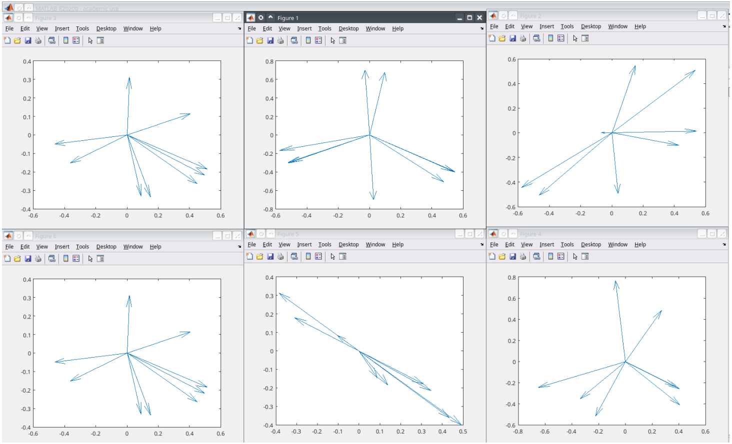
Some examples of designs in $\mathbb{R}$, constructed by Bramwell (2011), Hughes and Waldron (2018), and Mohammadpour and Waldron (2019):

- A spherical $(2,2)$-design of 16 vectors in $\mathbb{R}^5$: the union of
  - six equiangular vectors at an angle of $1/5$, of length $\sqrt[4]{20/21}$;
  - ten equiangular vectors at an angle of $1/3$, of length $\sqrt[4]{36/35}$

  where the angle between vectors of different families is $1/\sqrt{5}$.
- A $(3,3)$-design of 27 equal norm vectors of unknown structure (found numerically).
- A $(9,9)$-design of 32 vectors for $\mathbb{C}^2$, found as a union of orbits of a complex reflection group.
- A 19-design of 720 vectors for $\mathbb{R}^4$, found as a union of orbits of a real reflection group (obtained from a 360 vector $(9,9)$-design)

Union of four Mercedez-Benz frames

Every equal-norm $(2,2)$-design of 12 vectors in $\mathbb{R}^4$ is constructed as a union of four Mercedez-Benz frames.



(Here we project down to a plane by projecting orthogonally down the space spanned by $\dim \mathbb{R}^4 - 2 = 2$ vectors.)

The numerical search

We carried out a numerical search for minimal real spherical (t,t)-designs using the Manopt software package for optimisation over a manifold, searching for global minima of the polynomial

$$f_{t,d,n}(V) = \sum_{i=1}^{n}\sum_{j=1}^{n} |\langle v_i, v_j\rangle|^{2t} - c_{t,d}(\mathbb{R})\left(\sum_{i=1}^{n} \|v_i\|^{2t}\right)^2$$

in $d \times n$ real variables.

We refer to the value of $f_{t,d,n}$ on some set V as the **error** of that set; so a spherical (t,t)-design is a set with error 0.

In order to find designs numerically, a good threshold was found to be an error of 10^{-9}.

Minimal spherical (t,t)-designs for $\mathbb{R}^d$ (2018 list)

t	d	n_w	n_e	
1	d	d	d	orthonormal bases
t	2	$t+1$	$t+1$	equiangular lines in $\mathbb{R}^2$
2	3	6	6	equiangular lines in $\mathbb{R}^3$
2	4	11	12	wtd is due to Reznick
2	5	16	20	
2	6	22	24	
2	7	28	28	equiangular lines in $\mathbb{R}^4$
2	8	45	> 45	
3	3	11	16	wtd is due to Reznick
3	4	23	> 23	
3	5	41	> 41	
4	3	16	25	
4	4	43	> 43	
5	3	24	35	

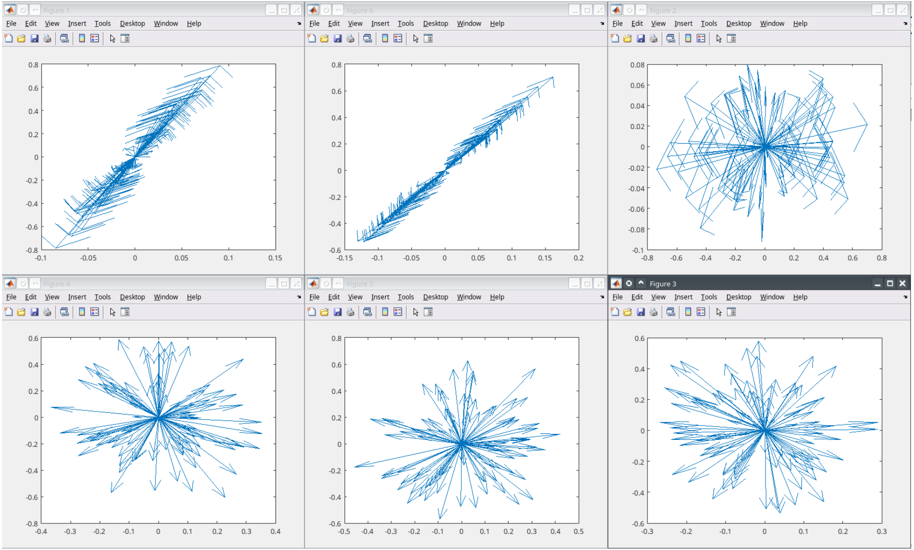
Minimal spherical (t,t)-designs for $\mathbb{R}^d$

t	d	n_w	n_e
1	d	d	d
t	2	$t+1$	$t+1$
2	3	6	6
2	4	11	12
2	5	16	20
2	6	22	24
2	7	28	28
2	8	45	51
2	9	55	67
2	10	76	85
2	11	95	
2	12	120	
3	3	11	16
3	4	23	24
3	5	41	55
3	6	63	96
3	7	99	158
3	8	120	120
3	9	236	
3	10	235	
4	3	16	25
4	4	43	57
4	5	57	126
4	6	53	261
4	7	54	504
4	8	62	
4	9	61	

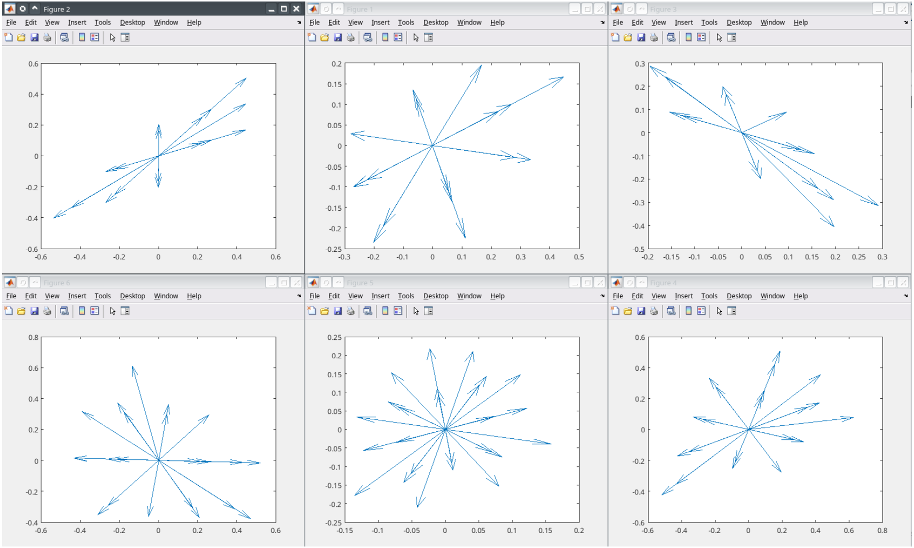
t	d	n_w	n_e
5	3	24	35
5	4	29	60
5	5	29	253
5	6	27	604
5	7	29	
5	8	31	
6	3	32	47
6	4	116	155
6	5	360	458
6	6	18	
6	7	18	
7	3	43	61
7	4	171	229
7	5	11	
7	6	15	
8	3	59	79
8	4	8	
8	5	13	
9	3	6	97
9	4	8	
10	3	11	

For large d, configurations of points of comparatively small size met the error threshold without being designs due to numerical instability. Items in the list coloured green are likely artifacts of this problem.

An equal norm $(3,3)$-design in $\mathbb{R}^6$ of 96 vectors

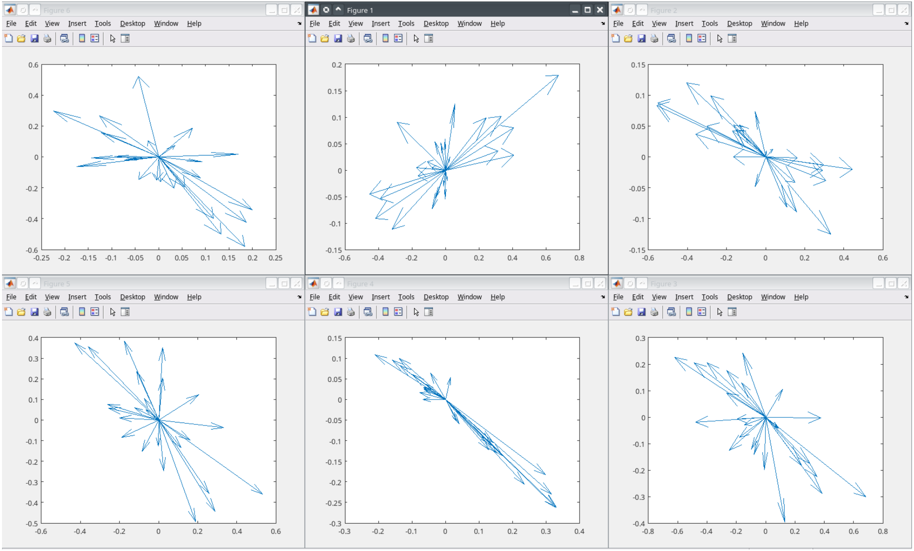


An weighted $(3,3)$-design in $\mathbb{R}^6$ of 63 vectors

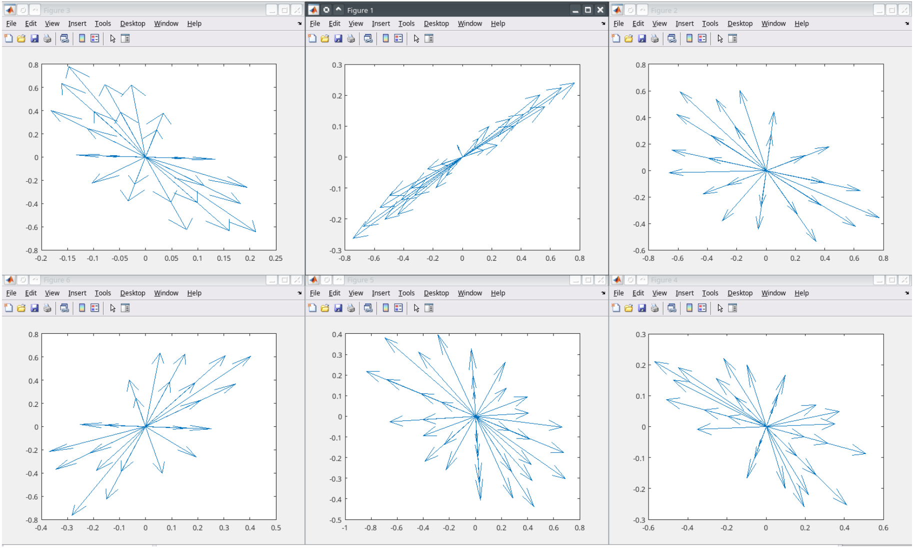


This has been constructed analytically as a union of orbits of two vectors

An weighted $(5,5)$-design in $\mathbb{R}^8$ of 31 vectors



An equal-norm $(5,5)$-design in $\mathbb{R}^4$ of 60 vectors



From Sheppard-Todd group 30

Other remarks on the examples found

- Some of the designs we found are unique up to isometry (e.g. the $(2, 2)$-design of 76 vectors in $\mathbb{R}^{10}$), others come in an infinite family.
- There is a $(3, 3)$-design in $\mathbb{R}^7$ of 91 vectors which has been constructed analytically but which we have not yet been able to find numerically with this method.
- The same method works for complex spherical designs (this is a work in progress), and can very likely be adapted to work for quaternionic and octonionic spherical designs.

The real varieties of spherical designs

Defining the real varieties

Recall that a real spherical design is a nontrivial zero of the following polynomial, where $k_{t,d}$ is some fixed number in $[0,1]$:

$$f_{t,d,n}(V) = \sum_{i=1}^{n}\sum_{j=1}^{n} \left\langle v_i \middle| v_j \right\rangle^{2t} - k_{t,d} \sum_{i=1}^{n}\sum_{j=1}^{n} \langle v_i | v_i \rangle^{t} \left\langle v_j \middle| v_j \right\rangle^{t}$$

We shall denote by $\mathbb{R}\mathscr{W}_{t,d,n}$ the variety of real (t,d,n)-designs: that is, $\mathbb{R}\mathscr{W}_{t,d,n} := \mathbf{Z}(f_{t,d,n}) \setminus \{0\}$.
We shall denote by $\mathbb{C}\mathscr{W}_{t,d,n}$ the *complex* variety associated with $f_{t,d,n}$: that is, $\mathbb{C}\mathscr{W}_{t,d,n} := \mathbf{Z}(f_{t,d,n})(\mathbb{C}) \setminus \{0\}$.
Essentially, there are two questions of interest:

1. For fixed t and d, what is the smallest n such that $\mathbb{R}\mathscr{W}_{t,d,n}$ is nonempty?
2. What is the structure of $\mathbb{R}\mathscr{W}_{t,d,n}$ when it is nonempty?

Newton polytope of $f_{t,d,n}$

It is a philosophy (e.g. due to Khovanskii) that enumerative results on real algebraic systems come from enumerating monomials. One useful object is the Newton polytope of a polynomial (the convex hull of the exponent vectors).

Theorem

Let $\Delta_{d\times n}$ denote the convex hull of the standard basis vectors of $\mathbb{R}^{d\times n}$. Then

$$\operatorname{newt} f_{t,d,n} = 4t\Delta_{d\times n} = \operatorname{conv}\{\pi \in \mathbb{Z}_{\geq 0}^{d\times n} : \pi \textit{ a composition of } 4t\},$$

and

$$|\operatorname{supp} f_{t,d,n}| = \binom{2t+d-1}{2t}\left(\binom{n}{2}+n\right) + \binom{t+d-1}{t}\binom{n}{2}\left(\binom{t+d-1}{t}-1\right).$$

Newton polytope of $f_{t,d,n}$

The count given for the number of terms of $f_{t,d,n}$ implies that $f_{t,d,n}$ is 'sparse' in the sense that as d and n increase for any fixed t, the ratio

$$\mu(t,d,n) \coloneqq \frac{\text{number of terms of } f_{t,d,n}}{\text{number of homogeneous monomials of degree} 4t \text{ in } dn \text{ variables}}$$

tends to zero.

Reducibility

Using the Macaulay2 commutative algebra package, we investigated the factorisation properties of $f_{t,d,n}$.

$$f_{2,2,1} = \frac{5}{8}X_{1,1}^8 + \frac{5}{2}X_{1,1}^6X_{2,1}^2 + \frac{15}{4}X_{1,1}^4X_{2,1}^4 + \frac{5}{2}X_{1,1}^2X_{2,1}^6 + \frac{5}{8}X_{2,1}^8$$

Experimentation suggests the following:

Conjecture

$f_{t,d,n}$ is reducible iff $(t,d,n) \in \{(1,2,1),(1,2,2),(2,2,1)\}$.

It is thus open whether $\mathscr{W}_{t,d,n}$ is reducible, beyond the following:

Theorem (Cahill/Mixon/Strawn, 2017)

When $t = 1$, $\mathbb{C}\mathscr{W}_{t,d,n}$ is always irreducible as a real variety for $n \geq d$, and $\mathbb{R}\mathscr{W}_{t,d,n}$ is irreducible for all $n \geq d+2 \geq 4$ except when $n = 4$ and $d = 2$.

Singular properties

Theorem

$\mathbb{R}\mathscr{W}_{t,d,n} \subseteq \operatorname{Sing} \mathscr{W}_{t,d,n}$.

Questions:

1. What is the structure of the embedding $\mathbb{R}\mathscr{W}_{t,d,n} \hookrightarrow \operatorname{Sing} \mathbb{C}\mathscr{W}_{t,d,n}$?
2. Is $\mathbb{R}\mathscr{W}_{t,d,n}$ always nonsingular as a real variety? What if $\mathbb{R}\mathscr{W}_{t,d,n}$ has some natural deformation structure? Do nonsingular points correspond to 'optimal' or 'degenerate' designs?

(Motivation for the second question: often when we have a continuous family of designs, there is some 'canonical member' of that family.)
In order to study the structure of the variety, we would like to decompose it.

Hilbert's 17th problem

Note that if f is a real polynomial such that $f = g_1^2 + \cdots + g_n^2$, then $f(x) = 0$ iff $g_i(x) = 0$ for all i. Thus decomposing a real variety is equivalent to finding sum-of-squares decompositions of polynomials.
Hilbert's 17th problem: If a polynomial is non-negative, can it be decomposed as a sum of rational squares?

Theorem (Artin, 1927)

Yes.

Strengthened problem: If a polynomial is non-negative, can it be decomposed as a sum of polynomial squares?

Theorem (Hilbert, 1888 (nonconstructive); Motzkin, 1967 (explicit example))

No.

Algorithms

There exists an algorithm for finding a polynomial sum-of-square decomposition of a polynomial, if it exists.
Idea is to reduce the problem to a matrix optimisation problem, specifically a **semidefinite programming problem**.

Case of $f_{t,d,n}$

Since the number of variables is large, computing sum-of-squares decompositions is slow. However, we have the following from the solver implemented in Macaulay2:

t	d	n	num. of squares	design exists
1	2	1	3	no
1	2	2	4	**yes**
1	2	3 to 10	2	yes
1	3	1	6	no
1	3	2	21	no
1	3	3	10	**yes**
1	3	4 to 5	5	yes
1	4	1	10	no
1	4	2	36	no
1	4	3	78	no
1	4	4	18	**yes**
1	5	1	15	no
1	5	2	55	no
1	5	3	120	no
1	6	1	21	no
1	6	2	78	no
1	7	1	28	no
1	7	2	105	no
1	8	1	36	no
1	8	2	crashes	no
1	9	1	45	no

t	d	n	num. of squares	design exists
2	2	1	5	no
2	2	2	35	no
2	2	3	86	**yes**
2	3	1	15	no
2	3	2	126	no
2	4	1	35	no
2	5	1	70	no
2	6	1	126	no
2	7	1	crashes	no
3	2	1	7	no
3	2	2	84	no
3	2	3	crashes	no
3	3	1	28	no
3	3	2	crashes	no
3	4	1	84	no
3	5	1	210	no
3	6	1	crashes	no
4	2	1	9	no
4	2	2	165	no
4	3	1	45	no
5	2	1	11	no

Case of $f_{t,d,n}$

For p a non-negative polynomial, write $\ell(p)$ for the length of the sum of squares representation given by the solver. (If p is not a sum of squares, set $\ell(p) = \infty$.)
Based on the data gathered, we make the following series of conjectures:

Conjecture

1. *The nonnegative polynomial $f_{t,d,n}$ is always a sum of squares.*
2. *For fixed t and d, there exist $N_{t,d}$ and $L_{t,d}$ natural numbers such that*

$$\ell(f_{t,d,n}) = \begin{cases} \binom{2t+nd-1}{2t} & n < N_{t,d} \\ \text{some fixed unknown number} & n = N_{t,d} \\ L_{t,d} & n > N_{t,d}. \end{cases}$$

3. *The integer $N_{t,d}$ is the smallest n such that $\mathbb{R}\mathscr{W}_{t,d,n}$ is nontrivial. (That is, $\ell(f_{t,d,n})$ stabilisers for all n strictly greater than the number of vectors of the smallest known design.)*
4. *We have an inequality*

$$L_{t,d} < \ell(f_{t,d,N_{t,d}}) < \min_{1 \le n < N_{t,d}} \ell(f_{t,d,n}).$$

Case of $f_{t,d,n;c}$

Recall that in the definition of $f_{t,d,n}$ there is a constant $k_{t,d}$ which is fixed. If we allow this constant to vary across $[0,1)$ (so we generalise from the specific case of spherical designs), we have

Conjecture

Consider the polynomials $f_{t,d,n;c}$ defined by replacing $k_{t,d}$ with $c \in [0,1)$ in the definition of $f_{t,d,n}$. Then:

$$\ell(f_{t,d,n;c}) = \begin{cases} \ell(f_{t,d,n}) & n < N_{t,d} \\ \text{some constant independent of } c & n \geq N_{t,d}, c < k_{t,d} \\ \ell(f_{t,d,n}) & n \geq N_{t,d}, c = k_{t,d} \\ \infty & n \geq N_{t,d}, c > k_{t,d}. \end{cases}$$

Case of $f_{t,d,n;c}$

To summarise the conjectures:

	$n < N_{t,d}$	$n = N_{t,d}$	$N_{t,d} > n$
$0 \leq c < K_{t,d}$	$\binom{2t+nd-1}{2t}$	$\binom{2t+nd-1}{2t}$	$\binom{2t+nd-1}{2t}$
$c = K_{t,d}$	$\binom{2t+nd-1}{2t}$	?	$L_{t,d}$
$K_{t,d} < c < 1$	$\binom{2t+nd-1}{2t}$	∞	∞
$c = 1$	$0 \ (n=1)$	$\infty \ (n>1)$	

It is surprising that we can detect existence of spherical designs by considering lengths of sum-of-squares decompositions, independent of the content of those decompositions. More precisely, existence of spherical designs may be detected from linear conditions on the entries of the polynomial $f_{t,d,n}$ together with a condition requiring a specific matrix to be positive semidefinite.

Reznick (1992) proved a result of the same type: namely, he constructed spherical t-designs from even power decompositions of a specific function,

$$h_{n,2s}(x) := (x_1^2 + \cdots + x_n^2)^s = \|x\|^{2s}.$$

This function has a similar, though simpler, form to $f_{t,d,n}$. Still looking for a way to relate the conjectures above to this theory of Reznick.

Possible generalisations

Observe that, since a given (t,t)-design is also a $(t-1,t-1)$ design, the parameter space

$$\varphi_{d,n} : \coprod_{t\in\mathbb{N}} \mathscr{W}_{t,d,n} \to \mathbb{Z}$$

where $\varphi_{d,n}$ is the obvious projection map sending each point of $\mathscr{W}_{t,d,n}$ to t has a cone-like structure.

Possible generalisations

Further, it may be profitable to consider the 'completion' of $\varphi_{d,n}$ given by

$$\varphi_{d,n} : \coprod_{t \in \mathbb{R}} \mathscr{W}_{t,d,n} \to \mathbb{R}$$

where now we define $\mathscr{W}_{t,d,n}$ for arbitrary t to be the zero set of

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \left\langle v_i | v_j \middle| v_i | v_j \right\rangle^{2t} - \left(\int_{x \in \Omega_d} x_1^{2t} \, d\omega \right) \sum_{i=1}^{n} \sum_{j=1}^{n} \langle v_i | v_i | v_i | v_i \rangle^{t} \left\langle v_j | v_j \middle| v_j | v_j \right\rangle^{t}$$

and the integral here generalises the definition of $k_{t,d}$ in the specific case of spherical designs.
(Remark: we consider fibres over $\mathbb{R}$ rather than over $\mathbb{C}$ as the integral is taken only over the real sphere; if we take the same integral over the complex sphere we obtain the variational constant for complex designs rather than real designs.)