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Putatively Optimal Projective Spherical Designs With Little Apparent Symmetry

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ABSTRACT

We give some new explicit examples of putatively optimal projective spherical designs, that is, ones for which there is numerical evidence that they are of minimal size. These form continuous families, and so have little apparent symmetry in general, which requires the introduction of new techniques for their construction. New examples of interest include an 11-point spherical (3, 3)-design for $\mathbb{R}^3$, and a 12-point spherical (2, 2)-design for $\mathbb{R}^4$ given by four Mercedes-Benz frames that lie on equi-isoclinic planes. The latter example shows that the set of optimal spherical designs can be uncountable. We also give results of an extensive numerical study to determine the nature of the real algebraic variety of optimal projective real spherical designs, and in particular when it is a single point (a unique design) or corresponds to an infinite family of designs.

AMS Classification: primary 05B30, 65D30, 65K10, 49Q12, 65H14, secondary 14Q10, 14Q65, 42C15, 94B25

1 | Introduction

Due to a wide range of applications, there is a large body of work on the general problem of constructing points (or lines) on a sphere that are optimally separated in some way. These configurations can be numerical or explicit, with the general hope being that numerical configurations of interest approximate explicit constructions that might be found. Some examples include Hardin and Sloane's list of numerical spherical t-designs [1], the numerical constructions of Weyl–Heisenberg SICs (d^2 equiangular lines in $\mathbb{C}^d$) [2] and exact constructions obtained from them [3], the "Game of Sloanes" optimal packings in complex projective space [4], and minimisers of the p-frame energy on the sphere [5].

Here we consider numerical and explicit constructions of a putatively optimal set of points (or lines) of what are variously called spherical (t, t)-designs for $\mathbb{R}^d$ [6], spherical half-designs [7] and projective t-designs [8]. These are given by a sequence of vectors $v_1, \ldots, v_n \in \mathbb{R}^d$ (not all zero) which give equality in the inequality

$$\sum_{j=1}^{n}\sum_{k=1}^{n}\left|\langle v_j, v_k\rangle\right|^{2t} \geq \frac{1\cdot 3\cdot 5\cdots(2t-1)}{d(d+2)\cdots(d+2(t-1))}\left(\sum_{\ell=1}^{n}\left\|v_\ell\right\|^{2t}\right)^2, \tag{1}$$

where $t = 1, 2, \ldots$. The case where all the vectors have unit length is variously referred to as an equal-norm/unweighted/classical design, and in general as a weighted design. We observe (see [9], [6]) that

- These are projective objects (lines), which are counted up to projective unitary equivalence, that is, for U unitary and c_j unit scalars, we have that (v_j) is a spherical (t, t)-design if and only if $(c_j U v_j)$ is, and these are considered to be equivalent.
- Spherical (t, t)-designs of n vectors in $\mathbb{R}^d$ exist for n sufficiently large, that is, the algebraic variety given by Equation (1) is nonempty for n sufficiently large. Designs for which n is minimal are of interest, and are said to be **optimal**.

- The existence of (optimal) spherical designs can be investigated numerically.

If (v_j) gives equality in Equation (1) up to machine precision, then we will call it a **numerical** design. We say a numerical or explicit design is **putatively optimal** if a numerical search (which finds it) suggests that there is no design with fewer points.

The examples of putatively optimal spherical (t, t)-designs for $\mathbb{R}^d$ found so far (see Table 6.1 of [10]) come from cases where the algebraic variety of spherical (t, t)-designs (up to equivalence) appears to consist of a finite number of points. This can be detected by considering the m-products

$$\delta(v_{j_1}, \ldots, v_{j_m}) := \langle v_{j_1}, v_{j_2}\rangle\langle v_{j_2}, v_{j_3}\rangle\cdots\langle v_{j_m}, v_{j_1}\rangle,\ 1 \le j_1, \ldots, j_m \le n,$$

which determine these vectors up to projective unitary equivalence [11]. From these, it is then possible to conjecture what the symmetry group of the design is [12], and ultimately to construct an explicit (putatively optimal) spherical (t, t)-design as the orbit of a few vectors under the unitary action of the symmetry group (cf. [13], [3]).

In this paper, we consider, for the first time, the case when the algebraic variety of optimal spherical (t, t)-designs appears to be uncountable (of positive dimension). In the examples that we consider, a generic numerical putatively optimal spherical (t, t)-design has a trivial symmetry group. However, there is often some structure, referred to as "*repeated angles*," that is some 2-products

$$\delta(v_j, v_k) = |\langle v_j, v_k\rangle|^2, j \ne k,$$

are repeated. This is just enough structure to tease out an uncountably infinite family of putatively optimal spherical (t, t)-designs, in some examples. In particular, the example of Theorem 4.1 does give a family of optimal spherical $(2, 2)$-designs for $\mathbb{R}^4$.

2 | Numerics

For $V = [v_1, \ldots, v_n] \in \mathbb{R}^{d\times n}$, let $f(V) = f_{t,d,n}(V) \ge 0$ be given by

$$f(V) := \sum_{j=1}^{n}\sum_{k=1}^{n}\left|\langle v_j, v_k\rangle|^{2t} - c_t(\mathbb{R}^d)\left(\sum_{\ell=1}^{n}\left\|v_\ell\right\|^{2t}\right)^2,\ c_t(\mathbb{R}^d) := \prod_{j=0}^{t-1}\frac{2j+1}{d+2j}. \tag{2}$$

We consider the real algebraic variety of spherical (t, t)-designs given by $f(V) = 0$, subject to the (algebraic) constraints

$$\begin{aligned}&\|v_1\|^2 = \cdots = \|v_n\|^2 = 1,\\ &\text{equal-norm/unweighted/classical designs}\\ &\|v_1\|^2 + \cdots + \|v_n\|^2 = n,\\ &\text{weighted designs} \quad (n \text{ chosen for convenience}).\end{aligned}$$

This has been studied in the case $t = 1$, where it gives the *tight frames* [14], [10]. In particular, local minimisers of f for $t = 1$ are global minimisers. It is not known if this is true for $t > 1$, and obviously this has an impact on the numerical search for designs, for example, a local minimiser which was not a global minimiser might be more easily found, leading to a false conclusion that there is no spherical (t, t)-design.

We are primarily interested in the minimal n for which the variety is nonempty (denoted by n_e and n_w, respectively), that is, the optimal spherical (t, t)-designs. We have

$$\binom{t+d-1}{t} = \dim(\mathrm{Hom}(t)) \le n_w \le n_e \le \dim(\mathrm{Hom}(2t)) = \binom{2t+d-1}{2t},$$

(see [10] for details). For d fixed, n_e and n_w are increasing functions of t.

A numerical search was done in [6] using an iterative method that moves in the direction of $-\nabla f(V)$. The results there, and in Table 1 of [5], have been duplicated and extended by using the `manopt` software [15] for optimisation on manifolds and matrices (implemented in Matlab). The putatively optimal numerical designs that we found are summarised in Table 1, and can be downloaded from [16] and viewed at

www.math.auckland.ac.nz/˜waldron/SphericalDesigns

Here are some details about our `manopt` calculations:

- The cost function f of Equation (2) was minimised using the `trustregions` solver.
- This requires the manifold over which the minimisation is done to be specified. We used `obliquefactory` for real equal-norm designs and `euclideanfactory` for real weighted designs, and `obliquecomplexfactory` and `euclideancomplexfactory` for complex designs.
- Since `euclideanfactory(d,n)` is the manifold $\mathbb{R}^{d\times n}$, minimising the homogeneous polynomial f tended to give minima of small norm. To avoid this, we added the term $(\|v_1\|^2 - 1)^2$ to the cost function, so that the weighted designs $V = [v_1, \ldots, v_n]$ obtained have the first vector v_1 of unit norm. For the purpose of calculating errors, V was normalised so that $\|v_1\|^2 + \cdots + \|v_n\|^2 = n$ (as for unit-norm designs).
- The solver requires the gradient and Hessian of f as parameters. The gradient function (page 140, [10]) was given explicitly, and the Hessian was calculated symbolically from f by `trustregion`.
- We used the default solver options, except for the `delta_bar` parameter, where setting `problem.delta_bar` to `problem.M.typicaldist()/10`, rather than the default `problem.M.typicaldist()` gave better results.

TABLE 1 | The minimum numbers n_w and n_e of vectors in a weighted and in a equal-norm spherical (t, t)-design for $\mathbb{R}^d$ (spherical half-design of order $2t$) as calculated numerically.

t	d	n_w	n_e	Remarks on n_w	Remarks on n_e
2	2	3	3	Mercedes-Benz frame	See Example 3.1
2	3	6	6	Equiangular lines in $\mathbb{R}^3$	
2	4	11	12	§6.3[19], [20], infinite family	Infinite family (Theorem 4.1)
2	5	16	20	§6.3 unique, group structure [21]	Infinite family (Example 5.1)
2	6	22	24	§6.3 unique, group structure [21]	Repeated angles (Example 5.2)
2	7	28	28	Equiangular lines in $\mathbb{R}^7$	
2	8	45	51	Infinite family, no structure	Infinite family, no structure
2	9	55	67	Infinite family, no structure	Infinite family, no structure
2	10	76	85	Infinite family, no structure	Infinite family, no structure
2	11	96	106	Infinite family, no structure	Infinite family, no structure
2	12	120	131	Infinite family, no structure	Infinite family, no structure
2	13	146	159	Infinite family, no structure	Infinite family, no structure
2	14	177	190	Infinite family, no structure	Infinite family, no structure
2	15	212	226		Infinite family, no structure
2	16	250	267		Infinite family, no structure
2	17	294	312		Infinite family, no structure
2	18	342	362		
3	2	4	4	Two real mutually unbiased bases	See Example 3.1
3	3	11	16	§6.1 Reznick, no structure	Infinite family, no structure
3	4	23	24	Group structure (Example 5.3)	Infinite family (Example 6.1)
3	5	41	55	Group structure (Example 5.4)	Infinite family, no structure
3	6	63	96	Unique, two orbits (Example 5.5)	Infinite family, no structure
3	7	91	158	Unique, two orbits (Example 5.5)	Infinite family, no structure
3	8	120	120	Unique (Example 6.2)	See Figure 4
3	9	338	380	Infinite family, no structure	Infinite family, no structure
4	2	5	5	Equally spaced lines	See Example 3.1
4	3	16	24	Unique, two orbits (Example 5.5)	Repeated angles (Example 5.6)
4	4	43	57	Infinite family, no structure	Infinite family, no structure
4	5	101	126	Infinite family, no structure	Infinite family, no structure
4	6	217	261		
4	7	433	504		
5	2	6	6	Equally spaced lines	See Example 3.1
5	3	24	35	Infinite family, no structure	Infinite family, no structure
5	4	60	60	Unique, one orbit [6]	See Figure 2 and Example 5.8
5	5	203	253		
5	6	503	604	Infinite family, no structure	
6	3	32	47	Infinite family, no structure	Infinite family, no structure
6	4	116	154	Infinite family, no structure	Infinite family, no structure
6	5	368	458		
7	3	41	61	Unique (Example 5.7)	Infinite family, no structure
7	4	173	229	Infinite family, no structure	
8	3	54	78	Infinite family, some structure	Infinite family, no structure

(Continues)

t	d	n_w	n_e	Remarks on n_w	Remarks on n_e
8	4	249			
9	3	70	97	Infinite family, no structure	
9	4	360		Unique, two orbits (Example 5.5)	
10	3	89	118	Infinite family, no structure	See Example 5.9

Note: The (t, t)-design of $(t+1)$ vectors in R^2 was obtained for all t (not all cases are listed).

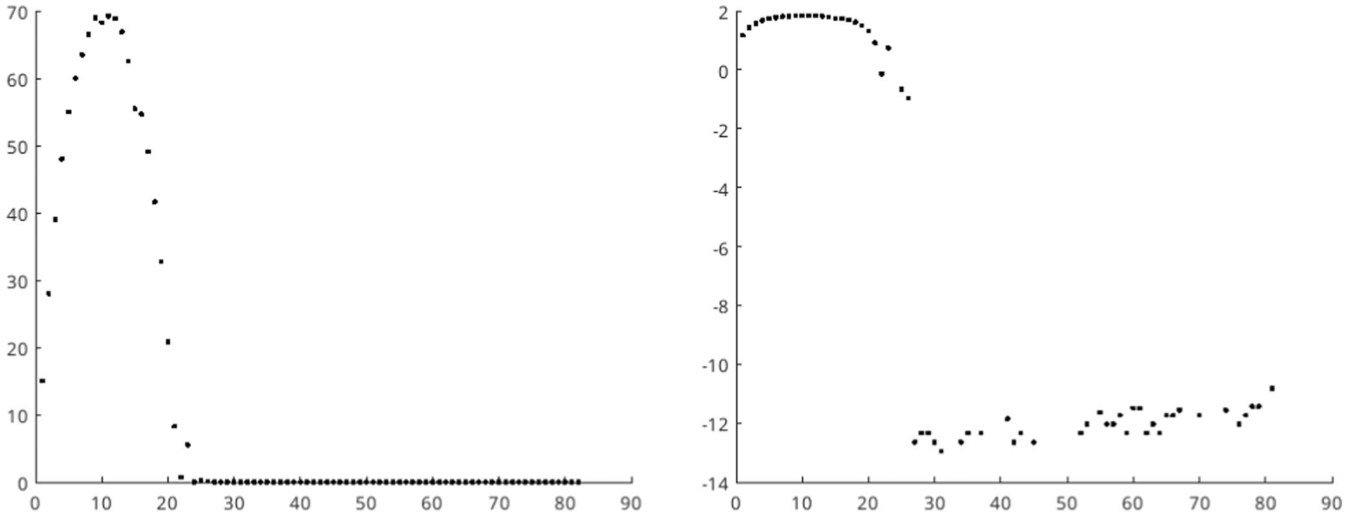

FIGURE 1 | The graphs of $n \mapsto f_{t,d,n}$ and $n \mapsto \log_{10} f_{t,d,,n}$ for $t = 2$, $d = 6$, that is, the error in numerical approximations to a unit-norm spherical (2, 2)-design of n vectors in $\mathbb{R}^6$.

- We considered the absolute error in V being a design, that is,

$$f_{t,d,n} = f_{t,d,n}(V) := \sum_j \sum_k \left| \langle v_j, v_k \rangle|^{2t} - c_t(\mathbb{R}^d) \left(\sum_\ell \left\| v_\ell \right\|^{2t} \right)^2 \right| \geq 0, \quad (3)$$

where $\mathrm{trace}(V^*V) = \|v_1\|^2 + \cdots + \|v_n\|^2 = n$.

See [17] for further details.

We now discuss the heuristics of determining when $f_{t,d,n}(V)$ is (numerically) zero.

3 | The Overall Picture

We use $f_{t,d,n}(V)$ for a numerically computed $V = [v_1, ..., v_n]$ as a proxy for

$$\alpha_{t,d,n} := \min_{\substack{V \in \mathbb{R}^{d \times n} \\ \mathrm{trace}(V^*V) = n}} f_{t,d,n}(V),$$

where the condition $\|v_j\| = 1$ is added for unit-norm designs. It is known that

- For equal-norm designs $n \mapsto \alpha_{t,d,n}$ is zero for some (large) n (see [18]).
- For unweighted designs $n \mapsto \alpha_{t,d,n}$ is decreasing, becoming zero for some (large) n.

Moreover

- For large n (relative to t and d), a random set of n points is close to being a spherical (t, t)-design, and hence has a small error $f_{t,d,n}(V)$.

A priori, these properties suggest that it may be difficult to identify (t, t)-designs, in the sense that the error $n \mapsto f_{t,d,n}(V)$ slowly approaches numerical zero. However, extensive calculations suggest that in the "generic" situation (see Figure 1) this is not the case:

- **Generic situation:** At the point where an optimal (t, t)-design is obtained the error "jumps down" to numerical zero.

There are also "special" situations (see Figures 2 and 4), where (by reasons of symmetry)

- **Special situation:** An equal-norm (t, t)-design with an unexpectedly small number of vectors exists. This design may or may not be obtained by calculating a single numerical design. Here the error jumps to zero, but then returns to roughly the generic situation (nonzero with an eventual jump to numerical zero).

The error graphs for unweighted (t, t)-designs share this "jump" phenomenon (see Figure 3), but are strictly decreasing (becoming constant once zero is obtained). This is because a zero weight

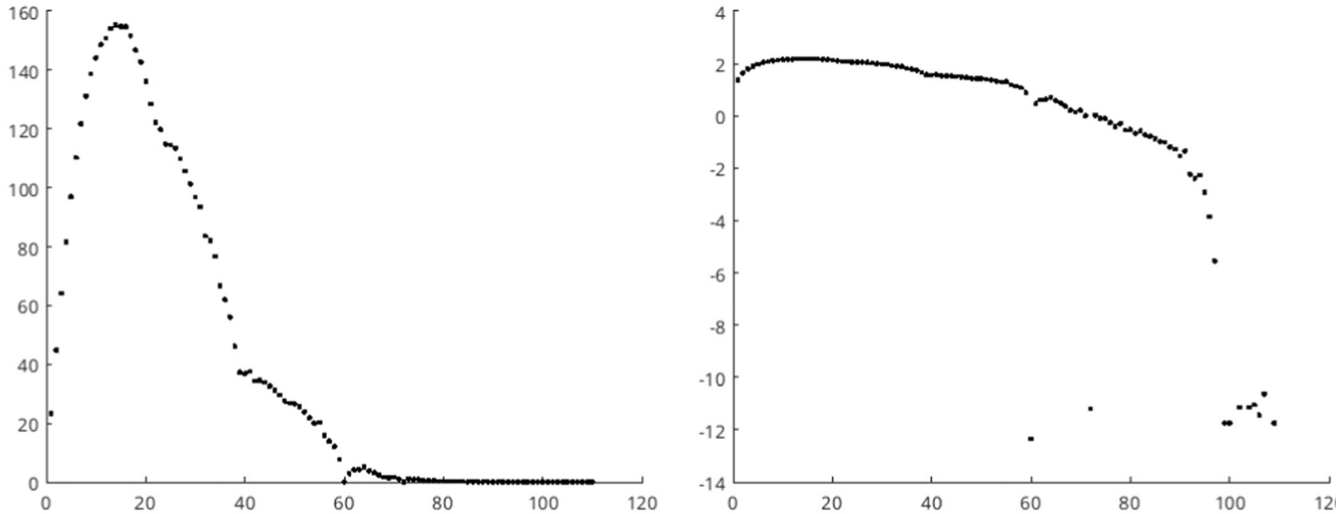

FIGURE 2 | The graphs of $n \mapsto f_{t,d,n}$ and $n \mapsto \log_{10} f_{t,d,,n}$ for $t = 5$, $d = 4$, that is, the error in numerical approximations to a unit-norm spherical $(5, 5)$-design of n vectors in $\mathbb{R}^4$.

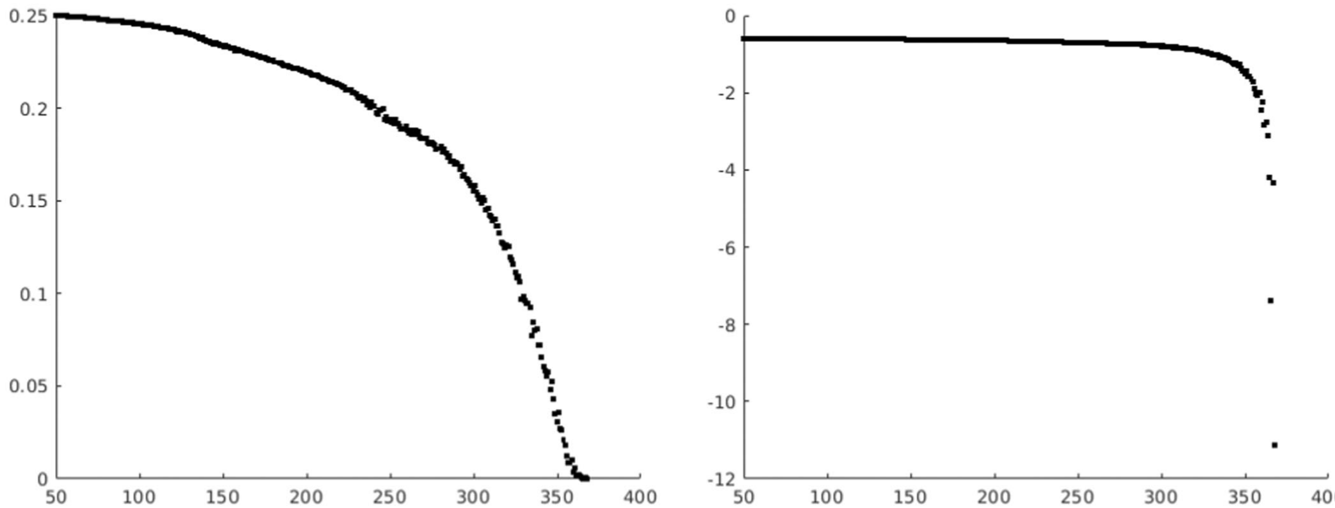

FIGURE 3 | The graphs $n \mapsto f_{t,d,n}$ and $n \mapsto \log_{10} f_{t,d,,n}$ of the error in approximations to weighted designs with $t = 6$ and $d = 5$, that is, $(6, 6)$-designs of n vectors in $\mathbb{R}^5$.

corresponds to a design with one fewer point (and so increasing the number of points enlarges the possible set of designs).

The cost of finding a numerical approximation to a spherical (t, t)-design in $\mathbb{R}^d$ grows with t and d. Therefore (like in previous studies) we could only calculate numerical designs up to a certain point. The previous calculations of [5] and [6] were replicated and extended. These are summarised in Table 1, with comments, for example,

- *structure* means some angles are repeated for equal-norm designs (*repeated angles*), and some norms are repeated for unweighted designs.
- *infinite family* means a different numerical design is obtained each time, and we infer that the algebraic variety of optimal designs has positive dimension.
- *group structure* means that a finite number of numerical designs are obtained, which are a union of orbits of some (symmetry) group.

A set of equal-norm vectors for which the angles $|\langle v_j, v_k\rangle|$, $j \neq k$, are all equal is said to be **equiangular**.

The following example shows that minimising $f_{t,d,n}$ over a larger number of points than for an optimal design can give a unique configuration.

Example 3.1. Minimisation of $f_{t,d,n}$ for $t = 2$ and n equal-norm vectors in $\mathbb{R}^2$ gives

- $n = 3$: the unique optimal configuration of three equiangular lines in $\mathbb{R}^2$, which is known as the Mercedes-Benz frame.
- $n = 4$: a unique configuration of two MUBs (mutually unbiased bases), equivalently, four equally spaced lines.
- $n = 5$: a unique configuration of five equally spaced lines.
- $n = 6$: configurations with six angles of $\frac{1}{2}$ and three other angles (each appearing 3 times), which are seen to be the union of two Mercedes-Benz frames.

The set of $t+1$ equally spaced lines in $\mathbb{R}^2$ is a known optimal spherical (t, t)-design.

We now describe some specific (t, t)-designs that we obtained during our calculations.

4 | A Family of 12-Point Spherical (2, 2)-Designs for $\mathbb{R}^4$

Putatively optimal unit-norm 12-point spherical (2, 2)-designs for $\mathbb{R}^4$ are easily found. These numerical designs appear to have trivial projective symmetry group. However, they all have the feature:

- *Each vector/line makes an angle of $\frac{1}{2}$ with two others,*

that is, each row and column of the Gramian has two entries of modulus $\frac{1}{2}$ (up to machine precision). We now outline how we went from this observation, to an infinite family of explicit putatively optimal designs (Theorem 4.1).

- The vector and the two making an angle $\frac{1}{2}$ with it were seen (numerically) to give three equiangular lines.
- These four sets of three equiangular lines, were seen to be Mercedes-Benz frames, that is, each lies in a 2-dimensional subspace.
- The four associated 2-dimensional subspaces are equi-isoclinic planes in $\mathbb{R}^4$.

Let $V_1, \ldots, V_4 \in \mathbb{R}^{4\times 2}$ have orthonormal columns. Then $P_j := V_j V_j^*$ is the orthogonal projection onto the 2-dimensional subspace of $\mathbb{R}^4$ spanned by the columns of V_j. These four subspaces (planes) are said to be **equi-isoclinic** if

$$P_j P_k P_j = \sigma^2 P_j, j \neq k, \text{ for some } \sigma. \tag{4}$$

There is a unique such configuration [22], [23] (up to a unitary map) given by

$$[V_1, V_2, V_3, V_4] = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{6} & 0 & \sqrt{2} & 0 & \sqrt{2} & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{6} & 0 & \sqrt{2} & 0 & \sqrt{2} & 0 & \sqrt{2} \\ 0 & 0 & -2 & 0 & 1 & -\sqrt{3} & 1 & \sqrt{3} \\ 0 & 0 & 0 & -2 & \sqrt{3} & 1 & -\sqrt{3} & 1 \end{pmatrix}. \tag{5}$$

A **Mercedes-Benz frame** is a set of three equiangular vectors/lines in a 2-dimensional subspace.

Theorem 4.1. *Let (v_j) consist of four Mercedes-Benz frames that lie in four equi-isoclinic planes in $\mathbb{R}^4$. Then (v_j) is a 12-vector spherical (2, 2)-design for $\mathbb{R}^4$.*

Proof. Let $M_j \in \mathbb{R}^{2\times 3}$ give a Mercedes-Benz frame (in $\mathbb{R}^2$), that is, have the form

$$M_j = [u_j, Ru_j, R^2 u_j], R = \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, u_j = \begin{pmatrix} \cos\theta_j \\ \sin\theta_j \end{pmatrix},$$

and $V_j \in \mathbb{R}^{4\times 2}$ be given by Equation (5). Then all such (v_j) are given up to projective unitary equivalence by $V = [V_1 M_1, \ldots, V_4 M_4]$. The variational condition to be such a design is

$$\sum_{j=1}^{12}\sum_{k=1}^{12} |\langle v_j, v_k\rangle|^4 = \frac{1\cdot 3}{4\cdot 6}\left(\sum_{\ell=1}^{12} \|v_\ell\|^4\right)^2 = \frac{1}{8}12^2 = 18, \tag{6}$$

which we now verify by considering the 16 blocks of the Gramian $V^*V = [(V_j M_j)^* V_k M_k]$.

The four diagonal blocks $(V_j M_j)^* V_j M_j = M_j^*\left(V_j^* V_j\right) M_j = M_j^* M_j$ are the Gramian of a Mercedes-Benz frame, and so each contributes $3\cdot 1 + 6\cdot(\frac{1}{2})^4 = \frac{27}{8}$ to the left-hand side of the sum (6). The off-diagonal blocks are all circulant (by a direct calculation)

$$(V_j M_j)^* V_k M_k = \begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix}, a^4 + b^4 + c^4 = \frac{1}{8}.$$

Thus Equation (6) holds as $4\cdot\frac{27}{8} + 12\cdot\frac{3}{8} = 18$. □

Corollary 4.1. *The minimal number of vectors in an equal-norm spherical (2, 2)-design for $\mathbb{R}^4$ is $n_e = 12$, and therefore the corresponding real algebraic variety of such optimal designs is uncountable (of positive dimension).*

Proof. It follows from [20] (Proposition 9.26, with $n = 4$ giving $w(h_{4,4}) = 11$) that the minimal number of vectors in a weighted spherical (2, 2)-design is $n_w = 11$ (the explicit construction is discussed in Section 6.3). Therefore, the minimal number of vectors in an equal-norm design satisfies $n_e \geq n_w = 11$. On the other hand, [24] has used linear programming bounds to prove that $n_e \neq 11$ (Theorem 5.3, with $n = 4$), so that $n_e \geq 12$. The construction of Theorem 4.1, shows that $n_e \leq 12$, and so $n_e = 12$, with the given designs contained within the real algebraic variety of optimal (12-point equal-norm) spherical (2, 2)-designs for $\mathbb{R}^4$. □

Here are some further observations on this example:

- Our calculations suggest this gives the entire variety of optimal designs.
- A simple calculation shows that $|\langle v_j, v_k\rangle|$ can take any value in the interval $[0, \frac{1}{\sqrt{3}}]$.

- The optimal designs $V = V_{\theta_1,\theta_2,\theta_3,\theta_4}$ described in the proof, up to unitary unitary equivalence, are a continuous family (depending on three real parameters).
- A generic design has no projective symmetries.
- There are designs with projective symmetries. In particular, $V_{0,\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2}}$ consists of three real MUBs (mutually unbiased orthonormal bases) for $\mathbb{R}^4$, that is, orthonormal bases for which vectors from different bases make an angle $|\langle v_j, v_k\rangle| = \frac{1}{2}$, and has a projective symmetry group of order 576. These have the nice presentation

$$[B_1, B_2, B_3] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 \end{pmatrix}$$

where Equation (6) holds as $12 \cdot 1 + (12 \cdot 8) \cdot (\frac{1}{2})^4 + (12 \cdot 3) \cdot 0^4 = 18$. This design can also be constructed as a union of one or two orbits of the Shephard-Todd group $G(2, 1, 4)$ (see [21]), the generating vectors being $(1, 1, 0, 0)$ and $(1, 0, 0, 0)$, $\frac{1}{2}(1, 1, 1, 1)$.

5 | Selected Calculations

5.1 | A Family of 24-Point Spherical (4, 4)-Designs for $\mathbb{R}^3$

A set of three equiangular vectors (v_j) is said to be **isogonal** if they span a 3-dimensional subspace, that is, by appropriately multiplying the vectors by ± 1 their Gramian has the form

$$\begin{pmatrix} 1 & a & a \\ a & 1 & a \\ a & a & 1 \end{pmatrix}, -\frac{1}{2} < a < 1.$$

The limiting case $a = -\frac{1}{2}$ gives a Mercedes-Benz frame and $a = 1$ gives three equal lines. These can be viewed as a *lift* of a Mercedes-Benz frame to three dimensions [10].

Putatively optimal 24-point spherical (4, 4)-designs for $\mathbb{R}^3$ are readily calculated, and all appear to have the following structure:

- Each is a union of eight sets of three isogonal lines.
- Each set of isogonal lines is the lift of a Mercedes-Benz frame in a fixed 2-dimensional subspace.
- This suggests an order three rotational symmetry.

We speculate that (up to projective unitary equivalence) every design has the form:

$$V = [v_1, gv_1, g^2v_1, ..., v_8, gv_8, g^2v_8],$$

where

$$g = \begin{pmatrix} 1 & \\ & R \end{pmatrix}, R = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, v_j = \begin{pmatrix} b_j \\ c_j \end{pmatrix}, b_j \in \mathbb{R}, c_j = \begin{pmatrix} y_j \\ z_j \end{pmatrix} \in \mathbb{R}^2.$$

The blocks of the Gramian have the (numerically observed) circulant form

$$[v_k, gv_k, g^2v_k]^*[v_j, gv_j, g^2v_j] = \begin{pmatrix} \langle v_j, v_k\rangle & \langle gv_j, v_k\rangle & \langle g^2v_j, v_k\rangle \\ \langle g^2v_j, v_k\rangle & \langle v_j, v_k\rangle & \langle gv_j, v_k\rangle \\ \langle gv_j, v_k\rangle & \langle g^2v_j, v_k\rangle & \langle v_j, v_k\rangle \end{pmatrix}.$$

In particular, since $|b_j|^2 + \|c_j\|^2 = 1$, the diagonal blocks are given by

$$\begin{pmatrix} 1 & a_j & a_j \\ a_j & 1 & a_j \\ a_j & a_j & 1 \end{pmatrix}, a_j := \langle v_j, gv_j\rangle = b_j^2 + \left(1 - b_j^2\right)\langle \frac{c_j}{\|c_j\|}, R\frac{c_j}{\|c_j\|}\rangle$$
$$= \frac{3}{2}\left(b_j^2 - \frac{1}{3}\right).$$

The definition $f(V) = 0$ for being a design gives a polynomial of degree 16 in the 24 variables b_j, c_j. The condition $|b_j|^2 + \|c_j\|^2 = 1$ allows this to be effectively reduced to 16 variables. We now indicate how the characterisation of a design as a cubature rule allows us to obtain a system of lower degree polynomials.

A unit-norm sequence of n vectors (v_j) in $\mathbb{R}^d$ is a spherical (t, t)-design if and only if it satisfies the cubature rule (see Theorem 6.7 [10])

$$\int_{\mathbb{S}} p \, d\sigma = \frac{1}{n}\sum_{j=1}^{n} p(v_j), \forall\, p \in \mathrm{Hom}(2t), \tag{7}$$

where σ is the normalised surface area measure on the unit sphere $\mathbb{S}$ in $\mathbb{R}^d$. and $\mathrm{Hom}(2t)$ are the homogeneous polynomials $\mathbb{R}^d \to \mathbb{R}$ of degree $2t$. The integral of any monomial $x^\alpha = x_1^{\alpha_1}\cdots x_d^{\alpha_d}$ is zero, unless the power of every coordinate is even, in which case

$$\int_{\mathbb{S}} x^{2\alpha} \, d\sigma(x) = \frac{(\frac{1}{2})_\alpha}{(\frac{d}{2})_{|\alpha|}}, \tag{8}$$

with $(a)_\alpha := \prod_j a_j(a_j+1)\cdots(a_j+\alpha_j-1)$ the Pochammer symbol.

We now consider our design. The cubature rule (7) for $\mathrm{Hom}(8)$ restricted to the sphere $x^2+y^2+z^2=1$, implies that the monomials x^2, x^4, x^6, x^8 are integrated, that is,

$$\frac{1}{8}\sum_j b_j^2 = \frac{1}{3}, \frac{1}{8}\sum_j b_j^4 = \frac{1}{5}, \frac{1}{8}\sum_j b_j^6 = \frac{1}{7}, \frac{1}{8}\sum_j b_j^8 = \frac{1}{9},$$

which implies that

$$\sum_j a_j = \frac{3}{2}\left(\sum_j b_j^2 - \frac{8}{3}\right) = 0, \sum_j a_j^2 = \frac{9}{4}\left(\sum_j b_j^4 - \frac{2}{3}\sum_j b_j^2 + \frac{8}{9}\right)$$
$$= \frac{8}{5}.$$

Since our design has the symmetry group $G = \{I, g, g^2\}$, it is sufficient to check the cubature rule holds for the polynomials $\text{Hom}(8)^G$, which are invariant under this group, that is, the image of Hom(8) under the Reynolds operator R_G given by

$$R_G(f) := \frac{1}{|G|}\sum\nolimits_{g\in G} f^g, f^g := f(g\cdot).$$

By computing the Molien series

$$\begin{aligned}\sum_{g\in G} \frac{1}{\det(I - tg)} &= \sum_{j=0}^{\infty} \dim(\text{Hom}(j)^G) t^j \\ &= 1 + t + 2t^2 + 4t^3 + 5t^4 + 7t^5 + 10t^6 \\ &\quad + 12t^7 + 15t^8 + 19t^9 + \cdots,\end{aligned}$$

we see that $\text{Hom}(8)^G$ has dimension 15 (we are only concerned with its restriction to the sphere, which happens to have the same dimension). We have

$$\text{Hom}(2)^G = \text{spam}\{x^2, y^2 + z^2\},$$

since x^2 (by our choice of b_j) and $x^2 + y^2 + z^2$ (which is 1 on the sphere) are integrated by the cubature rule, so is $\text{Hom}(2)^G$, and hence all of Hom(2). We now consider

$$\text{Hom}(4)^G = \text{spam}\{x^4, (y^2 + z^2)^2, x^2(y^2 + z^2), xy(3z^2 - y^2), xz(3y^2 - z^2)\}.$$

On the sphere $x^2 + y^2 + z^2 = 1$, the first three of the polynomials above can be written as $x^4, (1 - x^2)^2, x^2(1 - x^2)$ and so are integrated by the cubature rule. To integrate the fourth polynomial $xy(3z^2 - y^2)$, which can be written on the sphere as

$$xy(3z^2 - y^2)|_{\mathbb{S}} = xy(3 - 3x^2 - 4y^2),$$

we must have

$$\frac{1}{8}\sum\nolimits_j b_j y_j\left(3 - 3b_j^2 - 4y_j^2\right) = 0.$$

The fifth polynomial on the sphere cannot be written as a polynomial in x, y only, and so we get the condition

$$xz(3y^2 - z^2)|_{\mathbb{S}} = xz(3 - 3x^2 - 4z^2) \Rightarrow \frac{1}{8}\sum\nolimits_j b_j z_j\left(3 - 3b_j^2 - 4z_j^2\right) = 0.$$

Continuing in this way, we obtain the following condition.

Theorem 5.1. *Let*

$$g = \begin{pmatrix} 1 & \\ & R \end{pmatrix}, R = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, v_j = \begin{pmatrix} b_j \\ x_j \\ y_j \end{pmatrix} \in \mathbb{R}^3, b_j^2 + x_j^2 + y_j^2 = 1.$$

Then the orbit of the eight vectors $\{v_1, \ldots, v_8\}$ under the unitary action of the group $G = \{I, g, g^2\}$ is a 24-vector (4, 4)-design for $\mathbb{R}^3$ if and only if

$$\frac{1}{8}\sum\nolimits_j b_j^2 = \frac{1}{3}, \frac{1}{8}\sum\nolimits_j b_j^4 = \frac{1}{5}, \frac{1}{8}\sum\nolimits_j b_j^6 = \frac{1}{7}, \frac{1}{8}\sum\nolimits_j b_j^8 = \frac{1}{9},$$

$$\sum\nolimits_j b_j^{2k-1} y_j\left(3 - 3b_j^2 - 4y_j^2\right) = \sum\nolimits_j b_j^{2k-1} z_j\left(3 - 3b_j^2 - 4z_j^2\right) = 0, k = 1, 2, 3,$$

$$\frac{1}{8}\sum\nolimits_j b_j^2 y_j^2\left(3 - 3b_j^2 - 4y_j^2\right)^2 = \frac{8}{315}, \sum\nolimits_j b_j^{2k} y_j z_j\left(3z_j^2 - y_j^2\right)\left(3y_j^2 - z_j^2\right) = 0, k = 0, 1,$$

$$\sum\nolimits_j\left(y_j^4 - z_j^4\right)\left(y_j^4 - 14y_j^2 z_j^2 + z_j^4\right) = 0.$$

Proof. A basis for the $\text{Hom}(8)^G$ is given by the 15 polynomials

$$x^8, x^6(y^2 + z^2), x^4(y^2 + z^2)^2, x^2(y^2 + z^2)^3, (y^2 + z^2)^4,$$

$$x^5y(3z^2 - y^2), x^3y(3z^2 - y^2)(y^2 + z^2), xy(3z^2 - y^2)(y^2 + z^2)^2,$$

$$x^5z(3y^2 - z^2), x^3z(3y^2 - z^2)(y^2 + z^2), xz(3y^2 - z^2)(y^2 + z^2)^2,$$

$$x^2y^2(3z^2 - y^2)^2, x^2yz(3z^2 - y^2)(3y^2 - z^2), yz(3z^2 - y^2)(3y^2 - z^2)(y^2 + z^2),$$

$$(y^2 - z^2)(y^2 + z^2)(y^2 - 4yz + z^2)(y^2 + 4yz + z^2) = (y^4 - z^4)(y^4 - 14y^2z^2 + z^4).$$

By using $x^2 + y^2 + z^2 = 1$ on the sphere to eliminate variables, and taking appropriate linear combinations to simplify, we obtain the desired equations, for example, the polynomials in the first row restricted to the sphere span the same subspace as $1, x^2, x^4, x^6, x^8$, which gives the condition

$$\frac{1}{8}\sum_j b_j^{2k} = \int_{\mathbb{S}} x^{2k}\, d\sigma(x, y, z) = \frac{1}{2k + 1}, k = 0, 1, 2, 3, 4.$$

We omit the case $k = 0$, since it automatically holds. □

This gives 19 equations (the 11 derived and $b_j^2 + y_j^2 + z_j^2 = 1$) in the 24 variables $b_j, y_j, z_j, 1 \le j \le 8$. We were unable to solve these equations using numerical solvers, however, they are easily seen to hold for the numerical designs we obtained.

5.2 | Spherical (t, t)-Designs With Some Structure

Here is an example where designs with and without structure are commonly generated.

Example 5.1. The equal-norm 20-point (2, 2)-designs in $\mathbb{R}^5$ seem to split into two types:

- No apparent structure (repeated angles).
- Exactly 38 angles, each repeated five times.

Both appear to be continuous families. Further analysis of the numerical designs with repeated angles shows each is a union of four sets of five vectors, which have just two angles (each occurring five times) and projective symmetry group the dihedral group D_5.

Here is an example of the special situation.

Example 5.2. The search for equal-norm 24-point (2, 2)-designs in $\mathbb{R}^6$ returns either

- A set of vectors which is not a design, but does have repeated angles. This might indicate local minima which are not global minima.
- A design with repeated angles, specifically what appears to be $\frac{1}{2}$ (48 times or 32 times) and 0 (12 times or 20 times).

We also note that there are no numerical equal-norm designs with $n = 25, 26$, and the minimiser for 25 vectors appears to be a unique configuration with repeated angles.

Example 5.3. The unweighted 23-vector (3, 3)-designs in $\mathbb{R}^4$ seem to have some group structure: 12 vectors with equal-norms, which have just three angles between them (appearing with multiplicities 30, 30, 6).

Example 5.4. The unweighted 41-vector (3, 3)-designs in $\mathbb{R}^5$ seem to have a unique group structure. Two sets of 16 vectors with equal norms (the same in all examples), four pairs with equal norms, and one vector with a unique norm (the same in all examples). For those with largest norm, the (normalised) angles are 0 (48 times) or $\frac{1}{2}$ (72 times) (a MUB like configuration). The other 16 make angles $\frac{1}{5}$ (80 times) and $\frac{3}{5}$ (40 times).

Example 5.5. A number of spherical (t, t)-designs constructed in [21] as unions of two orbits that give lower order designs appear (from our numerical search) to be optimal. These include (3, 3)-designs of 63 vectors in $\mathbb{R}^6$ (orbits of size 27 and 36), 91 vectors in $\mathbb{R}^7$ (orbits of size 28 and 63), and a (4, 4)-design of 16 vectors in $\mathbb{R}^3$ (orbits of size 6 and 10). There is also a (9, 9)-design of 360 vectors in $\mathbb{R}^4$ (orbits of size 60 and 300). This is always detected in our numerical search, which is costly, and so it is assumed to be unique and optimal.

Example 5.6. The equal-norm 24-vector (4, 4)-designs in $\mathbb{R}^3$ have 92 different angles, each appearing three times. They either involve three or six vectors.

Example 5.7. There appears to be a unique unweighted 41-vector (7, 7)-design in $\mathbb{R}^3$. This appears in roughly half the searches. It consists of eight sets of five lines, each with the dihedral group of order 10 as its projective symmetry group, together with a single line. The sets of five lines present as two-angle frames, and can be viewed as nonunitary images of the unique harmonic frame of five lines in $\mathbb{R}^3$ (the lifted five equally spaced lines in $\mathbb{R}^2$).

We say that subspaces with orthogonal projections P_j and P_k are **equi-isoclinic** with **angle** σ if Equation (4) holds.

Example 5.8. The search for equal-norm (5, 5)-designs for $\mathbb{R}^4$ (see Figure 2) provided two examples of the special situation: a unique putatively optimal design of 60 points, and ones with 72 points. The 72-point designs appear to be part of an infinite family. Each numerical design has projective symmetry group $\mathbb{Z}_6$, and consists of 12 orbits of size 6. These orbits consist of six equally spaced lines in a plane (two-dimensional subspace). The 12 planes in $\mathbb{R}^4$ appear to have a unique geometric configuration: each plane is orthogonal to one other, that is, $\sigma = 0$, and makes the following angles with the other 10

$$\sigma_1^2 = \frac{5+\sqrt{5}}{10} \approx 0.72361 \quad (5 times), \sigma_2^2 = \frac{5-\sqrt{5}}{10} \approx 0.27640 \quad (5 times).$$

Example 5.9. For large values of t, the jump in the generic case can be less pronounced, for example, for (10, 10)-designs $\mathbb{R}^3$. A heuristic explanation for this is that for small angles, the terms $|\langle v_j, v_k\rangle|^{2t}$ are close to numerical zero, for example, for $|\langle v_j, v_k\rangle| \leq \frac{1}{3}$ and $t = 10$, we have

$$|\langle v_j, v_k\rangle|^{2t} \leq (\frac{1}{3})^{20} \approx 10^{-10}.$$

Motivated by our calculations, we will say that an equal-norm spherical (t, t)-design of n points for $\mathbb{R}^d$ is **exceptional** if there exists no (t, t)-design of $n-1$ or $n+1$ points. This is an easily checkable condition that can indicate the existence of interesting designs.

Example 5.10. Of the putatively optimal spherical (2, 2)-designs for $\mathbb{R}^d$ in Table 1, those for $d = 3, 4, 7$ are exceptional. There are exceptional (3, 3)-designs for $d = 4, 8$. The (5, 5)-designs for $\mathbb{R}^4$ of 60 and 72 points (Example 5.8) are exceptional.

6 | Designs From Number Theory and Cubature

We now consider some designs first obtained as algebraic formulas, and a completely new one.

6.1 | The Reznick 11-Point Spherical (3, 3)-Design for $\mathbb{R}^3$

The first putatively optimal design on the list of [6] for which an explicit design was not known is a weighted spherical (3, 3)-design of 11 points for $\mathbb{R}^3$, which was said to have "*no structure.*"

In [5], it is referred to as the *Reznick design*, due to the formula (9.36) of [20]

$$\begin{aligned}540(x^2+y^2+z^2)^3 &= 378x^6+378y^6+280z^6\\ &+(\sqrt{3}x+2z)^6+(\sqrt{3}x-2z)^6\\ &+(\sqrt{3}y+2z)^6+(\sqrt{3}y-2z)^6\\ &+(\sqrt{3}x+\sqrt{3}y+z)^6\\ &+(\sqrt{3}x-\sqrt{3}y+z)^6\\ &+(\sqrt{3}x+\sqrt{3}y-z)^6\\ &+(\sqrt{3}x-\sqrt{3}y-z)^6.\end{aligned} \tag{9}$$

Let us elaborate. The definition $f(V)=0$ for being a spherical (t,t)-design is equivalent to the "Bessel identity" (see Theorem 6.7 [10])

$$c_t(\mathbb{R}^d)\left\|x\right\|^{2t}=\frac{1}{\sum_{\ell=1}^n\|v_\ell\|^{2t}}\sum_{j=1}^n(\langle x,v_j\rangle)^{2t},\ \forall\, x\in\mathbb{R}^d, \tag{10}$$

which allows the *d-ary* $2t$*-ic form* $\|x\|^{2t}=\left(x_1^2+\cdots+x_d^2\right)^t$ to be written as a sum of $n2t$-powers. The converse is also true, that is if there is a constant C with

$$C\left\|x\right\|^{2t}=\sum_{j=1}^n(\langle x,v_j\rangle)^{2t},\ \forall\, x\in\mathbb{R}^d, \tag{11}$$

then integrating over the unit sphere in $\mathbb{R}^d$ using Equation (8) for $\alpha=(t,0,\ldots,0)$ gives

$$\begin{aligned}C&=\sum_{j=1}^n\left\|v_j\right\|^{2t}\int_{\mathbb{S}}(\langle x,\frac{v_j}{\|vj\|}\rangle)^{2t}\,d\sigma(x)=\sum_{j=1}^n\left\|v_j\right\|^{2t}\int_{\mathbb{S}}x_1^{2t}\,d\sigma(x)\\ &=c_t(\mathbb{R}^d)\sum_{j=1}^n\left\|v_j\right\|^{2t},\end{aligned}$$

so that (v_j) is a spherical (t,t)-design. Thus, Equation (9) gives an 11-point spherical (3, 3)-design

$$V=\begin{pmatrix}\sqrt[6]{378} & 0 & 0 & \sqrt{3} & \sqrt{3} & 0 & 0 & \sqrt{3} & \sqrt{3} & \sqrt{3} & \sqrt{3}\\ 0 & \sqrt[6]{378} & 0 & 0 & 0 & \sqrt{3} & \sqrt{3} & \sqrt{3} & -\sqrt{3} & \sqrt{3} & -\sqrt{3}\\ 0 & 0 & \sqrt[6]{280} & 2 & -2 & 2 & -2 & 1 & 1 & -1 & -1\end{pmatrix}.$$

Moreover, Theorem 9.28 of [20] implies that this design is optimal. We make some observations/comments based on our calculations:

- The algebraic variety of (optimal) 11-point weighted spherical (3, 3)-designs for $\mathbb{R}^3$ appears to have infinitely many points.
- A generic numerical design on it has no symmetry properties, with none of the norms $\|v_j\|$ repeated.
- The Reznick design has projective symmetry group of order 2 (exchange the x and y coordinates), and three different norms taken by 1, 2, 8 of the vectors.

6.2 | A New 11-Point (3, 3)-Design for $\mathbb{R}^3$

The search for numerical 11-point (3, 3)-designs for $\mathbb{R}^3$, with the condition that two of the vectors have equal norms, yielded the Reznick design (which appears to be unique) and also, frequently, a design with two sets of five vectors with equal norm. This new design has symmetry group the dihedral group D_5.

The projection of each set of five vectors onto the orthogonal complement of the other single vector gave sets of five equally spaced lines in $\mathbb{R}^2$, exactly the same up to a scalar multiple. Thus we came the conjectured analytic form of such a design:

$$V=\begin{pmatrix}a_1E & a_2E & 0\\ b_1e & -b_2e & -b_3\end{pmatrix},\ E=\left[\begin{pmatrix}\cos(\frac{2\pi}{5}k)\\ \sin(\frac{2\pi}{5}k)\end{pmatrix}\right]_{0\le k\le 4}, \tag{12}$$

$$e=[1]_{0\le k\le 4},$$

where, numerically,

$$a_1\approx 0.972824,\ b_1\approx 0.172322,\ a_2\approx 0.736481,\ b_2\approx 0.692954,\ b_3\approx 1.003311,$$

with the normalisation

$$5\left(a_1^2+b_1^2+a_2^2+b_2^2\right)+b_3^2=11. \tag{13}$$

From this assumed structural form, by substituting into the sum of squares formula (11), we deduce the necessary and sufficient conditions for such a design

$$\begin{aligned}5b_1^6+5b_2^6+b_3^6=\frac{25}{16}\left(a_1^6+a_2^6\right),\ a_1^6+a_2^6&=6\left(a_1^4b_1^2+a_2^4b_2^2\right)\\ &=8\left(a_1^2b_1^4+a_2^2b_2^4\right).\end{aligned}$$

A fourth more complicated equation is given by the variational condition $f_{3,3,11}(V)=0$. In the computer algebra package Maple, we attempted to solve these four equations for four of the variables a_1,a_2,b_1,b_2,b_3, with the other as a parameter. This yields some solutions with complex entries, some which are real but not numerically correct, and some which are numerically correct – often with very complicated formulas. With b_2 as the free parameter, we eventually came to

$$\begin{aligned}\frac{a_1}{b_2}=(3051-297\sqrt{105})^{\frac{1}{6}},\ \frac{a_2}{b_2}&=\frac{3\sqrt{5}-\sqrt{21}}{2}\\ &=\left(\frac{32373-3159\sqrt{105}}{2}\right)^{\frac{1}{6}},\end{aligned}$$

$$\frac{b_1}{b_2}=\left(\frac{135311-13205\sqrt{105}}{64}\right)^{\frac{1}{6}},$$

$$\frac{b_3}{b_2}=\left(\frac{1246875-121625\sqrt{105}}{64}\right)^{\frac{1}{6}}.$$

On putting these ratios with b_2 (presented as sixth roots) into Maple, the variational inequality and the sum of squares formula are seen to hold, with the sums of the 6-th powers of the 11 inner products with (x, y, z) giving

$$\frac{675}{32}(1425 - 139\sqrt{105})b_2^6\,(x^2 + y^2 + z^2)^3.$$

To obtain a neat formula for this design, with $(1425 - 139\sqrt{105})b_2^6$ rational, we choose

$$b_2 = (1425 + 139\sqrt{105})^{\frac{1}{6}}$$

to get

$$a_1 = (12960 + 864\sqrt{105})^{\frac{1}{6}},\ a_2 = (12960 - 864\sqrt{105})^{\frac{1}{6}},$$

$$b_1 = (1425 - 139\sqrt{105})^{\frac{1}{6}},\ b_2 = (1425 + 139\sqrt{105})^{\frac{1}{6}},$$
$$b_3 = 26250^{\frac{1}{6}}.$$

This gives an 11-point $(3, 3)$-design for $\mathbb{R}^3$ of the form (12), which does not satisfy the normalisation (13). The corresponding sum of squares can be written as

$$40500(x^2 + y^2 + z^2)^3 = \sum_{j=0}^{1}\sum_{k=0}^{4}(\alpha_j(c_k x + s_k y) + \beta_j z)^6 + 26250z^6, \tag{14}$$

where $c_k = \cos(\frac{2\pi}{5}k)$, $s_k = \sin(\frac{2\pi}{5}k)$, and

$$\alpha_j = (12960 + (-1)^j 864\sqrt{105})^{\frac{1}{6}},\ \beta_j = (-1)^j (1425 - (-1)^j 139\sqrt{105})^{\frac{1}{6}}.$$

This design and the Reznick design appear to be singular points on the algebraic variety of such designs. It would be interesting to study this variety further, for example, finding nice points on it (those giving designs with large symmetry groups), rational points, or explicitly giving an infinite family of these designs.

6.3 | The Reznick/Stroud Spherical (2, 2)-Designs for $\mathbb{R}^4$, $\mathbb{R}^5$, $\mathbb{R}^6$

The equation (9.27)(i) of [20] is

$$\begin{aligned}192&\left(x_1^2 + x_2^2 + x_3^2 + x_4^2\right)^2\\ &= 6(x_1 + x_2 + x_3 + x_4)^4 + \Sigma^4(3x_1 - x_2 - x_3 - x_4)^4\\ &\quad + \Sigma^6((1 + \sqrt{2})x_1 + (1 + \sqrt{2})x_2 + (1 - \sqrt{2})x_3 + (1 - \sqrt{2})x_4)^4,\end{aligned}$$

where $\Sigma^4(3x_1 - x_2 - x_3 - x_4)^4$ stands for the four terms obtained by making a permutation of the variables x_1, x_2, x_3, x_4 in $(3x_1 - x_2 - x_3 - x_4)$, and so on. Therefore

$$V = \begin{pmatrix} \sqrt[4]{6} & 3 & -1 & -1 & -1 & a & a & a & b & b & b\\ \sqrt[4]{6} & -1 & 3 & -1 & -1 & a & b & b & a & a & b\\ \sqrt[4]{6} & -1 & -1 & 3 & -1 & b & a & b & a & b & a\\ \sqrt[4]{6} & -1 & -1 & -1 & 3 & b & b & a & b & a & a\end{pmatrix},$$
$$a = 1 + \sqrt{2},\ b = 1 - \sqrt{2},$$

is an 11-point spherical $(2, 2)$-design for $\mathbb{R}^4$. This is the first in a family of three optimal spherical $(2, 2)$-designs for $\mathbb{R}^d$, $d = 4, 5, 6$ that can be obtained from Stroud's [19] antipodal cubature rules of degree 5 (five-designs) for the unit sphere, given by

$$C\left(x_1^2 + \cdots + x_d^2\right)^2 = a_1(\Sigma x_j)^4 + \Sigma^d(a_2\Sigma x_j + a_3 x_1)^4 + \Sigma^{\binom{d}{2}}(a_4\Sigma x_j + a_5(x_1 + x_2))^4,$$

$$g = (8 - d)^{\frac{1}{4}},\ a_1 = 8(g^4 - 1)(g^2 \pm \sqrt{2})^4,\ a_2 = 2g^2 \pm 2\sqrt{2},$$

$$a_3 = \mp 2\sqrt{2}g^4 - 8g^2,\ a_4 = 2g,\ a_5 = \mp 2\sqrt{2}g^3 - 8g,\ C = 3a_5^4.$$

The corresponding vectors are

$$V = \left[a_1^{\frac{1}{4}}u, \{a_2 u + a_3 e_j\}_{1\le j\le d}, \{a_4 u + a_5(e_j + e_k)\}_{1\le j<k\le d}\right],$$
$$u = e_1 + \cdots + e_d.$$

Our numerical search shows that for $d = 4$ there is an infinite family of designs, and for $d = 5, 6$ there is a unique design. The unique designs can be obtained as a union of two orbits (sizes 6, 10 and 6, 16 respectively) [21].

6.4 | Kempner's 24-Point Spherical (3, 3)-Design for $\mathbb{R}^4$

With the $\pm$ independent of each other and the previous notation, Kempner (1912) [25] gives

$$120\left(x_1^2 + x_2^2 + x_3^2 + x_4^2\right)^3 = \Sigma^4(2x_1)^6 + 8\Sigma^{12}(x_1 \pm x_2)^6 + \Sigma^8(x_1 \pm x_2 \pm x_3 \pm x_4)^6. \tag{15}$$

The vectors in the corresponding design have equal norms.

Example 6.1. Our search for equal-norm 24-point spherical $(3, 3)$-designs for $\mathbb{R}^4$ gave an infinite family, with repeated angles 0 (60 times), $\frac{1}{\sqrt{2}}$ (32 times) and 21 other angles (each four times). The exact example given by Equation (15) has just three angles 0 (108 times) $\frac{1}{\sqrt{2}}$ (72 times) and $\frac{1}{2}$ (96 times), and is the orbit of three vectors under the natural action of S_4. This design can also be obtained as the orbit of two vectors under the action of the real reflection group $W(F_4)$ (Shephard-Todd number 28) [21].

Interestingly, our search for equal-norm 23-point spherical $(3, 3)$-designs for $\mathbb{R}^4$ seemed to give a unique configuration, with repeated angles.

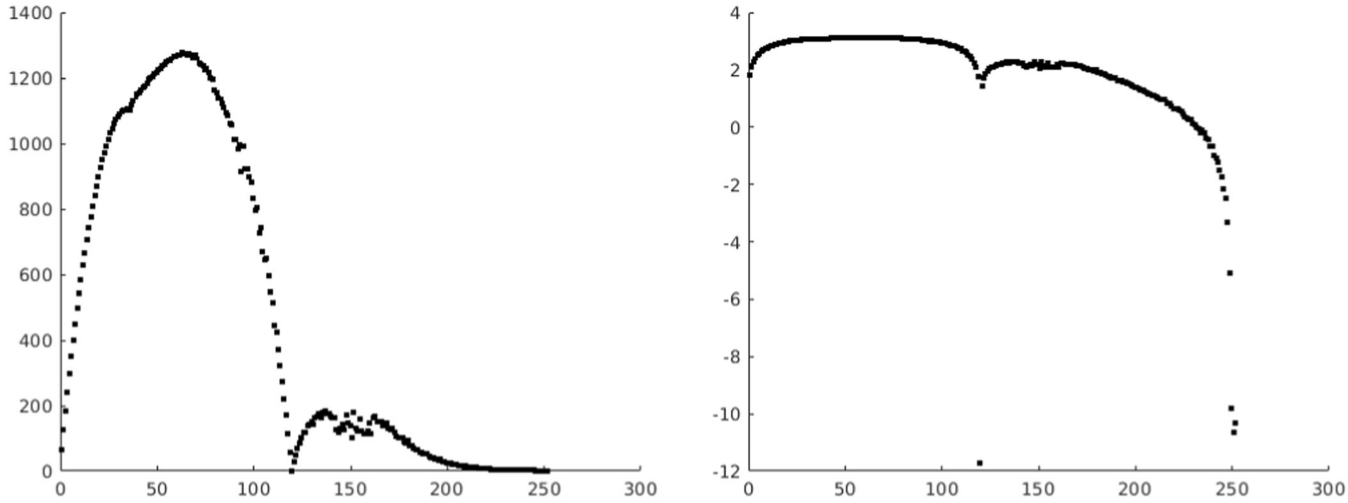

FIGURE 4 | Special situation: the graphs $n \mapsto f_{t,d,n}$ and $n \mapsto \log_{10} f_{t,d,,n}$ for $t = 3$, $d = 8$.

6.5 | Kotelina and Pevnyi's 120-Point (3, 3)-Design for $\mathbb{R}^8$

A similar formula to Equation (15) is given in [7], which leads to what appears to be the unique optimal 120-vector (3, 3)-design for $\mathbb{R}^8$.

Example 6.2. Our numerical search for equal-norm spherical (3, 3)-designs for $\mathbb{R}^8$ gave an optimal design of 120 points, with repeated angles 0 (3780 times) and $\frac{1}{2}$ (3360 times). This is easily recognised to be the design of [7]. This is an example of the special situation, see Figure 4. The next value of n for which there is a design is $n = 250$.

Intuitively, one would expect that for fixed t, the numbers $n_e = n_e(d)$ and $n_w = n_w(d)$ of vectors in optimal equal-norm and weighted (t, t)-designs in $\mathbb{R}^d$ should be increasing functions of d. The above example for $t = 3$ is so exceptional that it provides a counter example (see Table 1), for example,

$$n_e(7) = 158, n_e(8) = 120, n_e(9) = 380.$$

Nevertheless, we expect $d \mapsto n_e(d)$ and $d \mapsto n_w(d)$ to be asymptotically increasing.

7 | Conclusion

We used the `manopt` optimisation software to considerably enlarge the list of putatively optimal spherical (t, t)-designs (see Table 1).

The generic situation seems to be

- The algebraic variety of optimal equal-norm and weighted spherical (t, t)-designs for $\mathbb{R}^d$ has positive dimension. A typical (numerical) element in the variety has little or no structure/symmetry, though there may be such points on the variety. It is characterised by a significant "jump" down in the error $f_{t,d,n}$ to numerical zero from configurations with fewer points.

A highlight is the first full geometric description of the algebraic variety of optimal designs in the generic case of positive dimension (Theorem 4.1). The new 11-point (3, 3)-design for $\mathbb{R}^3$ of § is also of particular interest.

There are also special situations (previously the only explicit examples known) where

- The algebraic variety consists of a single point, or a finite set of points. These designs have a high degree of structure/symmetry, which may lead to explicit constructions (as group orbits).

Some other observations about our methods that may be of future use are:

- The special situation is not always detected by a single calculation (though it might be indicated by the graph of the minimum values obtained), and so could be missed by methods which do only one calculation for a given value of n.
- In the generic situation, the jump value of n is not always detected by one calculation, for example, for unweighted $(t, d, n) = (4, 5, 101), (6, 4, 116)$ and weighted $(2, 9, 45), (6, 4, 154), (8, 3, 78)$. Because of this, we suggest constructing several numerical designs of $n - 1$ points, where n is the presumed jump (optimal value).
- Adaptive methods could be used to find larger numerical designs, for example, instead of calculating $f_{t,d,n}$ for consecutive values of n until numerical zero is found, a bisection method could be used to find the "jump", or an interval in which it lies.
- The methods outlined apply to a wide class of configurations, and could for example be applied to the Game of Sloanes, for which the optimal solutions are strictly speaking not an algebraic variety.

- We came to no firm conclusions about the existence of local minimisers which are not optimal designs (for $t > 1$), when an optimal design exists.

Finally, we mention a couple of interesting connections.

- The idea of decomposing a tight frame (design) as a union of smaller dimensional ones, as was done in Theorem 4.1 (subsets of vectors which form a regular simplex in $\mathbb{R}^2$) is an old idea used to understand and construct them [26].
- Unique minimisers which are not spherical designs may also be of interest, for example, there appears to be a unique set of 16 vectors in $\mathbb{R}^5$ which minimise the potential for spherical $(2, 2)$-designs, which is related to the exact value of the fifth maximal projection constant [27].

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Data Availability Statement

The data that support the findings of this study are openly available in aelzenaar/tightframes at https://github.com/aelzenaar/tightframes.

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