Numerical construction of spherical (t,t)-designs

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Summer research scholarship
project report

Department of Mathematics
The University of Auckland
2019–2020

1 Career development statement

This scholarship has furthered my career development in two major ways: firstly, providing some research experience within the mathematics department before I begin my honours project in 2020; and secondly, enabling me to develop industry-relevant skills in software development, mathematical modelling, and analysis of large data sets using standard tools like Python and MATLAB.

2 Summary of research and its significance

A computer search was used to find approximate numerical values for a certain class of mathematical structures known as *spherical* (t,t)*-designs*. This work has importance both in pure mathematics (helping understand this class of structures in the abstract and allowing further development of the theory surrounding them that could have applications to open problems like Zauner's conjecture) and in applied fields like information theory (the topic is relevant to design of codes for information transfer) and quantum mechanics (where particular types of these structures, known as *SICs*, appear in the study of quantum information states).

3 Abstract

Numerical searches for (t,t)-designs of minimal size in each dimension have been carried out before for both weighted and equal-norm designs over $\mathbb{C}$ and $\mathbb{R}$; for example, by Hughes and Waldron [HW18]. The tables of such designs were verified and extended by a new search using the Manopt software package [Bou+14; ABG07], and uniqueness of such designs was checked up to projective unitary equivalence. Some conjectures were made regarding exact analytic forms of some families of designs found.

4 Theoretical preliminaries

4.1 Notation. Throughout, $\mathbb{F}$ will stand for a field which is either $\mathbb{R}$ or $\mathbb{C}$; and the bracket $(\cdot,\cdot)$ will stand for the usual inner product on $\mathbb{F}^d$. We say a function $f : \mathbb{F}^d \to \mathbb{F}$ is a **pseudo-polynomial** if it is a member of the $\mathbb{F}$-algebra given by the symbols $X_1, ..., X_d, \bar{X}_1, ..., \bar{X}_d$ together with the relation forcing $\bar{X}_i$ to be the complex conjugate of X_i upon evaluation. The degree of a pseudo-polynomial is defined in the obvious fashion, and we say a pseudo-polynomial f is (t,t)-**homogeneous** if it is homogeneous of degree t in the X_i and the $\bar{X}_i$ separately; so a (t,t)-homogeneous pseudo-polynomial is of degree $2t$. The set of (t,t)-homogeneous pseudo-polynomials over $\mathbb{F}^d$ will be denoted by $\Pi^\circ_{t,t}(\mathbb{F}^d)$.

For $t, d \in \mathbb{N}$ we set the coefficient $c_t(d, \mathbb{F})$ to be $\binom{d+t-1}{t}^{-1}$ in the case $\mathbb{F} = \mathbb{C}$, and $(1 \cdot 3 \cdot 5 \cdots (2t-1))/(d(d+2) \cdots (d+2(t-1)))$ in the case $\mathbb{F} = \mathbb{R}$.

A 'design' is a set with some additional structure which is 'balanced' in some sense. Many classical designs which arise in combinatorics have the additional structure imposed on subsets and intersections of those subsets and can often be viewed as arising geometrically (see, e.g. [Wal88; CD07]).

A fruitful definition for such a structure on finite subsets of the unit sphere in $\mathbb{F}^d$, was given in the real case in a 1977 paper by Delsarte, Goethals, and Seidel [DGS77]; a modern generalised definition is given here:

4.2 Proposition ([Wal18, theorems 6.5 and 6.7])**.** *If $t \in \mathbb{N}$ and X is a finite n-subset of $\mathbb{F}^d$ with at least one non-zero member, then*

$$\sum_{x,y \in X^2} |(x,y)|^{2t} \geq c_t(d, \mathbb{F}) \left(\sum_{x \in X} \|x\|^{2t} \right)^2 . \tag{1}$$

*For all t and all d there exists a finite set $X \subset \mathbb{F}^d$ containing a non-zero vector such that equality holds. Further, if equality holds for a set X, the set is called a **spherical** (t,t)**-design**, and the following integration rule also holds: for all homogeneous pseudo-polynomials $f \in \Pi^\circ_{t,t}(\mathbb{F}^d)$,*

$$\frac{1}{\sum_{x \in X} \|x\|^{2t}} \sum_{x \in X} f(x) = \frac{1}{\omega_d} \int_{\Omega_d} f(x) \, \mathrm{d}x. \tag{2}$$

where Ω_d is the unit sphere in $\mathbb{F}^d$, and ω_d is the surface area of Ω_d. □

It is clear that designs of small n will be better (since it is clear that as n increases, the sum will better approximate the integral); and that designs of large t will be better (as larger t is a stronger condition on the sets of functions we integrate). We call designs of smallest possible n (for fixed d, t) **minimal designs**.

Interestingly, this definition can be shown to correspond to classical $(t/2)$-designs defined using binary codes, when the integral is replaced with a finite sum and the transformation set $O_d(\mathbb{F})$ is replaced with S_n (the details may be found in the 1977 paper).

We normally view a spherical design as a set of lines together with a numerical weight per line, rather than a set of vectors. The most natural definition of equivalence for designs, then, is projective unitary equivalence: X and Y are said to be equivalent if there is a unitary transformation U that sets up a bijective correspondence between the lines determined by the vectors in X with the lines determined by Y. One can give several invariants to decide whether two designs are equivalent in this way (e.g. the so-called 'm-products', which are computed from the inner products of vectors in a design).

4.3 Examples.

1. Orthonormal bases in $\mathbb{C}$ and $\mathbb{R}$ are $(1,1)$-designs.
2. The lines joining the vertices of a regular $(t+1)$-gon (equivalently, the $(t+1)$th roots of unity) where t is odd form a real equal-norm t-design; it can be shown that such a design is not a $(t+k)$-design for any $k > 1$. The case $t = 2$ is known as the **Mercedez-Benz frame**.
3. The lines joining the vertices of an icosahedron form a 2-design in $\mathbb{R}^3$, of six vectors. More generally, sets of equi-angular lines in all dimensions are designs.
4. A particularly nice $(3,3)$-design can be found of 40 unit vectors in $\mathbb{C}^4$, such that every vector is orthogonal to 12 others and makes an angle of exactly $\arccos(1/\sqrt{3})$ with the other 27.

To elaborate on the third example, Zauner made the following conjecture in 1999 (see the citation and list of numerical evidence given on p.361 of [Wal18]):

4.4 Conjecture. *In $\mathbb{C}^d$, for all d, there is a set of d^2 equiangular lines. (It is known that d^2 is an upper bound on the size of the set of equiangular lines.)*

Such sets are called **SICs**, and arise naturally in the theory of quantum measurements; they are precisely the equal-norm $(2,2)$-designs in $\mathbb{C}^d$ of d^2 vectors.

5 The numerical search

Several tables of minimal designs can be found in the literature — such tables are scattered in various places, see section 6 — but tend to only give minimal designs for small n and d as the computations involved quickly become difficult. For this project, two methods were used to extend these tables and produce numerical examples of the designs. Both methods attempted to find designs by minimising the function

$$\varepsilon(X, \mathbb{F}^d, t) := c_t(d, \mathbb{F}) \sum_{x,y \in X^2} |(x,y)|^{2t} - \left(\sum_{x \in X} \|x\|^{2t} \right)^2 \tag{3}$$

(compare equation 1).

As a first attempt, a MATLAB programme implementing a slight variation of the ‘alternating projections’ algorithm given in [Tro08, §7.2] was used. This was somewhat successful, and was used to verify most of the entries given in the table of complex equi-norm designs given in [Wal18]; however, it was quite slow and was not able to refine numerical designs to sufficient accuracy to find analytic descriptions of them.

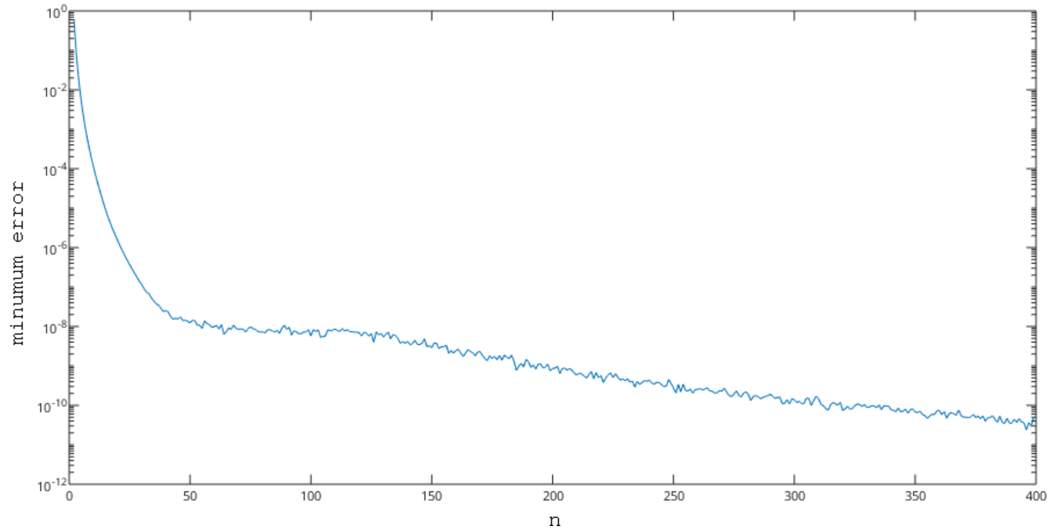

Figure 1: Minimal errors obtained for sets of size n with respect to $\varepsilon(\cdot, \mathbb{R}^5, 3)$.

The more successful implementation used the Manopt software package together with the `trust-regions` optimiser [Bou+14; ABG07]. This method was much faster for larger d, and produced designs of sufficient accuracy to (in some cases) compute the symmetry groups of the numerical example. The threshold for deciding whether a minimal set X of given size n was indeed a design was set at $\varepsilon(X, \mathbb{F}^d, t) < 10^{-9}$; random n-sets of vectors which have the same properties (e.g. unit-norm) tend to produce errors ≥ 1, and so this threshold is sufficiently low to ensure that we do not obtain false positives for minimal designs. However, for some parameters (e.g. $t = 3$ for weighted real designs — the obtained errors for various n in $\mathbb{R}^5$ are displayed in figure 1) this threshold seems to be a little low due to the optimiser having difficulty finding global rather than local minima of ε in these cases; experimentation is still being done in the cases where for low t larger than expected errors are being produced, in order to decide a better method for detecting designs (e.g. by looking at ratios of errors for consecutive n). It should be noted that for most parameters the sizes of minimal designs obtained are of the expected magnitude based on extrapolation from the lists that already exist.

Both implementations may be found on Github [Elz19], and the table of minimal designs that were found may be found in section 6.

Various other scripts, written in MATLAB and Python, were used to analyse the data obtained in an attempt to answer some basic questions:

1. What are the lower bounds on the size of a (t, t)-design? It is known that designs exist for sufficiently large n (proposition 4.2 cited above), and some very loose lower bounds are given in (for example) [DGS77, theorems 5.11 and 5.12], but a tight lower bound is not known.

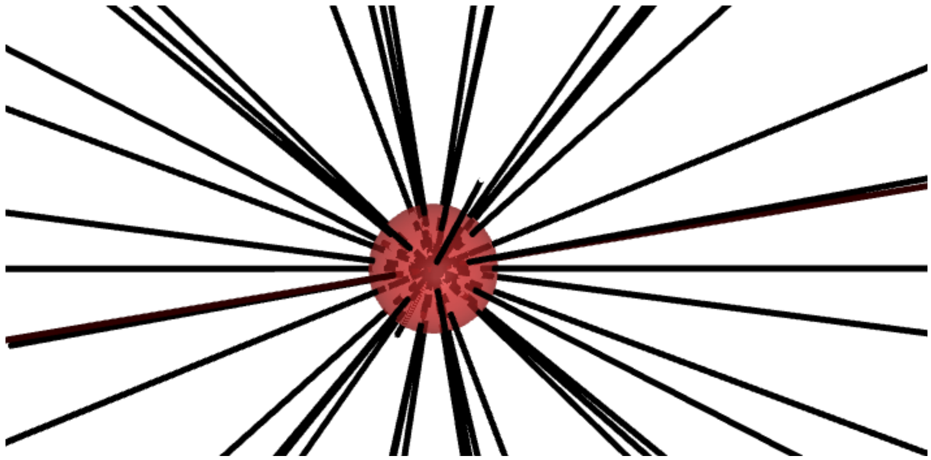

Figure 2: The lines of an equi-norm 24-vector $(4, 4)$-design in $\mathbb{R}^3$.

2. If a design is found with given parameters, is it unique up to unitary transformation?

3. If a design is found with given parameters, does it come from some other structure (e.g. a group action on the sphere, or from a 'classical' combinatorial design)?

This analysis is still on-going; however, some interesting new results have already been found using the numerical designs that were generated during this project.

5.1 Example. There is an uncountable family of $(2, 2)$-designs of 12 vectors in $\mathbb{R}^4$ which can be constructed by taking the four equi-isoclinic planes (planes which pairwise make equal angles with each other) in $\mathbb{R}^4$ and embedding a copy of the Mercedez-Benz frame in each plane. (There is a unique such set of four planes, and no set of five equi-isoclinic planes in $\mathbb{R}^4$ [LS73].)

It seems that a similar structure might appear for higher dimensions — there is a set of 20 vectors in $\mathbb{R}^5$ which appears to have a similar inner-product structure to the 4D design; it is known that there is a unique set of five equi-isoclinic planes in $\mathbb{R}^5$ (see [Et-06]), so it could be that this is obtained by taking five copies of a nice 4-vector set in $\mathbb{R}^2$ and embedding each into a plane in $\mathbb{R}^5$.

There are only a small number of continuous and uncountable families of designs known, so these examples are interesting.

5.2 Example. An equi-norm 24-vector $(4, 4)$-design in $\mathbb{R}^3$ was found (the previous minimal design known was of 25 vectors); in this case the sets of internal inner products seem to have a combinatorial design structure of some sort. The design is pictured in figure 2.

6 Tables of best known minimal designs

The below table lists the minimal known designs of equal-norm designs (n_e) and general (weighted) designs (n_w). Designs in regular type with no annotations are listed in one of [Bra11], [Wal18, §6.16], or [HW18]; those marked with * are listed in [MW19]; and those marked with $^{\dagger n}$ are listed in [CD07, §54] (where the number n is the line of the table; note that the parameters given in the book are based on the classical definition from [DGS77]). Designs in bold type are new or improved: more precisely, they are the sizes of the smallest set of vectors X produced by the computer programmes written for this project for which the corresponding value of $\varepsilon(X, \mathbb{F}^d, t)$ is less than 10^{-9}.

		$\mathbb{R}$		$\mathbb{C}$	
t	d	n_w	n_e	n_w	n_e
1	d	d	d	d	d
t	2	$t+1$	$t+1$		
2	d			d^2	d^2
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^*			
2	10	66^*			
2	11	**97**			
2	16	$256^{\dagger 20}$	$256^{\dagger 20}$		
2	22	$891^{\dagger 3}$	$891^{\dagger 3}$		
2	23	276	276		

		$\mathbb{R}$		$\mathbb{C}$	
t	d	n_w	n_e	n_w	n_e
3	2			6	6
3	3	11	16	21^*	27
3	4	23	**24**	40	40
3	5	41	**55**	45^*	**157**
3	6	63^*	**96**	126	126
3	7	91^*	**158**	**199**	
3	8	120	120	**212**	
3	9	**222**		**220**	
3	10	**229**		**230**	
3	11			**246**	
3	12	$378^{\dagger 30}$	$378^{\dagger 30}$	**254**	
3	23	2300	2300		

		$\mathbb{R}$		$\mathbb{C}$	
t	d	n_w	n_e	n_w	n_e
4	2			10	12
4	3	16	**24**	**43**	**58**
4	4	43	**57**	**48**	**207**
4	5	**54**	**126**	**50**	**617**
4	6	**58**	**261**	**53**	672
4	7	**60**		**54**	
4	8	**58**		**58**	
4	9	**61**		**57**	
4	10			**65**	
4	11			**77**	
4	12			**90**	
5	2			12	12
5	3	24	35	**19**	**113**
5	4	**29**	60	**23**	60
5	5	**30**	**253**	**30**	
5	6	**42**	**42**	**42**	
5	7	**56**		**56**	
5	8	**72**		**72**	
5	9			**90**	
5	10			**110**	
5	11			**132**	
5	24	98280	98280		
6	2			**13**	24
6	3	**16**	**47**	**16**	**198**
6	4	**30**	**154**	**30**	
6	5	**50**	**476**	**50**	
6	6	**77**		**77**	
6	7	**112**		**112**	
6	8			**156**	
6	9			**210**	
6	10			**275**	

		$\mathbb{R}$		$\mathbb{C}$	
t	d	n_w	n_e	n_w	n_e
7	2			**9**	24
7	3	**20**	**61**	**20**	**330**
7	4	**40**	**229**	**40**	
7	5	**70**		**70**	
7	6	**112**		**112**	
7	7			**168**	
7	8			**240**	
7	9			**330**	
8	2			**9**	**40**
8	3	**25**	**79**	**25**	
8	4	**55**		**55**	
8	5	**105**		**105**	
8	6			**182**	
8	7			**294**	
8	8			**450**	
9	2			**8**	**50**
9	3	**30**		**30**	
9	4	**70**		**70**	
9	5			**140**	
9	6			**252**	
9	7			**420**	
10	2			**11**	
10	3	**36**		**36**	
10	4			**91**	
10	5			**196**	
10	6			**378**	
11	2	**12**		**12**	
11	3			**42**	
11	4			**112**	
11	5			**252**	
12	2			**13**	
12	3			**49**	
12	4			**140**	
13	2	**14**	**14**	**14**	
13	3			**56**	
14	2			**15**	

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