On zonal Stiefel harmonics with applications in discrete geometry

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Proefschrift

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Symmetrie, ob man ihre Bedeutung weit oder eng faßt, ist ***eine*** *Idee, vermöge derer der Mensch durch die Jahrtausende seiner Geschichte versucht hat, Ordnung, Schönheit und Vollkommenheit zu begreifen und zu schaffen.*

— Hermann Weyl, *Symmetrie* (1955)

Contents

Samenvatting

We lossen stappen op van de hiërarchie van Lasserre voor verscheidene topologische stapelingsgrafen. Dit vereiste een aantal nieuwe technieken, en in dit proefschrift richten we ons voornamelijk op de berekening van de zonale Stiefelharmonischen. Eerst ontwikkelen we een harmonisch analytisch raamwerk. Voor het gebruik hiervan moeten de deelruimten van representaties van de orthogonale groep, die invariant zijn onder een deelgroep, bepaald worden. Vervolgens moeten de matrixcoëfficiënten berekend worden voor deze invarianten. Hiervoor geven we twee methoden. Voor het gelijkhoekige-lijnenprobleem met een vaste hoek leidt dit tot nieuwe bovengrenzen. Voor het kusgetalprobleem in dimensie vier wordt een scherpe optimale oplossing verkregen. Via complementariteitsvoorwaarden leidt dit tot het nieuwe resultaat dat het D_4 wortelsysteem de unieke optimale kusconfiguratie in dimensie vier vormt.

Summary

We solve steps of the Lasserre hierarchy for various topological packing graphs. New techniques were necessary to do so and this thesis focuses on the calculation of the zonal Stiefel harmonics. First, we develop an appropriate harmonic analytical framework. To use this, the subspaces of representations of the orthogonal group, which are invariant under a subgroup, have to be determined. Then, the matrix coefficients of these invariants have to be calculated in practice. We give two methods to do so. For the equiangular lines problem with a fixed angle this leads to new bounds. For the kissing number problem in dimension four, a sharp optimal solution is obtained. Via complementary slackness, this leads to the new result that the D_4 root system is the unique optimal kissing configuration in dimension four.

Introduction

Suppose that you have just turned on the dishwasher and you sit down on the couch to watch a cat video on your phone. In this seemingly innocuous situation, two interesting problems occurred. The first one occurred when you loaded the dishwasher. You tried to fit as many things into it as possible, but you also tried to ensure that there was enough space between everything so that it will be cleaned properly. The second one occurred when the video you wanted to watch was retrieved from a server in a data center, where, unbeknownst to you, a bit was flipped due to it being hit by a cosmic ray. Somehow, the video was not distorted.

To a mathematician, these problems are of a similar nature. In both cases, we try to fit as many objects as possible into a given space, while satisfying a separation condition. For instance, when transmitting or storing data, we leave, in an abstract sense, a little room around each data point. This room allows for error-correction. Leave a lot of room and you can correct a lot of errors, but less data can be stored in total and you will need a bigger data center. Don't leave enough room, and you can store loads of data, but you can't correct many errors and the video may get distorted. Similarly, if you put too many plates in your dishwasher, you may be left with a bit of muck. As usual, there is a fruitful collaboration between the real world and Mathematics. Mathematics has contributed to the problem described, but the ideas and experience from that area flow back. This allows one to tackle classical and long-standing problems in discrete geometry.

The problems which are studied in this thesis are of this kind. Firstly, we will study the equiangular lines problem with a fixed angle. For an angle α and dimension n, this asks what the maximum number of lines is in $\mathbb{R}^n$ such that the lines go through the origin and such that the acute angle between any pair of lines is α. The problem then is to write down as many points as possible in projective space, such that the separation condition, having exactly a given angle between the lines, is satisfied.

Secondly, we will study the kissing number problem. A kissing configuration in dimension n is a collection of nonoverlapping, equal-size spheres in $\mathbb{R}^n$ that touch (or "kiss") a central sphere of the same size. We assume the spheres have unit radius, and we identify a kissing configuration with the set C of contact points with the central sphere. Such a set C is a subset of the sphere such that any pair of points in C has an angle of at least $\pi/3$. The kissing number in dimension n is then the maximal size of a kissing configuration. Again, the problem is to write down as many points as possible, this time on the sphere, such that the separation condition, having at least an angle of $\pi/3$ between any two points, is satisfied.

It is useful to phrase these problems as the independent set problem of a graph. For the equiangular lines problem, we consider the graph with vertex set given by real projective space $\mathbb{P}^{n-1}$ and we say that there is an edge between two distinct vertices if the acute angle between the corresponding lines is not equal to α. For the kissing number problem, we consider the graph with vertex set the real sphere $\mathbb{S}^{n-1}$ and we say that there is an edge between two distinct vertices if the angle is smaller than $\pi/3$. We say a subset of a graph is independent if there are no edges between the elements of that subset. The independence number of a graph is the maximal size of an independent set. The independent set problem of a graph is the problem of determining the independence number. We see that both the equiangular lines problem and the kissing number problem then correspond to an independent set problem.

Now that we have phrased it as an independent set problem, we may use ideas from the theory of optimization. Finding the maximum size of an independent set in a finite graph can be written as a binary quadratic optimization problem, which may be tackled using the Lasserre hierarchy, also called the moment/sums of squares hierarchy [**71, 72**]. In our case, the graphs are of a continuous nature, but the approach has been adapted to this setting [**43**]. In summary, the size of an independent set may be bounded by a sequence of conic optimisation programs known as the Lasserre hierarchy. This sequence is indexed by a positive integer t and the calculation of this program for $t = 2$, and occasionally $t = 3$, is the principal goal of this thesis.

We now describe this optimisation program. The graphs we consider are examples of compact topological packing graphs, which is a type of graph endowed with a topology [**43**]. Let X be such a topological packing graph and let t be a positive integer. We then consider the set $\mathcal{I}_t$ of all independent sets of size at most t, which inherits a topology from X. We furthermore denote by $\mathcal{I}_{=t}$ the set of independent subsets with size t exactly. Let $C(X)$ be the space of real-valued continuous functions on a topological space X. Define the operator $A_t\colon C(\mathcal{I}_t \times \mathcal{I}_t)_{\mathrm{sym}} \to C(\mathcal{I}_{2t})$ by assigning to a function $K \in C(\mathcal{I}_t \times \mathcal{I}_t)_{\mathrm{sym}}$ the function $A_t K$, which assigns to $S \in \mathcal{I}_{2t}$ the number

$$A_t K(S) = \sum_{\substack{J_1, J_2 \in \mathcal{I}_t \\ J_1 \cup J_2 = S}} K(J_1, J_2).$$

Here $C(\mathcal{I}_t \times \mathcal{I}_t)_{\mathrm{sym}}$ is the space of continuous real-valued functions $K(J_1, J_2)$ that are symmetric in J_1 and J_2. We define $C(\mathcal{I}_t \times \mathcal{I}_t)_{\succeq 0}$ to be the cone of positive kernels, which is the set of $K \in C(\mathcal{I}_t \times \mathcal{I}_t)_{\mathrm{sym}}$ that satisfy

$$\sum_{i,j=1}^{N} c_i K(J_i, J_j) c_j \geq 0$$

for all $N \geq 0$, $c \in \mathbb{R}^N$, and $J_1, \ldots, J_N \in \mathcal{I}_t$. The Lasserre hierarchy for this problem is:

$$\begin{aligned} &\text{minimize} && K(\emptyset, \emptyset) \\ &\text{subject to} && A_t K(S) \leq -1_{\mathcal{I}_{=1}}(S), \qquad S \in \mathcal{I}_{2t} \setminus \{\emptyset\}, \\ &&& K \in C(\mathcal{I}_t \times \mathcal{I}_t)_{\succeq 0}, \end{aligned} \tag{1}$$

where $1_{\mathcal{I}_{=1}}$ is the indicator function of the set $\mathcal{I}_{=1}$ of independent sets of size 1. Let us verify that this program bounds the independence number. If C is an independent set and K a feasible kernel, then we have

$$0 \leq \sum_{\substack{J_1, J_2 \in \mathcal{I}_t \\ J_1, J_2 \subseteq C}} K(J_1, J_2) = \sum_{\substack{S \in \mathcal{I}_{2t} \\ S \subseteq C}} A_t K(S) \leq K(\emptyset, \emptyset) - |C|,$$

which shows any feasible solution to (1) gives an upper bound on the independence number. Suppose a compact group G acts on X and that this action preserves the edges. For the graphs we considered earlier, this is the natural action of the orthogonal group $\mathrm{O}(n)$. This action induces an action on $\mathcal{I}_t$ and $\mathcal{I}_{2t}$, and hence a linear action on $C(\mathcal{I}_t \times \mathcal{I}_t)$ and $C(\mathcal{I}_{2t})$ by $g \cdot K(J_1, J_2) = K(g^{-1}J_1, g^{-1}J_2)$ and $g \cdot f(S) = f(g^{-1}S)$. We say that a kernel K is G-invariant if $g \cdot K = K$ for all $g \in G$. By compactness of G and the symmetry of the above program, one may restrict without loss of optimality to G-invariant kernels, which results in a significant reduction of the size of the program. We will show how to parametrise the cone of G-invariant positive definite kernels by positive semidefinite matrices. Furthermore, the inequality constraint can be approached with sums of squares. Therefore, one may hope to calculate an approximation to the above program on a computer.

The parametrisation is of a harmonic analytic nature and requires a complete system of the space

$$\mathrm{Hom}_G(\mathcal{I}_t, V_\pi) \tag{2}$$

of continuous G-equivariant maps for every irreducible representation (π, V_π) of G. As mentioned, the group G, in which we are particularly interested, is the orthogonal group $\mathrm{O}(n)$. Let $\mathrm{O}(n-t)$ be the subgroup of $\mathrm{O}(n)$ which stabilises the first t standard basis vectors. We shall see that the parametrisation boils down to describing the space of invariants

$$V_\pi^{\mathrm{O}(n-t)} = \{v \in V_\pi \mid \pi(g)v = v \text{ for all } g \in \mathrm{O}(n-t)\} \tag{3}$$

and calculating the matrix coefficients. Matrix coefficients are defined to be the functions on G of the form $\langle v, \pi(g)w \rangle$ with $v, w \in V_\pi$. The collection of all such functions is loosely referred to as *the* matrix coefficients. Given a subgroup H of G, the matrix coefficients of the form $\langle v, \pi(g)w \rangle$ with $v \in V_\pi$ and $w \in V_\pi^H$ are of particular interest. As we will see in Chapter 1, these are precisely the matrix coefficients which appear in a Fourier series of a function on G/H. If $G = \mathrm{O}(n)$ and $H = \mathrm{O}(n-1)$, then the corresponding quotient $\mathrm{O}(n)/\mathrm{O}(n-1)$ is homeomorphic to the sphere and these matrix coefficients are known as spherical harmonics. For the more general case with $H = \mathrm{O}(n-t)$ with $t \geq 1$, the corresponding quotient $\mathrm{O}(n)/\mathrm{O}(n-t)$ is known as the Stiefel manifold and these matrix coefficients are known as the Stiefel harmonics [**54**]. Via an addition formula, the invariant kernels are described by a special case, namely matrix coefficients $\langle v, \pi(g)w \rangle$ with $w, v \in V_\pi^H$. For the sphere, these functions are known as the zonal spherical harmonics. Therefore, we refer to these functions for the Stiefel manifold as the zonal Stiefel harmonics. Given a basis v_i of the space V_π^H with $1 \leq i \leq \dim V_\pi^H$, we may gather the zonal Stiefel harmonics in a matrix $\langle v_i, \pi(g)v_j \rangle$, to which we will refer as the zonal matrix.

We now give an overview of the structure of this thesis, the main contributions and corresponding papers. Let X be a compact space with a continuous action of a compact group G, and let $C(X \times X)_{\succeq 0}^G$ be the cone of continuous G-invariant positive definite kernels. In Chapter 1, the main contribution is a density result for this cone in terms of a complete system of the space 2 under certain assumptions.

By "method" we shall mean a construction of the space of invariants (3) and an algorithm to compute the zonal Stiefel harmonics. We develop method I in Chapter 2 and method II in Chapter 3. The main contribution in Chapter 2 and method I is to make the construction of the spaces of invariants in expression (3) from a paper by Gross and Kunze [**57**], more concrete, accessible and ready for calculation. The main contribution in Chapter 3 and method II is a new construction of the space of invariants in expression (3) and a new algorithm to calculate the corresponding zonal Stiefel harmonics.

Method I is based on induced representations and it is in the spirit of the Borel-Weil theorem. Method II is based on Weyl's construction. Note that Weil rhymes with 'say' and Weyl with 'vile'. We have decided to use numerals to distinguish the methods.

Two chapters with applications to problems follow, and the context and history of these problems are described extensively in the introductions to the respective chapters. Chapter 4 is based on a paper by De Laat, Machado and the author of this thesis [**41**]. In this chapter, we calculate the above program for the equiangular lines problem with a fixed angle. This leads to new bounds and we give an asymptotic analysis of the bounds in terms of the dimension. Chapter 5 is based on a paper by De Laat, Leijenhorst and the author of this thesis [**40**]. In this chapter, we calculate the second step of the above program for the kissing number problem. In this case, a sharp optimal solution is obtained. Via complementary slackness, this yields a proof that the D_4 root system is the unique optimal kissing configuration in dimension four up to isometry.

Method I predates method II and it is the one originally used in these applications. Furthermore, considerable expense was made in these papers to make method I computationally efficient. We have decided to omit this part from this thesis, because method II deprecates method I for our purposes. It is both faster to calculate and the desired mathematical properties are more readily apparent. To see why it is mathematically simpler, compare the theory in Chapter 2 and the long calculations in [**40**, Section 3] and [**41**] to Chapter 3. To illustrate the speed, we provide an anecdote. Setting up the semidefinite program to be solved in Chapter 5 took two days with method I. With an implementation of method II, it took two hours. When implemented more carefully, this should improve further. Because of the above reasons, Chapters 4 and 5 have been rewritten so that method II is used. Those who are interested in additional techniques to make method I computationally efficient are referred to the corresponding papers.

These two methods to compute the zonal Stiefel harmonics are completely different, but we obtained the same zonal matrices using either method for all the representations up to degree 14. This serves as a mutual verification of the methods and of the semidefinite program with which our main results were proven. More applications of method II are currently under development. In a paper in preparation [**37**], we will study: other spherical coding problems; energy miminisation; and codes on the Stiefel manifold.

This thesis is part of a program of the last decades to apply semidefinite programming methods and symmetry in the area of discrete geometry. We are particularly interested in rotational symmetry and therefore the work of Weyl on classical groups is inescapable. Even with this in mind, his work on the subject features prominently in this thesis multiple times. Firstly, because of the Peter-Weyl theorem, which is the fundamental theorem for the Fourier transform on a compact group. Secondly, because of Weyl's construction of the representations of the classical groups. With the former, invariant positive definite kernels may be described and with the latter the zonal Stiefel harmonics.

CHAPTER 1

Harmonic analysis

In this chapter, we prove Theorem 1.16, in which we describe a dense subcone of the cone $C(X \times X)^G_{\succeq 0}$ of complex-valued, G-invariant, positive definite kernels on a compact space X with an action of a compact group G. We also discuss a real-valued version. This will allow us to parametrise the cone in optimisation program (1). To do so, we introduce a generalised notion of the Fourier transform. We first develop this theory, starting with the case of continuous functions on X. Our contribution is the development of this theory and the density result in Theorem 1.16. In Section 1.4, we also give a new proof of absolute, uniform convergence of the Fourier series in the case of finitely many orbits.

The density result may be summarised as follows. Suppose that for every irreducible representation (π, V_π) of G, we have a complete system for the space of equivariant continuous maps $\mathrm{Hom}_G(X, V_\pi)$. Theorem 1.16 then says that a certain subcone of $C(X \times X)^G_{\succeq 0}$, described in terms of that complete system, is dense.

In the thesis by David de Laat [**38**] a related density result is given. There the concept of a symmetry-adapted system is introduced and a density result is given in terms of symmetry-adapted system. The problem lies in the actual construction of a symmetry-adapted system, and we shed light on this by showing that a complete system of the space of continuous equivariant maps gives rise to a symmetry-adapted system. By approaching it from this angle from the beginning, we bypass the framework of general symmetry-adapted systems altogether. Furthermore, the connection to the classical theory of harmonic analysis on a compact group becomes more apparent. The precise conditions, under which this approach applies, are given in Section 1.1. At the end of the chapter, we discuss applicability and examples.

1.1. Preliminaries

The group action. For a topological space X, we denote by $C(X)$ the space of continuous, complex-valued functions on X and by $C(X, \mathbb{R})$ the space of continuous, real-valued functions on X. For a complex-valued function f, we will denote by $\overline{f}$ its pointwise complex conjugate. We will call a topological space separable if it contains a countable dense subset. We will call a subset of a normed linear space a complete system if it is countable and linearly independent and the span, consisting of finite linear combinations, is dense. One readily verifies that a normed linear space over $\mathbb{C}$ or $\mathbb{R}$ is separable if and only if it has a complete system. We are interested in finding a certain complete system, which is compatible with the group action. We also want to restrict our attention to the case where X is compact and Hausdorff, and we always make this assumption on X. Interestingly, if X is compact and Hausdorff, we then have, by the Riesz's theorem [**105**, Section 12.3], that $C(X)$ is separable if and only if X is metrisable. Therefore, if there is a complete system, it is necessary that X is metrisable. We are interested in finding a complete system with certain extra properties and therefore, we may restrict our attention to the case where X is a compact metric space.

Such a complete system, which is compatible with the group action, is often referred to as a symmetry-adapted system and a theory has been developed for it [**38**]. As mentioned in the introduction, we shall not use this existing framework and build up a theory from the ground. We now give our assumptions to do so. Let $p\colon X \to X/G$ be the canonical projection and let $R\colon X/G \to X$ be a function such that $pR = 1_{X/G}$, i.e. the identity on X/G. That is, choose from each orbit an element. For $t \in X/G$, we denote the stabiliser subgroup of $R(t)$ by $H(t)$. We assume:

(i) that X is a compact metric space with a continuous action of a compact group G;
(ii) that the function R can be chosen to be continuous;
(iii) that for each $t \in X/G$, there is an open neighbourhood U of t such that for all $u \in U$, we have $H(u) \subseteq H(t)$.

Assumption (ii) is nontrivial and there exist topological obstructions. Assumption (iii) is required to make the Stone-Weierstraß argument in Section 1.3 work. These assumptions appear to be related to the notion of a slice in differential geometry [**18**]. Further discussion and examples may be found in Section 1.5. These assumptions have some immediate consequences.

PROPOSITION 1.1. *Assumptions* (i) *and* (ii) *imply that X/G, with the quotient topology, is compact and metrisable.*

PROOF. Assume (i) and (ii). The space X/G is the quotient of a compact space and therefore compact. The map R is a continuous injection from a compact space into a Hausdorff space, and hence R is a homeomorphism onto the image with the subspace topology. Since X is a metric space, the result follows. □

By Riesz's theorem [**105**, Section 12.3], we then have

COROLLARY 1.2. *Assumptions* (i) *and* (ii) *imply that $C(X/G)$ is separable.*

PROPOSITION 1.3. *Assumption* (i) *implies that for each $t \in X/G$, the space $G/H(t)$ is Hausdorff.*

PROOF. Because the action is continuous, the subgroup $H(t)$ is closed for every $t \in X/G$. Hence, by compactness of G, the space $G/H(t)$ is Hausdorff [**45**, Proposition 1.2.1]. □

Measure theory. We will also need to introduce some measure-theoretic notions, for which we follow [**13**]. A measure is defined to be a countably additive nonnegative function on a σ-algebra. The Borel σ-algebra is the σ-algebra generated by the open sets of X. A Borel measure is defined to be a measure on the Borel σ-algebra such that every compact set has finite measure. A probability measure is a measure μ such that $\mu(X) = 1$. We will restrict our attention to probability measures and implicitly assume all measures are probability measures. Therefore, for us, any measure on the Borel σ-algebra is a Borel measure. We say that a measure has full support if for every non-empty open subset U of X, we have $\mu(U) > 0$.

PROPOSITION 1.4. *If X is a compact metric space, then there exists a Borel measure on X with full support.*

Proof. Since X is a compact metric space, it has a countable base [**87**, Exercise 30.4]. Therefore, X is separable [**87**, Theorem 30.3]. Let x_i with $i \in \mathbb{N}$ be countable dense subset and define

$$\mu_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$$

where δ_{x_i} is a Dirac measure centred at x_i. Since X is compact, the space of Borel measures in the weak topology is compact as well [**100**, Theorem II.6.4]. Thus, there exists a subsequential weak limit μ. By density of the x_i, the measure μ has full support. □

We now introduce the norms in which we are interested. For a topological space X, we will often consider the uniform norm on $C(X)$, which is defined by

$$\|f\|_\infty = \sup_{x\in X} |f(x)|.$$

When we speak of uniform convergence, it refers to convergence with respect to this norm. Furthermore, in the presence of a measure, we will consider the inner product on $C(X)$ defined by

$$\langle f, g\rangle = \int_X \overline{f(x)} g(x) dx$$

which depends implicitly on the measure. We then define the 2-norm to be

$$\|f\|_2 = \sqrt{\langle f, f\rangle}.$$

The space $L^2(X)$ may be defined as the space of measurable functions with finite 2-norm, or the completion of $C(X)$ with respect to the 2-norm. These definitions agree for a compact metric space [**13**, Theorem 29.14].

Representation theory. We finish this section with an overview of some conventions with regards to representation theory. We assume that the group is given a topology, and we define a representation to be a continuous group homomorphism from that group to the group of complex-linear invertible endomorphisms $\mathrm{GL}(V)$ of a complex vector space V. Let $\widehat{G}$ be a set containing one element of each isomorphism class of the irreducible representations of the group G. Because G is compact, the underlying vector space V_π of every irreducible representation π is finite-dimensional. Its dimension is denoted by d_π. An irreducible representation of a compact group has a unique, up to multiplication by a positive real number, inner product such that the equation $\pi(g)^* = \pi(g)^{-1}$ holds, where $(-)^*$ denotes the adjoint with respect to the inner product just described. A representation for which this property holds is called unitary. We assume every element of $\widehat{G}$ is unitary. We now define the contragradient representation. For every $\pi \in \widehat{G}$, we denote by $\overline{(-)}$ a conjugate-linear endomorphism of V_π which squares to the identity. This always exists by choosing a complex basis and conjugating each component. The contragradient representation $\overline{\pi}$ is then defined to act on the vector space V_π by $\overline{\pi}(g)v = \overline{\pi(g)\overline{v}}$.

1.2. A generalised Fourier transform

Define the space $\tilde{X} = X/G \times G$. We would like to define a notion of a Fourier transform for a function in $L^2(X)$. We will do this by treating $L^2(X)$ as a subalgebra of $L^2(\tilde{X})$. This will allow us to prove many properties of the space $L^2(X)$ using the known case $L^2(G)$. Under the assumptions from the previous section, we may define a surjection

$$\begin{aligned}\Phi\colon \tilde{X} &\to X\\ (t,g) &\mapsto gR(t).\end{aligned}$$

which is continuous, since it is the composition of the continuous map $R \times 1_G$ and the group action. The map Φ induces an embedding $C(X) \hookrightarrow C(\tilde{X})$ by sending a function f to the composition $\tilde{f} = f\Phi$. Any function $\tilde{f} = f\Phi$ in the image of the embedding satisfies the invariance property that for all (t, g), we have

$$\tilde{f}(t,g) = \tilde{f}(t,gh) \tag{4}$$

for all $h \in H(t)$. Let us show that any continuous function $\tilde{f}$ with the above invariance property is of the form $\tilde{f} = f\Phi$ for a unique continuous f. By the axiom of choice, there exists a function $s\colon X \to G$ such that $\Phi(p(x), s(x)) = x$ for all $x \in X$. Define the function f by $f(x) = \tilde{f}(p(x), s(x))$, so that $f\Phi = \tilde{f}$ by the invariance property of $\tilde{f}$. Let us now verify continuity of f. Since $\tilde{X}$ is compact and X is Hausdorff, the map Φ is closed. The map Φ is also surjective and hence to show continuity of f, it suffices to show continuity of $f\Phi$. Since we have $\tilde{f} = f\Phi$, this holds and hence f is continuous. Uniqueness of f follows from surjectivity of Φ.

We now give a Peter-Weyl type theorem for the space $\tilde{X}$. First, we need to define a measure. Recall that X/G has a measure with full support by Proposition 1.4. So does G, namely the Haar measure, as defined in [**45**, Chapter 1]. We define the measure μ on $\tilde{X} = X/G \times G$ as the product measure, in which case Fubini's theorem holds [**13**, Corollary 23.7]. The measure on X is defined to be the pullback via Φ. Notice that this measure is G-invariant and also has full support.

We now introduce the relevant spaces for the Fourier transform. The Hilbert space $L^2(\tilde{X})$ with inner product

$$\langle f_1, f_2 \rangle = \int_{\tilde{X}} \overline{f_1}(t,g) f_2(t,g) dtdg$$

is a unitary representation of $G \times G$ via the simultaneous left and right regular representation

$$(g_1, g_2) \cdot f(t,x) = f(t, g_1^{-1} x g_2).$$

For us, a countable direct sum of Hilbert spaces is the metric completion of the countable direct sum of vector spaces endowed with the sum of the inner products. The direct sum $\bigoplus_{\pi \in \widehat{G}} L^2(X/G, \mathrm{End}(V_\pi))$ of Hilbert spaces with inner product

$$\langle (A_\pi)_\pi, (B_\pi)_\pi \rangle = \sum_{\pi \in \widehat{G}} d_\pi \int_{X/G} \mathrm{Tr}\, A_\pi^*(t) B_\pi(t) dt$$

is also a unitary representation of $G \times G$ via simultaneous post- and precomposition

$$(g_1, g_2) \cdot (A_\pi(t))_\pi = (\pi(g_1) A_\pi(t) \pi^*(g_2))_\pi.$$

For $f \in L^2(\tilde{X})$ and $\pi \in \widehat{G}$, define the Fourier coefficient at π to be the Bochner integral [**45**, B.6]

$$\widehat{f}_\pi(t) = \int_G f(t,g) \pi(g)\, dg,$$

which is a square-integrable function on X/G with values in $\mathrm{End}(V_\pi)$. Recall V_π is finite dimensional. On the space V_π we may define a norm

$$\|v\|_2 = \sqrt{\langle v, v\rangle}$$

for $v \in V_\pi$ and we give $\mathrm{End}(V_\pi)$ the corresponding operator norm. When we speak of continuity of a function with values in either V_π or $\mathrm{End}(V_\pi)$, it is with respect to the topology induced by these norms. It is straightforward to verify that $\widehat{f}_\pi$ is continuous if f is. For an element f of $L^2(\tilde{X})$, denote by $\widehat{f}$ the element of $\bigoplus_{\pi\in\widehat{G}} L^2(X/G, \mathrm{End}(V_\pi))$ with π-component $\widehat{f}_\pi$. For an element A of $\bigoplus_{\pi\in\widehat{G}} L^2(X/G, \mathrm{End}(V_\pi))$ with π-component A_π, denote by $\widehat{A}$ the function in $L^2(\tilde{X})$, which sends $(t, g) \in \tilde{X}$ to the complex number $\sum_{\pi\in\widehat{G}} d_\pi \operatorname{Tr} A_\pi(t)\pi^*(g)$. Convergence is part of the statement of the following theorem.

Theorem 1.5. *The maps*

$$L^2(\tilde{X}) \leftrightarrow \bigoplus_{\pi\in\widehat{G}} L^2(X/G, \mathrm{End}(V_\pi))$$
$$f \mapsto \widehat{f}$$
$$\widehat{A} \leftarrow\!\shortmid A$$

are mutually inverse isometric isomorphisms of $(G \times G)$*-representations.*

We will denote by $\otimes$ the tensor product of vector spaces. We will define the tensor product of Hilbert spaces to be the metric completion of the tensor product of vector spaces and denote it by $\widehat{\otimes}$.

Lemma 1.6. *Let H be a separable Hilbert space and for each $i \in \mathbb{N}$, let H_i be a separable Hilbert space. The natural map $H\widehat{\otimes}\bigoplus_{i\in\mathbb{N}} H_i \to \bigoplus_{i\in\mathbb{N}} H\widehat{\otimes}H_i$ is an isomorphism.*

Proof. Let v_j with $j \in \mathbb{N}$ be a complete system of H and for each $i \in \mathbb{N}$, let w_{ik} with $k \in \mathbb{N}$ be a complete system of H_i. Let us denote by $\iota_{H_i} : H_i \to \bigoplus_{i\in\mathbb{N}} H_i$ and $\iota_{H\otimes H_i} : H \otimes H_i \to \bigoplus_{i\in\mathbb{N}} H \otimes H_i$ the natural inclusions. A complete system of $H \otimes \bigoplus_{i\in\mathbb{N}} H_i$ is given by $v_j \otimes \iota_{H_i}(w_{ik})$ and a complete system of $\bigoplus_{i\in\mathbb{N}} H \otimes H_i$ is given by $\iota_{H\otimes H_i}(v_j \otimes w_{ik})$. These are mapped to one another by the natural map, which is therefore an isomorphism of Hilbert spaces. □

Proof of Theorem 1.5. The natural map

$$L^2(X/G)\widehat{\otimes}L^2(G) \to L^2(X/G \times G) \tag{5}$$

is well-defined by Fubini's theorem [**13**, Corollary 23.7] and has dense image. Therefore, it is an isomorphism. By the Peter-Weyl theorem for a compact group [**45**, Theorem 7.2.3], we have $L^2(G) \cong \bigoplus_{\pi\in\widehat{G}} \mathrm{End}(V_\pi)$. Because of this, by Lemma 1.6 and by finite-dimensionality of V_π, the following morphisms

$$\begin{aligned} &L^2(X/G)\widehat{\otimes}L^2(G) \\ &\to L^2(X/G)\widehat{\otimes} \bigoplus_{\pi\in\widehat{G}} \mathrm{End}(V_\pi) \\ &\to \bigoplus\nolimits_{\pi\in\widehat{G}} L^2(X/G)\widehat{\otimes}\mathrm{End}(V_\pi) \\ &\to \bigoplus\nolimits_{\pi\in\widehat{G}} L^2(X/G, \mathrm{End}(V_\pi)) \end{aligned}$$

are isomorphisms and this gives the correct map. The statement now follows from the isomorphism (5). $\square$

To the maps in either direction we shall refer as the Fourier transform and for both maps we will use $\widehat{(-)}$. For a fixed π, we have a natural embedding of $L^2(X/G, \mathrm{End}(V_\pi))$ into $\bigoplus_{\pi\in\widehat{G}} L^2(X/G, \mathrm{End}(V_\pi))$. If $A_\pi \in L^2(X/G, \mathrm{End}(V_\pi))$, we will abuse notation slightly and denote by $\widehat{A_\pi}$ the Fourier transform via this embedding, i.e.

$$\widehat{A_\pi}(t, g) = d_\pi \operatorname{Tr} A_\pi(t)\pi^*(g).$$

Precomposition with Φ provides an embedding of $L^2(X)$ into $L^2(\tilde{X})$ and the Fourier transform of an element in $L^2(X)$ is defined via this embedding. Being an element of $C(X)$ constrains the Fourier coefficients. For an element $A \in C(X/G, \mathrm{End}(V_\pi))$, we may consider the condition that for all $t \in X/G$, $A(t)\pi^*(h) = A(t)$ holds for all $h \in H(t)$. That is, for all $t \in X/G$, we have

$$A(t) \in \mathrm{End}(V_\pi)^{H(t)}. \tag{6}$$

For the right regular action by $h \in G$ acting on a function $f \in C(X)$, we have,

$$\widehat{f \cdot h}_\pi(t) = \widehat{f}_\pi(t)\pi^*(h)$$

and hence the invariance condition (4) implies $\widehat{f}_\pi(t)$ satisfies (6) for all $\pi \in \widehat{G}$. As a partial converse, if the Fourier series converges pointwise to a continuous function f and for all $\pi \in \widehat{G}$, $\widehat{f}_\pi$ satisfies condition (6), then f satisfies (4). For instance, if all but finitely many Fourier coefficients vanish.

Let us give a different characterisation of condition (6). For $\pi \in \widehat{G}$, we define the space $E(X, V_\pi)$ to consist of those continuous functions $\phi \in C(X/G, V_\pi)$ such that

$$\phi(t) \in V_\pi^{H(t)} \tag{7}$$

holds for all $t \in X/G$. Recall $\overline{\pi}$ is the contragredient representation.

Proposition 1.7. *The image of the* $(G \times G)$*-morphism* $V_\pi \otimes E(X, V_{\overline{\pi}}) \to C(X/G, \mathrm{End}(V_\pi))$*, defined by* $v \otimes \phi \mapsto v\langle\overline{\phi}, -\rangle$*, is the set of functions which satisfy* (6).

Proof. Let us first show that elements in the image satisfy (6). Suppose $v \in V_\pi$ and $\phi \in E(X, V_\pi)$. For every $w \in V_\pi$, every $t \in X/G$ and every $h \in H(t)$, we then have

$$v\langle\overline{\phi(t)}, \pi^*(h)w\rangle = v\langle\overline{\overline{\pi}(h)\phi(t)}, w\rangle = v\langle\overline{\phi(t)}, w\rangle,$$

from which we see that elements in the image satisfy (6).

Now let $A \in C(X/G, \mathrm{End}(V_\pi))$ satisfy (6). Let v_i with $i = 1, \ldots, d_\pi$ be an orthonormal basis of V_π. There exist unique functions $A_{ij} \in C(X/G, V_\pi)$ such that

$$A(t) = \sum_{i,j=1}^{d_\pi} A_{ij}(t)v_i\langle v_j, -\rangle = \sum_{i=1}^{d_\pi} v_i\langle\overline{\phi_i(t)}, -\rangle,$$

where we have defined $\phi_i(t) = \sum_{j=1}^{d_\pi} A_{ij}(t)\overline{v_j}$. One readily verifies that ϕ_i for fixed i satisfies (7) if A satisfies (6). Therfore, A is in the image. $\square$

We may give the space $E(X, V_\pi)$ a norm by

$$\sup_{t \in X/G} \|\phi(t)\|_2$$

for $\phi \in E(X, V_\pi)$. Condition (7) is closed under limits for this norm, and, therefore, this gives $E(X, V_\pi)$ the structure of a Banach space. We now define the space of continuous equivariant functions $\mathrm{Hom}_G(X, V_\pi)$ to be the space of all continuous functions $\psi\colon X \to V_\pi$ such that $\psi(g \cdot x) = \pi(g)\psi(x)$ for all $g \in G$ and $x \in X$. Similarly, we give this space the norm

$$\sup_{x \in X} \|\psi(x)\|_2,$$

which gives the space $\mathrm{Hom}_G(X, V_\pi)$ the structure of a Banach space.

Proposition 1.8. *The following maps define isomorphisms of Banach spaces*

$$\begin{aligned} E(X, V_\pi) &\leftrightarrow \mathrm{Hom}_G(X, V_\pi) \\ \phi &\mapsto \pi(s(x))\phi(p(x)) \\ \psi(R(t)) &\leftarrow\!\shortmid \psi. \end{aligned}$$

Proof. Let $\phi \in E(X, V_\pi)$ and let us verify continuity of $\pi(s(x))\phi(p(x))$. It is necessary and sufficient that for all $v \in V_\pi$, the function $\langle v, \pi(s(x))\phi(p(x))\rangle$ is a continuous complex-valued function on X. By Section 1.2, it suffices to show, that the function $\langle v, \pi(g)\phi(t)\rangle$ on $\tilde{X}$ is continuous and satisfies (4). Both these requirement follow from the fact that ϕ is an element of $E(X, V_\pi)$. Therefore, $\pi(s(x))\phi(p(x))$ defines a continuous function on X. If $\psi \in \mathrm{Hom}_G(X, V_\pi)$, then ψR is also continuous, since R is. Therefore, the maps in both directions are well-defined. Linearity of both maps is easily checked. Let us now verify that the maps are mutual inverses. Let $\phi \in E(X, V_\pi)$. We have

$$s(R(t))R(t) = s(R(t))R(p(R(t))) = R(t)$$

by the definitions of s and p, and hence $s(R(t))$ stabilises $R(t)$. By the definition of $E(X, V_\pi)$ and by $p(R(t)) = t$ we have

$$\pi(s(R(t)))\phi(p(R(t))) = \pi(s(R(t)))\phi(t) = \phi(t)$$

which shows one direction. Now let $\psi \in \mathrm{Hom}_G(X, V_\pi)$. We then have

$$\pi(s(x))\psi(R(p(x))) = \psi(s(x)R(p(x))) = \psi(x),$$

which shows the other direction. By the open mapping theorem, it suffices to show that only one of the maps is bounded. The function R is continuous and therefore the map $\psi \mapsto \psi R$ is bounded with respect to these norms. Therefore the maps are mutually inverse isomorphisms of Banach spaces. □

Using the above correspondence, we will phrase our results in terms of equivariant continuous maps as well.

1.3. Uniform density

Let $\mathcal{E}(G) \subseteq C(G)$ be the algebra of functions such that the Fourier coefficients vanish for almost every $\pi \in \widehat{G}$, i.e. for all but finitely many. The algebra $\mathcal{E}(G)$ is dense in $C(G)$ with respect to the uniform norm [**50**]. We make a similar definition. For $\pi \in \widehat{G}$, we say that the Fourier coefficient of a function $f \in C(X)$ vanishes for π if the Fourier coefficient $\widehat{f}_\pi \in C(X/G, V_\pi)$ vanishes identically on X/G. We then define $\mathcal{E}(X)$ to be the vector subspace of $C(X)$ of functions f such that the Fourier coefficients of f vanish for almost every $\pi \in \widehat{G}$.

THEOREM 1.9. *$\mathcal{E}(X)$ is dense in $C(X)$ with respect to the uniform norm.*

We will show that $\mathcal{E}(X)$ is an algebra which separates points. Therefore, by the Stone-Weierstraß theorem [**45**, Theorem A.10.1], it must be dense.

LEMMA 1.10. *The subspace $\mathcal{E}(X)$ is an algebra.*

PROOF. It is obviously closed under sums and multiplication by a complex number. It is also closed under complex conjugation by considering the contragradient representation $\bar{\pi}$ of π. What is left is showing that it is closed under multiplication. Let $F_1 \in C(X/G, \mathrm{End}(V_{\pi_1}))$ and $F_2 \in C(X/G, \mathrm{End}(V_{\pi_1}))$ both satisfy condition (6). It suffices to show that the product of the functions $\mathrm{Tr}\, F_1(t)\pi_1(g)$ and $\mathrm{Tr}\, F_2(t)\pi_2(g)$ has the property that the Fourier coefficient vanishes for almost every $\pi \in \widehat{G}$, and that the Fourier coefficients satisfy condition (6). We have

$$\begin{aligned} &\mathrm{Tr}\, F_1\pi_1 \,\mathrm{Tr}\, F_2\pi_2 \\ &= \mathrm{Tr}(F_1\pi_1 \otimes F_2\pi_2) \\ &= \mathrm{Tr}(F_1 \otimes F_2)(\pi_1 \otimes \pi_2) \\ &= \mathrm{Tr}\, A\pi, \end{aligned}$$

where we have defined $A = F_1 \otimes F_2$ and $\pi = \pi_1 \otimes \pi_2$. Let $(\pi, V_\pi) = \oplus_{i=1}^r (\rho_i, V_i)$ be a decomposition into irreducibles and decompose A into blocks A_{ij} accordingly. By this we mean that $A_{ij} : V_j \to V_i$ is the canonical map obtained from A by inclusion and projection. Furthermore, define $A_j = \sum_{i=1}^n A_{ij}$. We then have

$$\mathrm{Tr}\, F_1\pi_1 \,\mathrm{Tr}\, F_2\pi_2 = \sum_j \mathrm{Tr}\, A_j \rho_j.$$

Because the left-hand side satisfies (4), so does the right-hand side. By Theorem 1.5, the Fourier coefficients of the right-hand side are given by the A_j and satisfy (6). $\square$

LEMMA 1.11. *The algebra $\mathcal{E}(X)$ separates points.*

PROOF. Let $x, y \in X$. First, suppose $p(x) \neq p(y)$. Recall that the trivial representation sends every element of G to the complex number 1, which acts on the vector space $\mathbb{C}$. For the trivial representation π and for any continuous complex-valued function f on X/G, the invariance condition is satisfied and hence $\mathrm{Tr}\, f(p(x))\pi(s(x)) = f(p(x)) \in \mathcal{E}(X)$. The space X/G is a compact metric space by Proposition 1.1. Therefore, by Urysohn's lemma [**87**, Theorem 33.1], there is a continuous function separating $p(x)$ and $p(y)$ and hence a function in $\mathcal{E}(X)$ doing so.

Second, suppose $p(x) = p(y)$. For notation, define $H = H(p(x))$. If $s(x)H = s(y)H$ then we have $x = s(x)R(p(x)) = s(y)R(p(y)) = y$, which cannot be. Hence we may assume $s(x)H \neq s(y)H$. By Proposition 1.3, G/H is compact Hausdorff. Therefore, again by Urysohn's lemma, there is a continuous function on G/H separating $s(x)H$ and $s(y)H$, corresponding to an H-invariant function f on $C(G)$. We now appeal to the known case for $C(G)$ [**50**, Theorem 5.11] and we let f_i be functions on G such that $f_i \in \mathcal{E}(G)$ and $f_i \to f$ in the uniform norm.

The only problem that's left is that f_i may not satisfy the invariance condition $\widehat{f_i}_\pi \in \mathrm{End}(V_\pi)^H$ for every $\pi \in \widehat{G}$. The projection operator $P_H : C(G) \to C(G)^H$ may be calculated explicitly with the formula $P_H f = \int_H h\cdot f dh$ and P_H is continuous with respect the uniform norm [**45**, Section 1.5]. Therefore, by the classical Peter-Weyl theorem or Theorem 1.5 with $X = G$, the operator P_H maps $\mathcal{E}(G)$ to itself. Thus, $P_H f_i \to f$ in the uniform norm and $P_H f_i \in \mathcal{E}(G)$. Therefore, by approximating and renaming f, we deduce the existence of a function $f \in C(G)$ such that $\widehat{f}_\pi$ vanishes for almost every $\pi \in \widehat{G}$, $\widehat{f}_\pi \in \mathrm{End}(V_\pi)^H$, and $f(s(x)) \neq f(s(y))$.

To construct the function function on X separating x and y we need one more element. By condition (iii) on the action, let U be a neighbourhood of $p(x)$ in X/G such that for all $u \in U$ we have $H(u) \subseteq H$. The space X/G is a compact metric space by Proposition 1.1. Therefore, again by Urysohn's lemma, there is a continuous function ψ on X/G such that ψ vanishes on the complement of U in X/G and is 1 on $p(x)$.

Consider the function $F(t, g) = \psi(t)f(g)$ in $C(\tilde{X})$, for which we have $\widehat{F}_\pi(t) = \psi(t)\widehat{f}_\pi$. Because $\widehat{f}_\pi$ vanishes for almost every $\pi \in \widehat{G}$, $\widehat{F}_\pi$ vanishes for almost every $\pi \in \widehat{G}$. For $t \in U$, $\widehat{F}_\pi(t)$ satisfies condition (6), because of $\widehat{f}_\pi \in \mathrm{End}(V_\pi)^H$ and condition (iii). For $t \notin U$, $\widehat{F}_\pi(t)$ vanishes and therefore $\widehat{F}_\pi$ satisfies condition (6). Therefore, F satisfies the correct invariance condition and can be identified with an element of $\mathcal{E}(X)$. Since $p(x) = p(y)$, we have

$$F(p(x), s(x)) = f(s(x)) \neq f(s(y)) = F(p(y), s(y))$$

and therefore F separates x and y. □

We may now define our desired complete system for $C(X)$. By Corollary 1.2, the space $C(X/G)$ is separable and therefore, for any $\pi \in \widehat{G}$, the space $C(X/G, V_\pi)$ is separable, since the dimension d_π is finite. A subset of a separable metric space is separable. We have $E(X, V_\pi) \subseteq C(X/G, V_\pi)$ and, therefore, $E(X, V_\pi)$ is separable. Given a complete system, we may perform the Gram-Schmidt procedure and assume that the elements are orthonormal. Let k_π denote the cardinality of the complete system for $E(X, V_\pi)$, which is either finite or countably infinite. Define

$$\Xi = \{(\pi, i, j) \in \widehat{G} \times \mathbb{N} \times \mathbb{N} \mid i \leq k_\pi, j \leq d_\pi\}.$$

Denote by $\phi_{\pi,i}$ the orthonormal complete system of $E(X, V_\pi)$ and denote by $\psi_{\pi,i}$ the corresponding orthonormal complete system of $\mathrm{Hom}_G(X, V_\pi)$. Let $v_{\pi,j}$ with $j = 1, \ldots, d_\pi$ denote an orthonormal basis of V_π. By Proposition 1.7, we may make the identification

$$v_{\pi,j} \otimes \phi_{\overline{\pi},i} = v_j \langle \overline{\phi_{\overline{\pi},i}}, - \rangle,$$

which is an element of $C(X/G, \mathrm{End}(V_\pi))$ satisfying (6). Therefore, the Fourier transform of such a function defines a function on X. For $\xi = (\pi, i, j) \in \Xi$, define

$$e_\xi = \frac{1}{\sqrt{d_\pi}} \widehat{v_j \otimes \phi_{\overline{\pi},i}}.$$

Furthermore, the functions $v_{\pi,j} \otimes \phi_{\overline{\pi},i}$ give a complete system of the subspace of functions in $C(X/G, \mathrm{End}(V_\pi))$ satisfying (6). Therefore, by taking the Fourier transform, we see that a function f for which only one Fourier coefficient does not vanish may be approximated uniformly by a finite linear combination of e_ξ with $\xi \in \Xi$. Therefore, an element of $\mathcal{E}(X)$ may be approximated uniformly in this way, and therefore, an element of $C(X)$. We see that e_ξ with $\xi \in \Xi$ give a complete system of $C(X)$.

Let us show they are orthonormal. The adjoint of $v_{j_1}\langle\overline{\phi_{\overline{\pi_1},j_1}},-\rangle$ is given by $\overline{\phi_{\overline{\pi_1},j_1}}\langle v_{j_1},-\rangle$. Thus, for the inner product introduced in Section 1.2, we have

$$\langle v_{j_1}\otimes\phi_{\overline{\pi},i_1}, v_{j_2}\otimes\phi_{\overline{\pi},i_2}\rangle = d_\pi\langle v_{j_1},v_{j_2}\rangle\langle\overline{\phi_{\overline{\pi_1},i_1}},\overline{\phi_{\overline{\pi_2},i_2}}\rangle.$$

We see that the e_ξ are orthonormal for this inner product. The function e_ξ, as a function on X, is given by

$$e_\xi(x) = \sqrt{d_\pi}\operatorname{Tr} v_{\pi,j}\otimes\phi_{\overline{\pi},i}(p(x))\pi^*(s(x)) = \sqrt{d_\pi}\langle\overline{\psi_{\overline{\pi},i}}(x), v_{\pi,j}\rangle.$$

We note that, ranging over all $\xi\in\Xi$, these functions define a symmetry adapted system [**38**, §3.2].

We now introduce some notation to work with this basis. Let Ξ be as above and endow it with the discrete topology. We will denote by $C_c(\Xi)$ the space of continuous functions with compact support, i.e. the space of functions with finite support. We have an embedding of $C_c(\Xi)$ into $C(X)$ defined by $a\mapsto\sum_{\xi\in\Xi}a_\xi e_\xi$ and by the above, the image is dense with respect to the uniform norm. We have

$$\widehat{g\cdot e_{\pi,i,j}} = \pi(g)\frac{1}{\sqrt{d_\pi}}v_{\pi,j}\otimes\phi_{\overline{\pi},i} = \sum_{k=1}^{d_\pi}\langle v_{\pi,k},\pi(g)v_{\pi,j}\rangle\widehat{e_{\pi,i,k}},$$

and hence

$$g\cdot e_{\pi,i,j} = \sum_{k=1}^{d_\pi}\pi_{kj}(g)e_{\pi,i,k}, \tag{8}$$

where we have defined $\pi_{kj}(g) = \langle v_{\pi,k},\pi(g)v_{\pi,j}\rangle$. From this, we see that image of the embedding $C_c(\Xi)$ into $C(X)$ is closed under the action of G. As such, we view $C_c(\Xi)$ as a representation of G.

Cave. The functions e_ξ are dense with respect to the uniform norm and therefore with respect to the 2-norm. Therefore, for $f\in L^2(X)$, we have, as square-integrable functions, an equality

$$f = \sum_{\xi\in\Xi}\widehat{f}_\xi e_\xi,$$

where $\widehat{f}_\xi = \langle e_\xi, f\rangle$. However, despite the fact that $C_c(\Xi)$ is dense, this is not necessarily an equality when considering the uniform norm. For example, there exists a continuous functions on the circle such that the Fourier series does not converge to the original function pointwise.

1.4. Kernels

We now turn our attention to $C(X\times X)$ and the operators on $L^2(X)$ that such function define. We may consider the action of $G\times G$ on $X\times X$. Given the previous section, there is a natural choice of complete system. By the Stone-Weierstraß theorem, the natural map $C(X)\otimes C(X)\to C(X\times X)$ has dense image with respect to the uniform norm. The functions e_ξ with $\xi\in\Xi$ are a complete system for $C(X)$, and therefore the pointwise products $e_{\xi_2}\overline{e_{\xi_1}}(x,y) = e_{\xi_2}(x)\overline{e_{\xi_1}}(y)$ with $\xi_1,\xi_2\in\Xi$ are a complete system for $C(X\times X)$. Recall the e_ξ are an orthonormal basis of $L^2(X)$. Therefore, the functions $e_{\xi_2}\overline{e_{\xi_1}}$ are an orthonormal basis of $L^2(X\times X)$ and hence with respect to the 2-norm, we have an equality

$$K = \sum_{\xi_1,\xi_2\in\Xi}\widehat{K}_{\xi_1,\xi_2}e_{\xi_1}\overline{e_{\xi_2}}, \tag{9}$$

where we have defined $\widehat{K}_{\xi_1,\xi_2} = \langle e_{\xi_1}\overline{e_{\xi_2}}, K\rangle$. As before, this is not necessarily an equality in the sense of continuous functions with the uniform norm, but the image of $C_c(\Xi \times \Xi)$ in $C(X \times X)$ defined by $a \mapsto A = \sum_{\xi_1,\xi_2\in\Xi} a_{\xi_1,\xi_2} e_{\xi_1}\overline{e_{\xi_2}}$ is dense with respect to the uniform norm. We immediately have $\widehat{A}_{\xi_1,\xi_2} = a_{\xi_1,\xi_2}$. A kernel $K \in C(X \times X)$ defines an operator $T_K : L^2(X) \to L^2(X)$ by

$$T_K f(x) = \int_X K(x,y)f(y)dy.$$

and we have

$$\widehat{T_K f}_{\xi_1} = \sum_{\xi_2\in\Xi} \widehat{K}_{\xi_1,\xi_2}\widehat{f}_{\xi_2}.$$

Given two kernels K_1 and K_2, it is easy to verify that to $T_{K_1}T_{K_2} = T_{K_1*K_2}$, where

$$K_1 * K_2 = \int_X K_1(x,z)K_2(z,y)dz.$$

Furthermore, for the adjoint operator T_K^*, we have $T_K^* = T_{K^*}$, where we have defined $K^*(x,y) = \overline{K(y,x)}$. For $a, b \in C_c(\Xi \times \Xi)$ and associated kernels $A, B \in C(X \times X)$, we have

$$\widehat{A * B}_{\xi_1,\xi_2} = \sum_{\xi_3\in\Xi} a_{\xi_1,\xi_3} b_{\xi_3,\xi_2}. \tag{10}$$

Similarly, for $a \in C_c(\Xi \times \Xi)$, we have

$$\widehat{A^*}_{\xi_1,\xi_2} = \overline{a_{\xi_2,\xi_1}}. \tag{11}$$

Positivity. Recall X is a compact metric space with a measure with full support. We have

PROPOSITION 1.12. *The kernel $K \in C(X \times X)$ satisfies*

$$\sum_{i,j}^{n} \overline{c_i} K(x_i,x_j)c_j \geq 0 \tag{12}$$

for all n, for all $c \in \mathbb{C}^n$ and all $x \in X^n$ if and only if

$$\int \overline{f(x)}K(x,y)f(y)dxdy \geq 0 \tag{13}$$

for all f in $L^2(X)$.

PROOF. Assume the kernel K satisfies (12). Let U_i with $i = 1, \dots n$ be open, disjoint subsets of X and for each i choose an element x_i of U_i. Define

$$f' = \sum_{i=1}^{n} f(x_i)1_{U_i},$$

where 1_{U_i} is the indicator function of U_i, and define

$$K' = \sum_{i,j=1}^{n} K(x_i,x_j)1_{U_i\times U_j}.$$

We then have

$$\int \overline{f'(x)}K'(x,y)f'(y)dxdy = \sum_{i,j=1}^{n} \overline{f'(x_i)}|U_i|K'(x_i,x_j)f'(x_j)|U_j| \geq 0 \tag{14}$$

We may choose U_i such that the integral in (13) is approximated arbitrarily well by the integral in (14) and therefore (13) holds.

Now assume (13) and let c and x be as described. Recall X is a metric space and the measure has full support. For each $i = 1, \ldots, n$ and $k \in \mathbb{N}$, let $U_{i,k} = B(x_i, \epsilon_k)$ be a ball with centre x_i and radius ϵ_k, where ϵ_k is a sequence converging to zero. For each k, define

$$f_k = \sum_{i=1}^{n} c_i \frac{1}{|U_{i,k}|} 1_{U_{i,k}}.$$

We then have

$$\int \overline{f_k(x)} K(x,y) f_k(y) dx dy = \sum_{i,j=1}^{n} \overline{c_i} c_j \frac{1}{|U_{i,k} \times U_{j,k}|} \int_{U_{i,k} \times U_{j,k}} K(x,y) dx dy \geq 0,$$

which converges to (13) as $k \to \infty$ by continuity of K. □

A kernel which satisfies any and hence both of these conditions is called positive definite. We call an infinite matrix positive semidefinite if every finite principal submatrix is positive semidefinite. Denote by $C_{\succeq 0}(\Xi \times \Xi)$ those elements of $C(\Xi \times \Xi)$ such that the matrix is positive semidefinite. Consider the embedding of $C_{\succeq 0}(\Xi \times \Xi)$ into $C(X \times X)$. By Proposition 1.12, and the fact that the e_ξ are an orthonormal basis of $L^2(X)$, a positive semidefinite matrix is mapped to a positive definite kernel and any positive definite kernel that is in the image of the embedding comes from a positive definite matrix. We also have the following characterisation.

Theorem 1.13 (Mercer). *Suppose $K \in C(X \times X)_{\succeq 0}$. Then there is an orthonormal basis ϕ_i with $i \in \mathbb{N}$ of $L^2(X)$ consisting of eigenfunctions of T_K such that the corresponding sequence of eigenvalues λ_i is nonnegative. The eigenfunctions corresponding to nonzero eigenvalues are continuous on X and K has the representation*

$$K(x,y) = \sum_{j=1}^{\infty} \lambda_j \phi_j(x) \overline{\phi_j(y)},$$

where the convergence is uniform.

Proof. In [**104**, Section 98], a proof is given where X is an interval, but the proof readily adapts to the case where X is a compact Hausdorff space and X has a measure with full support. The spectral theorem required for this case follows from [**45**, Theorem 5.2.2 and Section 5.3]. □

For a natural number n, define $R = \sum_{j=1}^{n} \sqrt{\lambda_j}\, \phi_j(x) \overline{\phi_j(y)}$. We have $R^* * R = \sum_{j=1}^{n} \lambda_j \phi_j(x) \overline{\phi_j(y)}$. In the uniform norm, we may approximate R by the kernel S associated to an element of $s \in C_c(\Xi \times \Xi)$. By equations (10) and (11), we have

$$\widehat{S^* * S}_{\xi_1,\xi_2} = \sum_{\xi_3 \in \Xi} \overline{s_{\xi_3,\xi_1}} s_{\xi_3,\xi_2}$$

which is a positive definite matrix in $C_c(\Xi \times \Xi)$. We can let n be big enough so that $R^* * R$ is as close as we like to K in the uniform norm. Choosing S close enough to R will ensure $S^* * S$ is as close as we like to $R^* * R$ in the uniform norm. We obtain

Corollary 1.14. *The image of $C_c(\Xi \times \Xi)_{\succeq 0}$ in $C(X \times X)_{\succeq 0}$ is dense with respect to the uniform norm.*

Invariance. Consider the closed subgroup $G \subseteq G \times G$ via the diagonal embedding and the projection P_G onto the G-invariants $C(X \times X)^G$. Explicitly, this projection is given by

$$P_G K = \int_G g \cdot K dg.$$

Firstly, the projection is bounded with respect to the uniform norm. It is also bounded with respect to the 2-norm, which may be seen as follows. Recall from Section 1.2 that the measure on X is G-invariant and therefore, we have $\|g \cdot K\|_2 = \|K\|_2$. We then have

$$\| \int_G g \cdot K dg\|_2 \leq \int_G \|g \cdot K\|_2 dg = \int_G \|K\|_2 dg = \|K\|_2.$$

Hence the projection is bounded with respect to the 2-norm.

Let us study the explicit form of the projection in terms of the complete system from earlier. By equation (8) and the Peter-Weyl theorem [**45**, Theorem 7.2.1], we have

$$\begin{aligned}
&\int_G g \cdot e_{\pi_1,i_1,j_1} \overline{e_{\pi_2,i_2,j_2}} dg \\
&= \sum_{k_1,k_2} e_{\pi_1,i_1,k_1} \overline{e_{\pi_2,i_2,k_2}} \int_G \pi_{1,k_1,j_1}(g) \overline{\pi_{2,k_2,j_2}(g)} dg \\
&= \delta_{\pi_1,\pi_2} \delta_{j_1,j_2} \frac{1}{d_{\pi_1}} \sum_{k_1=1}^{d_{\pi_1}} e_{\pi_1,i_1,k_1} \overline{e_{\pi_2,i_2,k_1}},
\end{aligned}$$

where we have used Kronecker-delta notation. With this fact at hand, we define the zonal matrices. We have

$$\begin{aligned}
&\frac{1}{\sqrt{d_\pi}} \sum_{k=1}^{d_\pi} e_{\pi,i_1,k}(x) \overline{e_{\pi,i_2,k}}(y) \\
&= \sqrt{d_\pi} \sum_{k=1}^{d_\pi} \langle \overline{\psi_{\overline{\pi},i_1}}(x), v_k \rangle \langle v_k, \overline{\psi_{\overline{\pi},i_2}}(y) \rangle \\
&= \sqrt{d_\pi}\, \overline{\langle \psi_{\overline{\pi},i_1}(x), \psi_{\overline{\pi},i_2}(y) \rangle},
\end{aligned}$$

a step which is known as the addition formula. Hence we define the functions

$$Z_{\pi,i_1,i_2}(x,y) = \sqrt{d_\pi}\, \langle \psi_{\pi,i_1}(x), \psi_{\pi,i_2}(y) \rangle.$$

Since the e_ξ are orthonormal, so are the Z_{π,i_1,i_2}. The, possibly infinite, matrix-valued kernel Z_π with entries as above is commonly referred to as the zonal matrix. It is the generalisation of the zonal matrix which was defined in the introduction of this thesis. The change between π and $\overline{\pi}$ is done for convenience in the next section on absolute convergence.

We may deduce several facts from the above calculation. Firstly, we will focus on statements regarding the 2-norm. Projection of (9) implies that every kernel K in $C(X \times X)^G$ has an expansion

$$K = \sum_{\pi \in \widehat{G}} \sum_{i_1,i_2=1}^{k_\pi} \widehat{K}_{\pi,i_1,i_2} \overline{Z_{\pi,i_1,i_2}}, \tag{15}$$

which converges with respect to the 2-norm, where we have

$$\widehat{K}_{\pi,i_1,i_2} = \langle \overline{Z_{\pi,i_1,i_2}}, K\rangle = \frac{1}{\sqrt{d_\pi}} \sum_{k=1}^{d_\pi} \widehat{K}_{(\overline{\pi},i_1,k),(\overline{\pi},i_2,k)}. \tag{16}$$

Proposition 1.15. *A G-invariant kernel K is positive definite if and only if for every $\pi \in \widehat{G}$, the matrix $\left(\widehat{K}_{\pi,i_1,i_2}\right)_{i_1,i_2=1}^{k_\pi}$ is positive semidefinite.*

Proof. Fix $\pi \in \widehat{G}$. Let K be a positive definite G-invariant kernel and let c_i be a sequence indexed by $i \in \mathbb{N}$ with $i \le k_\pi$ and assume only finitely many c_i are nonzero. Let $f_k = \sum_{i=1}^{\infty} c_i e_{\overline{\pi},i,k}(x)$. We then have

$$\sum_{k=1}^{d_\pi} \int \overline{f_k(x)} K(x,y) f_k(y) dx dy = \frac{1}{\sqrt{d_\pi}} \sum_{i_1,i_2}^{k_\pi} \widehat{K}_{\pi,i_1,i_2} \overline{c_{i_1}} c_{i_2} \ge 0,$$

and hence every finite principal submatrix is positive semidefinite. Conversely, assume every finite principal submatrix is positive semidefinite. For $f \in C_c(\Xi)$, using (15), we have

$$\int \overline{f(x)} K(x,y) f(y) dx dy = \sum_{\pi \in \widehat{G}} \frac{1}{\sqrt{d_\pi}} \sum_{k=1}^{d_\pi} \sum_{i_1,i_2} \overline{\widehat{f}_{\overline{\pi},i_1,k}} \widehat{K}_{\pi,i_1,i_2} \widehat{f}_{\overline{\pi},i_2,k} \ge 0,$$

since every finite principal submatrix is positive semidefinite. By density of $C_c(\Xi)$ in $L^2(X)$, this holds for $f \in L^2(X)$ too and hence K is positive definite. □

We now turn our attention to statements regarding the uniform norm. The projection is bounded with respect to the uniform norm and hence we deduce that $C_c(\Xi \times \Xi)^G$ is a dense subspace of $C(X \times X)^G$. Furthermore, the projection preserves positivity, and so we deduce, using Corollary 1.14, that $C_c(\Xi \times \Xi)^G_{\succeq 0}$ is a dense subcone of $C(X \times X)^G_{\succeq 0}$. By equation 16 and Proposition 1.15, the projection of an element of $C_c(\Xi \times \Xi)_{\succeq 0}$ is a kernel of the form

$$K = \sum_{\pi \in \widehat{G}} \sum_{i_1,i_2=1}^{k_\pi} \widehat{K}_{\pi,i_1,i_2} \overline{Z_{\pi,i_1,i_2}},$$

where for every $\pi \in \widehat{G}$ the matrix $(\widehat{K}_{\pi,i_1,i_2})_{i_1,i_2=1}^{k_\pi}$ is positive semidefinite and has finitely many nonzero entries; and for almost every $\pi \in \widehat{G}$, the matrix vanishes identically. Define

$$\langle Z_\pi, \widehat{K}_\pi \rangle = \sum_{i_1,i_2=1}^{k_\pi} \widehat{K}_{\pi,i_1,i_2} \overline{Z_{\pi,i_1,i_2}}.$$

We then have

Theorem 1.16. *The set of kernels of the form*

$$K = \sum_{\pi \in \widehat{G}} \langle Z_\pi, \widehat{K}_\pi \rangle, \tag{17}$$

forms a dense subcone of $C(X \times X)^G_{\succeq 0}$

Furthermore, the parametrisation also holds if the complete system is not orthonormal. This follows from the fact that if a matrix B is positive semidefinite and C is an invertible matrix, then B^*CB is also positive semidefinite and every positive semidefinite matrix is of this form.

Absolute convergence. On a compact group, absolute uniform convergence of the Fourier series is intimately related to positivity [**59**, §34]. In particular, if a function on a compact group G is of positive type, then the Fourier series converges absolutely uniformly. Using this, we will deduce that (15) converges absolutely uniformly if K is positive definite and G-invariant and X/G is finite. The case with finitely many orbits is known in the literature [**38**], but a different derivation is given below. For G compact and X consisting of one orbit, this result is due to Bochner.

Let $X/G \cong \{1, \dots, N\}$ be finite. Denote by X_i the orbit such that $p(X_i) = i$. Since X_i/G is a single point, there is a natural isomorphism $C(X_i/G, V_\pi) \cong V_\pi$ given by evaluation at that point and the invariance condition then gives $E(X, V_\pi) \cong V_\pi^{H(i)}$. Therefore, a complete system is given by an orthonormal basis $v_{\pi,i,j}$ of $V_\pi^{H(i)}$ with $1 \leq j \leq \dim V_\pi^{H(i)}$. We have $\bigoplus_{i=1}^{N} E(X_i, V_\pi) \cong E(X, V_\pi)$, where the maps $E(X_i, V_\pi) \to E(X, V_\pi)$ are given by extension by zero. The images of the complete systems for $E(X_i, V_\pi)$ then give a complete system for $E(X, V_\pi)$. This is the complete system we will use.

For a kernel $C(X \times X)^G$, we have uniform convergence of the expansion (15) if and only if this holds for the restriction to $X_{i_1} \times X_{i_2}$. For notation, it is convenient to recall the identification of $C(X \times X)$ with a subspace of $C(\tilde{X} \times \tilde{X})$. We may define a map $C(X_{i_1} \times X_{i_2})^G$ to $C(G)$ by

$$K \mapsto K((i_1, e), (i_2, g)) = k_{i_1,i_2}(g), \tag{18}$$

where e is the unit of the group G. Since K is G-invariant, this map is isometric with respect to both the uniform norm and the 2-norm. We will now show that the expansion (15), restricted to $X_{i_1} \times X_{i_2}$, is mapped to the Fourier series of $k_{i_1 i_2}$, thereby reducing the uniform convergence of (15) to the uniform convergence of the Fourier series of the $k_{i_1 i_2}$. We have

$$\begin{aligned} &Z_{\pi,i_1,j_1,i_2,j_2}((i_1, e), (i_2, g)) \\ &= \sqrt{d_\pi}\, \langle \psi_{\pi,i_1,j_1}(i_1, e), \psi_{\pi,i_2,j_2}(i_2, g) \rangle \\ &= \sqrt{d_\pi}\, \langle v_{\pi,i_1,j_1}, \pi(g) v_{\pi,i_2,j_2} \rangle. \end{aligned}$$

For a G-invariant kernel, (15) is the inner product expansion with respect to the orthonormal functions $\overline{Z_{\pi,(i_1,j_1),(i_2,j_2)}}$. For a function on G, the Fourier series is the inner product expansion with respect to the orthonormal functions $\sqrt{d_\pi}\, \overline{\langle v_{\pi,i_1,j_1}, \pi(g) v_{\pi,i_2,j_2} \rangle}$. The map from equation (18) is an isometry with respect to the uniform norm, and therefore, it is equivalent to show that the Fourier series of the functions k_{i_1,i_2} converges uniformly.

We do so now. For a finite-dimensional complex vector space V with an inner product, we may define a norm on the space of complex-linear endomorphisms $\mathrm{End}(V)$ [**59**, §D.37] by

$$\|X\|_{\phi_1} = \sum_{i=1}^{d} \lambda_i,$$

where λ_i are the eigenvalues of the positive semidefinite operator $|X|$. Note that this is equal to the sum of the singular values of X.

LEMMA 1.17. *Let V be a finite-dimensional complex vector space with an inner product. Let $A, B, C \in \mathrm{End}(V)$. If the matrix*

$$\begin{bmatrix} A & B^* \\ B & C \end{bmatrix} \tag{19}$$

is positive semidefinite, then we have $2\|B\|_{\phi_1} \leq \|A\|_{\phi_1} + \|C\|_{\phi_1}$.

PROOF. Let $U, V \in \mathrm{End}(V)$ be unitary. Composition of the matrix (19) on the left by the matrix $\left[\begin{smallmatrix} U & 0 \\ 0 & V \end{smallmatrix}\right]$ and on the right by the matrix $\left[\begin{smallmatrix} U & 0 \\ 0 & V \end{smallmatrix}\right]^{-1}$ gives the positive semidefinite matrix

$$\begin{bmatrix} UAU^{-1} & UB^*V^{-1} \\ VBU^{-1} & VCV^{-1} \end{bmatrix}. \tag{20}$$

Now let $I \in \mathrm{End}(V)$ be the identity map. Pairing the matrix (20) with the positive semidefinite matrix $\left[\begin{smallmatrix} I & -I \\ -I & I \end{smallmatrix}\right]$, using the trace inner product, gives

$$\operatorname{Tr} UAU^{-1} + \operatorname{Tr} VCV^{-1} \geq \operatorname{Tr} VBU^{-1} + \operatorname{Tr} UB^*V^{-1}.$$

Using that U and V are unitary and using the cyclic property of trace, we have

$$\operatorname{Tr} A + \operatorname{Tr} C \geq 2\operatorname{Re}(\operatorname{Tr} VBU^{-1}).$$

We now choose U and V so that VBU^{-1} is the singular value decomposition of B. Therefore, we have $2\operatorname{Re}(\operatorname{Tr} VBU^{-1}) = 2\|B\|_{\phi_1}$. A and C are positive semidefinite, being principal submatrices of a positive semidefinite matrix. Therefore, We also have $\operatorname{Tr} A = \|A\|_{\phi_1}$ and $\operatorname{Tr} C = \|C\|_{\phi_1}$. The result follows. □

Because K is a continuous positive definite kernel, the functions k_{i_1,i_1} are continuous functions of positive type and hence the Fourier series converges absolutely uniformly to the original function [**59**, Theorem 34.5]. For k_{i_1,i_2}, we have, by Lemma 1.17 with $V = V_\pi$, $A = \widehat{k_{i_1,i_1}}_\pi$, $C = \widehat{k_{i_2,i_2}}_\pi$, $B = \widehat{k_{i_1,i_2}}_\pi$, the inequality

$$2\|\widehat{k_{i_1,i_2}}_\pi\|_{\phi_1} \leq \|\widehat{k_{i_1,i_1}}_\pi\|_{\phi_1} + \|\widehat{k_{i_2,i_2}}_\pi\|_{\phi_1}.$$

Hence the Fourier series of k_{i_1,i_2} converges absolutely uniformly as well [**59**, Theorem 34.10].

Realness. A representation is of real type if $\pi \cong \overline{\pi}$. This is equivalent to the existence of a basis v_i of V_π such that the matrix coefficients $\langle v_i, \pi(g)v_j\rangle$ are real-valued on G. With such a choice of basis, the functions e_ξ with $\xi \in \Xi$ are real-valued and we obtain an inclusion $C_c(\Xi \times \Xi, \mathbb{R}) \subseteq C(X \times X, \mathbb{R})$. This also has a dense image, because sending a kernel to its real part $K \mapsto \frac{1}{2}(K + \overline{K})$ is bounded with respect to the uniform norm. Sending an element of $C_c(\Xi \times \Xi)$ to its real part preserves such properties as G-invariance and positivity and hence we also deduce density of $C_c(\Xi \times \Xi, \mathbb{R})^G_{\succeq 0}$ in $C(X \times X, \mathbb{R})^G_{\succeq 0}$. If there exists a representation π which is not of real type and $\mathrm{Hom}_G(X, V_\pi) \neq 0$, then the functions e_ξ are not necessarily real-valued and we may not restrict to real-valued kernels in the above way. However, a semidefinite program over the complex numbers can be written as a semidefinite program over the real numbers, albeit of twice the size.

1.5. Discussion

There exist topological obstructions to condition (ii). Consider singular homology with integral coefficients. If $pR = 1_{X/G}$, then this induces maps on homology groups $H_i(p)H_i(R) = 1_{H_i(X/G)}$ for all $i \geq 0$. Consider the double cover of the circle and the group action by $\mathbb{Z}/2\mathbb{Z}$ on this space. Then the quotient space is given by the circle as well and $p : X \to X/G$ is a self-map of the circle. We have $H_1(\mathbb{S}) \cong \mathbb{Z}$ and the map $H_1(p)$ is given by multiplication by 2. Hence, there cannot be such a function R, since in this case $H_1(p)$ would be surjective. We see that conditions (i) and (iii) are satisfied, but condition (ii) is not.

Let us now mention some cases for which the conditions are always satisfied. If X is a connected manifold of dimension $n+1$, G is a connected Lie group, and the action of G is smooth with at least one n-dimensional orbit, all conditions are satisfied; see [**86**]. If X/G is finite, then all conditions are satisfied. Therefore, we will see in Chapter 4, that for any natural number t, the space $\mathcal{I}_t$ for the equiangular lines problem satisfies all conditions. In Chapter 5, we will show that the space $\mathcal{I}_2$ for the kissing number problem satisfies all conditions.

What about general $\mathcal{I}_t$? Suppose V is a topological packing graph with the structure of a differentiable manifold and it has a smooth transitive action by a compact group G. For such a graph V, this space $\mathcal{I}_t$ may be constructed as a G-subspace of a quotient of V^t by the permutation group $\mathfrak{S}_t$, and $\mathcal{I}_t$ inherits the diagonal action of G on V^t. Someone with sufficient interest may wish to investigate when the conditions of this chapter are satisfied. Let us note some properties which may be useful in this regard. If a pair (X, G) satisfies the assumptions, then so does the pair $(X \times X, G \times G)$ defined by the product action. If Y is a G-invariant and closed subspace of X, then it also satisfies the conditions. Let us finally mention again that conditions (ii) and (iii) appear to bear a close relation to the notion of a slice in differential geometry [**18**].

Perhaps it would also be interesting to find a global version of these statements. By this we mean, vaguely speaking, the following. Assume such functions R exist locally on X/G. Then we can perform a Fourier transform locally. A global Fourier transform would then be defined by an appropriate way of agreeing on overlaps. In this context, perhaps it is worthwhile to have a look at a paper by Kuryatnikova and Vera [**68**].

CHAPTER 2

Method I

Recall that by “method” we shall mean a construction of the space of invariants (3) and an algorithm to compute the zonal Stiefel harmonics. As we have seen in Chapter 1, this is what is required to describe the cone of invariant positive definite kernels and, by extension, to calculate the program (1). For our applications, we will be interested in the space

$$V_\pi^{\mathrm{O}(n-t)} = \{v \in V_\pi \mid \pi(g)v = v \text{ for all } g \in \mathrm{O}(n-t)\} \tag{21}$$

for every irreducible representation (π, V_π) of $\mathrm{O}(n)$. Here, the group $\mathrm{O}(n-t)$ is defined to be group which stabilises the first t standard basis elements $e_1, \ldots, e_t$ pointwise. Such invariants for certain pairs of classical groups are described in a paper by Gross and Kunze [**57**]. This paper, however, is of such a general nature that is difficult to verify for nonspecialists. This chapter is intended to serve as a vademecum in the case of the orthogonal group. By working out this case, we hope to have made their result, namely the complete description of the space (21), more concrete, accessible and ready to use. That is the main contribution of this chapter.

We also deduce some minor additional facts. We show realness of the matrix coefficients and work out the relationship between invariants of the real versus the complex orthogonal group; these calculations are taken from the paper on equiangular lines by De Laat, Machado and the author of this thesis [**41**]. We also give a slightly different description of the case $n = 2t$. At the end, we give a summary.

Let us motivate the construction. Let G be the general linear group, which is the group of invertible $n \times n$ matrices with entries from $\mathbb{C}$. Let D be the subgroup of diagonal matrices and let N_1 and N_3 be the subgroup of upper, respectively lower, triangular matrices with 1s on the diagonal. Given an irreducible representation S of G, the space S^{N_1} of N_1-invariants is an irreducible, one-dimensional representation λ of D called the highest weight. It may be shown that two irreducible representations of G are isomorphic if and only their highest weights are isomorphic. Let us call an irreducible representation λ of D inductive if it arises as a highest weight. To construct all irreducible representations of G, it then suffices to characterise which λ are inductive and give a construction of the irreducible representation with that weight. For this bitriangular structure, that is the content of the Borel-Weil theorem. The functor $(-)^{N_1}$ defined by $S \mapsto S^{N_1}$ has a left adjoint, to which we shall refer as the induced representation Ind_D^G. For inductive λ, the induced representation $\mathrm{Ind}_D^G\lambda$ is the irreducible representation of G with highest weight λ. It is given explicitly by

$$\mathrm{Ind}_D^G\lambda = \{f : G \to \mathbb{C} | \, f \text{ is regular and } f(n_3 dx) = \lambda(d)f(x)\}.$$

where the equation should hold for all $d \in D, n_3 \in N_3$ and $x \in G$. For a proof of the above statements, we refer to [**57**, Theorem 6.11 and Section 6.18]. The above is an example of bitriangular structures, which are studied more generally in the paper by Gross and Kunze. The representations of $\mathrm{O}(n)$ with nontrivial $\mathrm{O}(n-t)$-invariants are given by the induced representations for a different choice of bitriangular structure for $\mathrm{O}(n)$.

2.1. Orthogonal geometry

Let us review some definitions and facts from the theory of vector spaces with a bilinear form [**3**]. Let V be a vector space over $\mathbb{C}$ and let F be a symmetric bilinear form on V, by which we mean a bilinear function from $V \times V$ to $\mathbb{C}$ symmetric under interchanging the two components. When a symmetric bilinear form F is in mind for a vector space V, we say V has orthogonal geometry. If a space V has orthogonal geometry, it is called nonsingular if there is no nonzero $v \in V$ such that $F(v, w) = 0$ for all $w \in V$. An element $v \in V$ is called isotropic if $F(v, v) = 0$. A space V is called isotropic if every element of V is isotropic. For a subspace U of V, we denote by $U^\perp$ the subspace of all $w \in V$ such that for all $u \in U$, we have $F(w, u) = 0$. For a vector space V, we denote by V^* the dual vector space of all $\mathbb{C}$-linear maps from V into $\mathbb{C}$. Notice a space V is nonsingular if and only if the map $V \to V^*$ defined by $v \mapsto F(v, -)$ is injective. We now prove some basic facts.

Proposition 2.1. *If V is nonsingular and U is a nonsingular subspace, then $V = U \oplus U^\perp$.*

Proof. We may define a map $V \to U^*$ by $v \mapsto F(v, -)$, which factorises through a map $V/U^\perp \to U^*$. Since U is nonsingular, this map is injective and hence we have $\operatorname{codim} U^\perp \leq \dim U$. Furthermore, we may define an injective map $U^\perp \to V^*$ by $w \mapsto F(w, -)$, which factorises through the injective map $(V/U)^* \to V^*$. Hence we have $\dim U^\perp \leq \operatorname{codim} U$. We then have $\dim U^{\perp\perp} \leq \operatorname{codim} U^\perp \leq \dim U$. Since we also have $U \subseteq U^{\perp\perp}$, equality must occur throughout. The map $U \oplus U^\perp \to V$ defined by $(u, w) \mapsto u + w$ is injective, since U is nonsingular. By the above result on dimension, it must be surjective too and we have $V = U \oplus U^\perp$. □

Proposition 2.2. *If V is nonsingular and U is a nonsingular subspace, then $U^\perp$ is nonsingular.*

Proof. Let $w \in U^\perp$ and $F(w, w') = 0$ for all $w' \in U^\perp$. Since $V = U \oplus U^\perp$, we then have $F(w, v) = 0$ for all $v \in V$. Hence $w = 0$. □

Let V have orthogonal geometry and let U be a subspace. A basis

$$\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n$$

of V will be called hyperbolic if the subspaces spanned by $\alpha_1, \ldots, \alpha_n$ and $\beta_1, \ldots, \beta_n$ are isotropic and

$$F(\alpha_i, \beta_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases} \tag{22}$$

We call the vector space V hyperbolic if it has a hyperbolic basis. A hyperbolic vector space is necessarily nonsingular.

Let V be a nonsingular vector space and let U be a subspace. In the rest of this chapter, we define $\dim V = n$ and $\dim U = t$. We say U has a hyperbolic resolution if there is a hyperbolic basis $(\alpha_1, \ldots, \alpha_t, \beta_1, \ldots, \beta_t)$ of a subspace W of V such that

$$U = \operatorname{Span}\{\alpha_i + \beta_i \mid 1 \leq i \leq t\}.$$

If a subspace U of V has a hyperbolic resolution, then U is nonsingular and we have

$$n \geq 2t \tag{23}$$

Conversely, we have

PROPOSITION 2.3. *Let V be a nonsingular vector space and U a nonsingular subspace satisfying* 23. *Then U has a hyperbolic resolution.*

PROOF. By [**3**, Theorem 3.7], U has an orthogonal basis $\sigma_1, \dots, \sigma_t$ and $U^\perp$ has an orthogonal basis $\tau_1, \dots, \tau_{n-t}$ such that none of the elements of the bases is isotropic. Note $n - t \geq t$. We may normalise so that

$$F(\sigma_j, \sigma_j) = \frac{1}{2}, \quad F(\tau_j, \tau_j) = -\frac{1}{2}, \quad 1 \leq j \leq t$$

Let $\alpha_j = \sigma_j + \tau_j$ and $\beta_j = \sigma_j - \tau_j$ for $1 \leq j \leq t$. Then $\alpha_1, \dots, \alpha_t, \beta_1, \dots, \beta_t$ is a hyperbolic basis for a submodule of V and U is spanned by $\alpha_1 + \beta_1, \dots, \alpha_t + \beta_t$. $\square$

2.2. Bitriangular structure

Throughout this section, let (V, F) be a nonsingular vector space. We suppose that U is a subspace of V of dimension t with a hyperbolic resolution given by a hyperbolic basis $\alpha_1, \dots, \alpha_t; \beta_1, \dots, \beta_t$ of a subspace as in 2.1. Thus, $\alpha_1 + \beta_1, \dots, \alpha_t + \beta_t$ is an orthogonal base for U such that $F(\alpha_j + \beta_j, \alpha_j + \beta_j) = 2$ $(1 \leq j \leq t)$. Let V_1 be the vector space spanned by $\alpha_1, \dots, \alpha_t$ and V_3 the vector space spanned by $\beta_1, \dots, \beta_t$. Then $V_1 \oplus V_3$ is a hyperbolic, hence nonsingular, subspace of V. By the Proposition 2.1, we then have

$$V = V_1 \oplus V_2 \oplus V_3, \tag{24}$$

where $V_2 = (V_1 \oplus V_3)^\perp$. The decomposition (24) will be fixed throughout this section and called the decomposition of V given by the hyperbolic resolution of U. A linear map $g \in \mathrm{End}(V)$ decomposes into a matrix (g_{ij}) with $g_{ij} \in \mathrm{Hom}(V_i, V_j)$ accordingly.

We now study duality and adjoints. We may define a map $V_3 \to V_1^*$ by $\beta \mapsto F(\beta, -)$. By (22), this is injective and by $\dim V_3 = \dim V_1$, it must be bijective. The same is true if the indices 1 and 3 are interchanged. The subspace $V_1 \oplus V_3$ is nonsingular and hence V_2 is too by Proposition 2.2. Hence the map $V_2 \to V_2^*$ defined by $v \mapsto F(v, -)$ is bijective. To study the adjoint with respect to F, it is convenient to adopt the following convention in regard to subscripts:

$$1' = 3, \quad 3' = 1, \quad \text{and} \quad 2' = 2.$$

Then to each linear transformation $h : V_i \to V_j$ $(1 \leq i, j \leq 3)$ there corresponds a unique linear transformation $h' : V_{j'} \to V_{i'}$, defined by

$$F(h\phi_i, \phi_{j'}) = F(\phi_i, h'\phi_{j'}) \tag{25}$$

for all $\phi_i \in V_i$ and $\phi_{j'} \in V_{j'}$. Since V is nonsingular, we define the adjoint of $g \in \mathrm{End}(V)$ with respect to F as the unique linear map g^* such that $F(\phi, g\psi) = F(g^*\phi, \psi)$ for all $\phi, \psi \in V$.

LEMMA 2.4. *Let $g \in \mathrm{End}(V)$. Then the matrix of g^* is given by*

$$(g^*)_{ij} = (g_{j'i'})' \tag{26}$$

for $1 \leq i, j \leq 3$.

Proof. Let $\phi_i \in V_i$ and $\phi_j \in V_j$. On the one hand, we have

$$F(g\phi_i, \psi_{j'}) = F(\phi_i, g^* \psi_{j'}) = F(\phi_i, g^*_{i'j'} \psi_{j'}).$$

On the other hand, we have

$$F(g\phi_i, \psi_{j'}) = F(g_{ji}\phi_i, \psi_{j'}) = F(\phi_i, (g_{ji})' \psi_{j'}).$$

Thus, $(g^*)_{i'j'} = (g_{ji})'$, which proves the lemma. $\square$

Proposition 2.5 ([**57**, Proposition 4.5]). *Let g be an linear transformation of V. The following are equivalent:*

(i) *g is an isometry;*
(ii) *$gg^* = 1$;*
(iii) *$\delta_{ij'} = g_{i1}g'_{j3} + g_{i2}g'_{j2} + g_{i3}g'_{j1}$ for all $i, j = 1, 2, 3$;*
(iv) *$g^*g = 1$;*
(v) *$\delta_{i'j} = g'_{3i}g_{1j} + g'_{2i}g_{2j} + g'_{1i}g_{3j}$ for all $i, j = 1, 2, 3$.*

Here, (g_{ij}) is the matrix of g and (δ_{ij}) denotes the matrix of the identity transformation 1_V of V.

To simplify notation, we drop parentheses and write g_{ij} and g'_{ij}. The form (26) for the adjoint of g can be remembered as follows: The matrix of g^* is obtained from that of g by placing a prime on each entry and reflecting the entries across the off-diagonal. Thus, a linear transformation

$$g = \begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$$

is an isometry if and only if

$$g^* = \begin{bmatrix} g'_{33} & g'_{23} & g'_{13} \\ g'_{32} & g'_{22} & g'_{12} \\ g'_{31} & g'_{21} & g'_{11} \end{bmatrix}$$

Throughout the rest of this section, we denote the isometry group by $\mathrm{O}(V)$. The group of those isometries with determinant 1 will be denoted by $\mathrm{SO}(V)$. Note that this group depends on F implicitly.

Occasionaly, we will refer to closed subgroups of the orthogonal group as a group of isometries: a group of which every element is an isometry. We are principally concerned with a bitriangular structure for the groups $\mathrm{O}(V)$ and $\mathrm{SO}(V)$. In the following, we use G to denote either. Let D denote the set of all $g \in G$ which map V_i to V_i for all $i = 1, 2, 3$. Next, for $i = 1$ and $i = 3$, define N_i to be the collection of all $g \in G$ which satisfy the following three conditions:

(i) $gv_i = v_i$ for all $v_i \in V_i$;
(ii) $gv_2 \in V_i + V_2$ for $v_2 \in V_2$;
(iii) g acts as the identity on both $(V_i + V_2)/V_i$ and $V/(V_i + V_2)$.

Clearly, N_1, D, N_3 are subgroups of G that depend on the given hyperbolic resolution of the subspace U. However, they depend in a sensible manner up to conjugacy on U. In any case, these groups will be fixed once and for all, and for brevity, the triple (N_1, D, N_3) will be called the bitriangular structure for G associated with U.

These groups can be characterized in terms of matrices as follows: D consists of all transformations in G whose matrices are diagonal. N_1 consists of all transformations g in G having upper triangular matrices such that $g_{11} = g_{22} = g_{33} = 1$. N_3 consists of the transformations analogous to those in N_1 but having lower triangular matrices. We now work this out in a bit more detail, partly by providing references.

LEMMA 2.6. *The map $g \in G$ is in D if and only if its matrix (g_{ij}) is diagonal and*

$$g_{33}^* = g_{11}^{-1}, \quad \text{and} \quad g_{22}^* = g_{22}^{-1}.$$

PROOF. The lemma follows immediately from the fact that g maps V_j to V_j for all j, and from Proposition 2.5. □

We define a map $\Phi_1 : \mathrm{GL}(V_1) \to \mathrm{O}(V)$

$$\delta_1 \mapsto d_1 = \mathrm{diag}(\delta_1, 1, \delta_1^\vee) \tag{27}$$

and a map $\Phi_2 : \mathrm{O}(V_2) \to \mathrm{O}(V)$

$$\delta_2 \mapsto d_2 = \mathrm{diag}(1, \delta_2, 1). \tag{28}$$

Here

$$\delta_1^\vee = (\delta_1')^{-1}. \tag{29}$$

We then define $D_1 = \mathrm{im}(\Phi_1)$. The definition of D_2 depends on G: If $G = \mathrm{O}(V)$, we define $D_2 = \Phi_2(\mathrm{O}(V_2))$ and if $G = \mathrm{SO}(V)$, we define $D_2 = \Phi_2(\mathrm{SO}(V_2))$. From the previous lemmas, we then see $D = D_1 D_2$. Thus, the general element of D is

$$d = d_1 d_2 = d(\delta_1, \delta_2) = \mathrm{diag}(\delta_1, \delta_2, \delta_1^\vee). \tag{30}$$

for $\delta_1 \in \mathrm{GL}(V_1)$ and $\delta_2 \in \mathrm{O}(V_2)$, respectively $\delta_2 \in \mathrm{SO}(V_2)$. Furthermore, for any $d \in D$, we have $\det d = \det \delta_1 \det \delta_2 \det \delta_1^\vee = \det \delta_2$. Hence $d \in \mathrm{SO}(V)$ if and only if $\delta_2 \in \mathrm{SO}(V)$. Here we used

LEMMA 2.7. *We have $\det g = \det g'$ for all $g \in \mathrm{End}(V_1)$.*

PROOF. We have

$$(g')_{ij} = F(\alpha_i, g'\beta_j) = F(g\alpha_i, \beta_j) = g_{ji}$$

and the result follows from the usual formula of the determinant. □

By [**57**, Lemma 4.9], The subgroup N_1 consists of the elements

$$n_1 = n_1(\eta_1, \eta_2) = \begin{bmatrix} 1 & \eta_1 & \eta_2 \\ 0 & 1 & -\eta_1' \\ 0 & 0 & 1 \end{bmatrix} \tag{31}$$

where $\eta_1 \in \mathrm{Hom}(V_2, V_1)$, $\eta_2 \in \mathrm{Hom}(V_3, V_1)$, and

$$\eta_2' + \eta_2 + \eta_1\eta_1' = 0. \tag{32}$$

Similarly, by [**57**, Lemma 4.10], N_3 consists of the elements

$$n_3 = n_3(\xi_1, \xi_2) = \begin{bmatrix} 1 & 0 & 0 \\ \xi_1 & 1 & 0 \\ \xi_2 & -\xi_1' & 1 \end{bmatrix} \tag{33}$$

with $\xi_1 \in \mathrm{Hom}(V_1, V_2)$, $\xi_2 \in \mathrm{Hom}(V_1, V_3)$, and

$$\xi_2 + \xi_2' + \xi_1\xi_1' = 0. \tag{34}$$

Let k be an infinite field. In the book by Waterhouse [**112**], an algebraic matrix group is defined to be a closed subgroup of $\mathrm{SL}(n, k)$ and an affine algebraic group as a Zariski closed subset of k^n with a group law. These are then shown to be equivalent notions. We mention this here, since we will reference this book for some facts, such as

PROPOSITION 2.8 ([**112**, Section 5.2]). *The affine varieties* $\mathrm{SO}(V)$ *and* $\nu\mathrm{SO}(V)$ *over* $\mathbb{C}$ *are irreducible.*

Let G be an affine algebraic group over $\mathbb{C}$ and N_1, D, N_3 algebraic subgroups of G. We say that (N_1, D, N_3) is a bitriangular structure for G if we have:

(i) that N_1 and N_3 are unipotent subgroups normalized by D;
(ii) that $N_i D$ is the semidirect product of D and N_i for $i = 1, 3$;
(iii) that the product $(n_1, d, n_3) \to n_3 d n_1$ is a biregular map of $N_1 \times D \times N_3$ onto an open dense subset of G.

PROPOSITION 2.9. *The bitriangular structure associated to* U *is a bitriangular structure for* $\mathrm{O}(V)$ *if* $n > 2t$ *and for* $\mathrm{SO}(V)$ *if* $n \geq 2t$.

Since the determinant of elements of the subgroups N_1 and N_3 is always 1, these subgroups agree for the cases $\mathrm{O}(V)$ and $\mathrm{SO}(V)$. However, D differs.

PROOF. For (i), recall that a subgroup of the general linear group is unipotent if all its elements are unipotent and an element r is unipotent if $r-1$ is nilpotent, i.e. $(r-1)^m = 0$ for a natural number m. The fact that N_1 and N_3 are unipotent follows immediately from equations 31 and 33. For (ii), recall that $N_i D$ is the semidirect product of N_i and D if $N_i \cap D = \{1\}$. This follows immediately from lemmas 2.6, 31 and 33.

We now show (iii). By [**57**, Theorem 4.14], the image of multiplication is equal to the Zariski open subset $D(\det g_{11}) = G \backslash V(\det g_{11})$. We first consider the case with $G = \mathrm{SO}(V)$ and $n \geq 2t$. We have $1 \in D(\det g_{11}) \cap \mathrm{SO}(V)$ and hence $D(\det g_{11}) \cap \mathrm{SO}(V)$ is a nonempty open subset of $\mathrm{SO}(V)$. Because $\mathrm{SO}(V)$, is irreducible, the subset $D(\det g_{11}) \cap \mathrm{SO}(V)$ is dense in $\mathrm{SO}(V)$, which is what we wanted to show. We now consider the case with $G = \mathrm{O}(V)$ and $n > 2t$. As before, $1 \in D(\det g_{11}) \cap \mathrm{SO}(V)$, and hence $D(\det g_{11}) \cap \mathrm{SO}(V)$ is a dense subset of $\mathrm{SO}(V)$. Since $n > 2t$, we may choose $\delta_2 \in \mathrm{O}(V_2)$ with $\det \delta_2 = -1$. We then have $d_2(\delta_2) \in D(\det g_{11}) \cap \nu\mathrm{SO}(V)$ and as before $D(\det g_{11}) \cap \nu\mathrm{SO}(V)$ is dense in $\nu\mathrm{SO}(V)$. Since $\mathrm{O}(V) = \mathrm{SO}(V) \cup \nu\mathrm{SO}(V)$, $D(\det g_{11})$ is dense in $\mathrm{O}(V)$. Biregularity follows from [**57**, Theorem 4.14]. □

2.3. Induced representations

Let G be an affine algebraic group over $\mathbb{C}$. Here and throughout the rest of the paper, it will be understood that all representations of G are algebraic. We say that a representation (π, S) of G is algebraic if S is a $\mathbb{C}$-vector space of finite dimension and the matrix entries of π are regular functions on G. If (π, S) is a representation of G, we write $x \cdot \phi$ for $\pi(x)\phi$ ($x \in G, \phi \in S$) and simply call S a G-module whenever it is unnecessary to emphasize π.

Suppose G has a specified bitriangular structure (N_1, D, N_3), and let S be a G-module. Then the space

$$S^{N_i} = \{\phi \in S : n_i \cdot \phi = \phi \text{ for all } n_i \in N_i\}$$

of N_i-invariants of S will be denoted by S_i (where $i = 1, 3$). The subspace of S spanned by

$$\{n_i \cdot \phi - \phi : n_i \in N_i, \phi \in S\}$$

will be denoted by $S^{(i)}$. We now give a characterisation of the spaces $S^{(i)}$. Let S^* be the dual vector space as in Section 2.1 and let the duality $S \times S^*$ define an adjoint: for $A \in \mathrm{End}(S)$ and $\psi \in S^*$, we define $A^*\psi = \psi \circ A$. The dual representation $\pi^\vee : G \to \mathrm{GL}(S^*)$ is then defined as $\pi^\vee(g) = (\pi(g^{-1}))^*$. We verify that the space $S^{(i)}$ is annihilated by $(S^*)_i$, which is the space of N_i-invariants in S^*. Indeed, for $\psi \in S^*$ and $\phi \in S$, we have

$$\langle \pi(n_i)\phi - \phi, \psi \rangle = \langle \phi, \pi^\vee(n_i)\psi \rangle - \langle \phi, \psi \rangle$$

Showing that $S^{(i)}$ is annihilated by $(S^*)_i$. Moreover, in the paper by Gross and Kunze it is stated that $S^{(i)}$ exactly the space of all elements which are annihilated by $(S^*)_i$. We remark that for the results that follow, only the inclusion of $S^{(i)}$ in the space annihilated by $(S^*)_i$ is required. Finally, we set $S_2 = S^{(1)} \cap S^{(3)}$. These spaces play an important role in the results that follow.

Lemma 2.10. *Let G be an affine algebraic group with a specified bitriangular structure (N_1, D, N_3) and S a G-module. Then S_i $(1 \le i \le 3)$ is a D-submodule of S, and S_1 and S_3 are always nonzero. Moreover, $S^{(i)}$ is a proper N_iD-submodule of S and $S^{(i)} \neq 0$ if and only if $S_i \neq S$ $(i = 1, 3)$.*

Proof. Since N_1 and N_3 are unipotent, they act by unipotent transformations on S [**112**, Section 8.1]. Hence, Kolchin's theorem [**112**, Section 8.2] implies that S_1 and S_3 are nonzero. Hence the space $(S^*)_i$ is nonzero too. By the inclusion of $S_{(i)}$ in the subspace annihilated by $(S^*)_i$, we obtain $\dim S^{(i)} + \dim(S^*)_i = \dim S$. Hence we see that $S^{(1)}$ and $S^{(3)}$ are proper subspaces (possibly 0) of S. For $i = 1$ and $i = 3$, the invariance of S_i under D and that of $S^{(i)}$ under N_iD is a straightforward consequence of (i). It follows that S_2 is also stable under D. The final statement follows immediately from the definitions of $S^{(i)}$ and S_i. □

We give the main structure theorem.

Theorem 2.11 ([**57**, Theorem 6.6]). *Let G be an affine algebraic group with a specified bitriangular structure (N_1, D, N_3) and S a G-module. If S is an irreducible G-module, then the space S_i of N_i invariants in S is an irreducible D-module, and*

$$S = S_1 \oplus S^{(3)} = S^{(1)} \oplus S_3. \tag{35}$$

If S is an irreducible G-module and $S_1 \neq S$ or $S_3 \neq S$, then

$$S^{(1)} = S_1 \oplus S_2, \quad S^{(3)} = S_2 \oplus S_3, \tag{36}$$

and

$$S = S_1 \oplus S_2 \oplus S_3. \tag{37}$$

Conversely, if S_1 or S_3 is an irreducible D-module and S is generated as a G-module by S_1 or S_3 respectively, then S is an irreducible G-module.

Given a group G and a subgroup D of G, one may define a functor Res_D^G from the category of G-modules to the category of D-modules by restriction. This functor has a left-adjoint, which is commonly referred to as the induced representation. We shall consider a slightly different notion of induced representation. Consider the functor $(-)_1$ from the category of G-modules to the category of D-modules given by sending S to the space of N_1-invariants S_1. We will now show that this functor has a left-adjoint, which we will denote by Ind_D^G. This does not appear explicitly in [**57**], though it follows straightforwardly from their results.

Theorem 2.12. *The functor* $(-)_1$ *has a left adjoint* Ind_D^G *and for a* G*-module* S *we have* $S \cong \mathrm{Ind}_D^G(S_1)$.

Proof. Recall [**75**, Section 2.1] for the definition of an adjoint functor. We have to show an isomorphism

$$\mathrm{Hom}(\mathrm{Ind}_D^G W, S) \cong \mathrm{Hom}(W, S_1), \tag{38}$$

which is natural in U and S. The functor $(-)_1$ preserves sums, and therefore it is sufficient to prove this for S irreducible. By Theorem 2.11, S_1 is then irreducible too. We first define the functor Ind_D^G on objects, starting with irreducible representations. Let W be an irreducible representation of D. If W is inductive, we define $\mathrm{Ind}_D^G W$ to be any representation such that $(\mathrm{Ind}_D^G W)_1 = W$. Since W is irreducible, we may, by Theorem 2.11, choose $\mathrm{Ind}_D^G W$ to be irreducible. If W is not inductive, we define $\mathrm{Ind}_D^G W = 0$. If $W \cong S_1$, then W is inductive and by [**57**, Theorem 6.8], we have $\mathrm{Ind}_D^G W \cong S$. Therefore, by Schur's lemma, equation (38) holds. If $W \ncong S_1$ and W is not inductive, then again by Schur's lemma, equation (38) holds. If $W \ncong S_1$ and W is inductive, then we cannot have $\mathrm{Ind}_D^G W \cong S$, since then $W \cong S_1$. Therefore, again by Schur's lemma, equation (38) holds. We now define Ind_D^G for general objects W. Let $W = \oplus_i W_i$ be a decomposition into irreducibles. We then define $\mathrm{Ind}_D^G(W) = \oplus_i \mathrm{Ind}_D^G(W_i)$. By compatibility of Hom with direct sums, equation (38) holds. What's left is to define Ind_D^G for morphisms. Again, by compatibility of Hom with direct sums, it suffices to do so for $p\colon W \to W'$ with W and W' both irreducible. By Schur's lemma, either $p = 0$, or it is an isomorphism. If $p = 0$, we define $\mathrm{Ind}_D^G(p) = 0$ too. We therefore assume p is an isomorphism. If W and W' are not inductive, we define $\mathrm{Ind}_D^G(p)$ to be zero. If W and W' are inductive, then $\mathrm{Ind}_D^G(p)$ is defined by equation (38).

We now show naturality. Recall that the isomorphism (38) in either direction is denoted by $\overline{(-)}$ and is referred to as the transpose. We have to show the equalities

$$\overline{\left(\mathrm{Ind}_D^G(W) \xrightarrow{g} S \xrightarrow{q} S'\right)} = \left(W \xrightarrow{\bar{g}} S_1 \xrightarrow{q_1} S_1'\right)$$

and

$$\overline{\left(W' \xrightarrow{p} W \xrightarrow{f} S_1\right)} = \left(\mathrm{Ind}_D^G(W') \xrightarrow{\mathrm{Ind}_D^G(p)} \mathrm{Ind}_D^G(W) \xrightarrow{\bar{f}} S\right)$$

for all $p\colon W \to W'$, $q\colon S \to S'$, $f\colon \mathrm{Ind}_D^G(W) \to S$ and $g\colon W \to S_1$. By compatibility of $\mathrm{Ind}_D^G, (-)_1$, Hom and $\overline{(-)}$ with direct sums, we may assume without loss that S, S', W, W' are all irreducible. These equations then follow from the construction and Schur's lemma.

Finally, we show $S \cong \mathrm{Ind}_D^G(S_1)$ for every G-module S. Again, by compatibility with direct sums, we may assume S is irreducible. Therefore $\mathrm{Ind}_D^G(S_1)$ is an irreducible representation of G and we have $(\mathrm{Ind}_D^G(S_1))_1 \cong S_1$. The isomorphism $S \cong \mathrm{Ind}_D^G(S_1)$ then follows from [**57**, Theorem 6.8]. $\square$

The preceding theorem shows that an irreducible representation (π, S) of a group G with a bitriangular structure (N_1, D, N_3) is determined up to equivalence by the corresponding representation

$$\lambda_1 : d \mapsto \pi(d)|_{S_1}, \quad d \in D$$

of D. Let λ_2 and λ_3 denote the representations of D that are defined by S_2 and S_3, respectively. We call λ_1 the highest D-type of π, λ_2 the intermediate D-type of π, and λ_3 the lowest D-type of π for the bitriangular structure (N_1, D, N_3).

If (λ, W_λ) is an irreducible representation of D, we say that λ is *inductive* for (N_1, D, N_3) if there is an irreducible representation of G with highest D-type equivalent to λ. Thus, a D-module W is inductive for (N_1, D, N_3) if there is an irreducible G-module S such that S_1 and W are isomorphic D-modules. Since D may have irreducible representations that are not inductive for (N_1, D, N_3), it is important to find criteria for inductivity.

Let $F(\lambda)$ denote the set of regular maps $f : G \to W$ which satisfy

$$f(n_3 dx) = \lambda(d) f(x), \tag{39}$$

for all $n_1 \in N_1$, $d \in D$, and $x \in G$. Then $F(\lambda)$ is a vector space on which G acts by right translation.

Proposition 2.13. *Let λ be an irreducible representation of D. If λ_1 is polynomial and λ_2 is trivial, then λ is inductive. Furthermore, $F(\lambda)$ is the irreducible representation with highest D-type equivalent to λ.*

2.4. Invariants

As in Section 2.2, let U be a subspace of V of dimension t and H the subgroup of G consisting of elements that leave U pointwise fixed. In this section, we summarise the results on H-invariants in irreducible representations of G. If S is a G-module, let S^H denote the subspace of H-invariants. If (π, S) is an irreducible representation of G with highest D-type λ, we give a sufficient condition on λ for the existence of nonzero H-invariants. Whether this condition is necessary depends on whether the orthogonal and special orthogonal group is considered. This will be studied in the subsequent subsections. Moreover, when π is realized as an induced representation, this correspondence is given explicitly and provides a construction for all the H-invariants in the induced module $F(\lambda)$.

We will need to introduce the isometry e. Recall that V_1 and V_3 are isotropic subspaces with bases $\alpha_1, \ldots, \alpha_t$ and $\beta_1, \ldots, \beta_t$ respectively, that $\alpha_1, \ldots, \alpha_t, \beta_1, \ldots, \beta_t$ is a hyperbolic basis for $V_1 \oplus V_3$, and that $V_2 = (V_1 \oplus V_3)^\perp$. Let e be the complex-linear transformation on V defined by

$$e\alpha_i = \beta_i, \quad e\beta_i = \alpha_i, \quad e\gamma = \gamma$$

for $1 \le i \le r$ and $\gamma \in V_2$. In the decomposition according to (24), the matrix (e_{ij}) of e has the form

$$\begin{bmatrix} 0 & 0 & e_{13} \\ 0 & e_{22} & 0 \\ e_{31} & 0 & 0 \end{bmatrix}$$

where $e_{13}\beta_i = \alpha_i$, $e_{22} = 1_{V_2}$, and $e_{31}\alpha_i = \beta_i$. Furthermore, recall that the group D is the direct product of the subgroups D_1 and D_2, where D_1 is isomorphic to $\mathrm{GL}(V_1)$ and $D_2 = \mathrm{O}(V_2)$, respectively $D_2 = \mathrm{SO}(V_2)$, is a subgroup of H.

LEMMA 2.14 ([**57**, Lemma 7.2]). *Let (π, S) be an irreducible representation of G with highest D-type λ. If $S^H \neq 0$, then λ_2 is trivial.*

THEOREM 2.15 ([**57**, Theorem 7.6]). *Let $F(\lambda)$ be the irreducible representation of G with highest D-type equivalent to λ and let λ_2 be trivial and λ_1 be polynomial. The linear mapping $T\colon W \to F(\lambda)$ defined for $\phi \in W$ by*

$$T(\phi)(x) = \lambda_1(x_{11} + x_{13}e_{31})\phi, \quad x \in G$$

is an isomorphism from the space W of λ_1 onto the space $\mathcal{S}^H$ of H-invariants.

We occasionally denote $T(\phi)$ by f_ϕ to reduce visual clutter.

The orthogonal group with $n > 2t$. We first consider the orthogonal group with $n > 2t$. We give a proof which is slightly different from the corresponding statement in the paper, which is [**57**, Theorem 7.5].

THEOREM 2.16. *Let $F(\lambda)$ be an irreducible representation of $\mathrm{O}(n)$ with highest D-type λ and let $n > 2t$. Then $F(\lambda)^H \neq 0$ if and only if λ_2 is trivial and λ_1 is polynomial.*

PROOF. If λ_2 is trivial and λ_1 is polynomial, then $F(\lambda)^H \neq 0$ by Theorem 2.15. Let $F(\lambda)^H \neq 0$. Then λ_2 is trivial by 2.14 and it suffices to show λ_1 is polynomial.

Then by [**57**, Theorem 6.10], there is a regular map $\lambda^{\#} : G \to \mathrm{End}(W)$ such that

$$\lambda^{\#}(x) = \lambda_1(x_{11}), \quad x \in G,\ x_{11} \in \mathrm{GL}(V_1) \tag{40}$$

Every irreducible representation of the general linear group is the tensor product of a polynomial representation with the dual of a power of the determinant [**52**, Proposition 15.47]. Hence $\lambda_1(x_{11}) = \det(x_{11})^k \lambda_1'(x_{11})$ for some k with λ_1' polynomial and λ_1' is not divisible by a further power of det. If $k \geq 0$, then λ_1 is polynomial. We will now assume $k < 0$ and show a contradiction. We have

$$\det(x_{11})^{-k}\lambda^{\#}(x) = \lambda_1'(x_{11}) \tag{41}$$

For x in the Cayley set. Now the left and right hand side are polynomial maps which agree on the Cayley set, and hence agree on G. Let ν be the map of V which interchanges α_t and β_t and leaves the rest of V fixed. In terms of the standard basis, this is the map which sends e_n to $-e_n$ and leaves the rest of the standard basis of V fixed. Then $\nu_{11}\alpha_t = 0$ and we have $\det(\nu_{11}) = 0$. Since λ_1' is not divisible by a power of k, we may fill a semistandard tableau T with numbers 1 up to $n-1$. We then have $\lambda_1'(\nu_{11})e_T = e_T$ and $\lambda_1'(\nu_{11}) \neq 0$. We see that the left and right hand side of (41) do not agree, which is a contradiction. □

Note that this proof would not work for the special orthogonal group, since ν has determinant -1.

The special orthogonal group with $n = 2t$. We now consider the special orthogonal group with $n = 2t$. We use the notation $G^+ = \mathrm{SO}(V)$ for the complex special orthogonal group and $H^+ = \mathrm{SO}(U^\perp)$. With the representations of G^+ we describe here, the irreducible representations of G with nontrivial H-invariants may be constructed. Let ν be the matrix which interchanges α_t and β_t and leaves all other α_i and β_i fixed. In the standard basis, this is the matrix such that $\nu e_i = e_i$ for all $1 \leq i < n$ and $\nu e_n = -e_n$. Then $\nu \notin G^+$ and

$$x \mapsto \nu x \nu^{-1}, \quad x \in G^+$$

is an automorphism of G^+. If $(\pi, \mathcal{S})$ is a representation of G^+, the representation $(\pi^\nu, \mathcal{S})$ defined by

$$\pi^\nu(x) = \pi(\nu x \nu^{-1}), \quad x \in G^+$$

will be called the conjugate representation of π. From [**57**, Theorem 8.2] it follows that the conjugate representation of $F(\lambda)$ is isomorphic to $F(\lambda')$, where $\lambda' = (\lambda_1, \ldots, \lambda_{t-1}, -\lambda_t)$ and every irreducible representation of G^+ is isomorphic to either $F(\lambda)$ as constructed above or its conjugate $F(\lambda')$. Furthermore, by [**57**, Theorem 8.4], we have $F(\lambda)^{H^+} = F(\lambda')^{H^+}$.

A representation of the orthogonal group G may be described by the action of G^+ together with the action of the element ν.

THEOREM 2.17 ([**57**, Theorem 8.8]). *Let $(\pi, \mathcal{S})$ be an irreducible representation of G^+ such that π is not equivalent to its conjugate π^ν. Then there is a unique irreducible representation τ of G on $\mathcal{S} \oplus \mathcal{S}$ such that $\tau = \pi \oplus \pi^\nu$ on G^+ and $\tau(\nu)$ is the transposition on $\mathcal{S} \oplus \mathcal{S}$ that interchanges components. An irreducible representation of G that is reducible upon restriction to G^+ is always equivalent to some such τ.*

THEOREM 2.18 ([**57**, Theorem 8.9]). *Let $(\pi, \mathcal{S})$ be an irreducible representation of G^+ such that π is equivalent to its conjugate π^ν. Then there is an operator A that intertwines π and π^ν such that $A^2 = I$, and A is unique up to sign. There are exactly two extensions π_ϵ, $\epsilon = 0, 1$, of π to a representation of G on $\mathcal{S}$. They are characterised by the property that*

$$\pi_\epsilon(\nu) = (-1)^\epsilon A, \quad \epsilon = 0, 1.$$

An irreducible representation of G that remains irreducible on restriction to G^+ is always equivalent to some π_ϵ.

We turn now to the problem of determining the H-invariants in irreducible G-representations. By Theorems 2.17 and 2.18, it suffices to do this for the representations given there.

THEOREM 2.19 ([**57**, Theorem 8.10]). *Let $(\pi, \mathcal{S})$ be an irreducible representation of G^+ such that π is not equivalent to its conjugate π^ν. Let τ be the corresponding representation of G on $\mathcal{S} \oplus \mathcal{S}$ described in Theorem 2.17. Then the subspace of invariants is given by*

$$(\mathcal{S} \oplus \mathcal{S})^H = \{(w, w) \mid w \in \mathcal{S}^{H^+}\}.$$

THEOREM 2.20 ([**57**, Theorem 8.12]). *Let $(\pi, \mathcal{S})$ be an irreducible representation of G^+ such that π is equivalent to its conjugate π^ν, let π_0 and π_1 be the associated representations of G, and normalize the operator A in 2.18 that intertwines π and π^ν so that A fixes every vector in $\mathcal{S}^{H^+}$. Then $\mathcal{S}^{H^+}$ is the space of $\pi_0(H)$ invariants, and there are no nonzero $\pi_1(H)$-invariants.*

The orthogonal group with $n = 2t$. We finally consider the orthogonal group with $n = 2t$. Let us note that this construction does not appear explicitly in the paper by Gross and Kunze [**57**]. As before, let

$$F(\lambda) = \{f : G \to W \mid f(n_3 d x) = \lambda(d) f(x)\},$$

where f is assumed to be regular and the equation should hold for all $d \in D, n_3 \in N_3$ and $x \in G$. Note the framework we developed does not apply directly, since in this case, we do not have a bitriangular structure for the orthogonal group; Proposition 2.9 no longer applies. However, we may use the case for the special orthogonal group with $n = 2t$. In the case $\pi \ncong \pi_\nu$, we define the maps

$$\begin{aligned} \Phi\colon F(\lambda) &\leftrightarrow S \oplus S \colon \Psi \\ f &\mapsto (f|_{G^+}, R_\nu f|_{G^+}) \\ g_1 \coprod R_\nu g_2 &\leftarrow\!\shortmid (g_1, g_2) \end{aligned}$$

and in the case $\pi \cong \pi_\nu$, we define the maps

$$\begin{aligned} \Phi\colon F(\lambda) &\leftrightarrow S \colon \Psi \\ f &\mapsto f|_{G^+} \\ g \coprod R_\nu A g &\leftarrow\!\shortmid g. \end{aligned}$$

In both cases, these maps define morphisms of representations of G. Furthermore, we have $\Phi\Psi = 1$ and hence Ψ is injective. The image of S^H resp. $(S \oplus S)^H$ under Ψ gives precisely the H-invariants in $\mathrm{im}(\Psi)$. Recall S^H is given by the regular W-valued functions on G^+ of the form

$$g_\phi(x) = \lambda_1(x_{11} + x_{13} e_{31})\phi \tag{42}$$

with $\phi \in W$. Notice, this equation defines a function on G too which we shall denote by f_ϕ. One may verify $f_\phi = R_\nu f_\phi$. If $\pi \ncong \pi_\nu$, we have

$$\Psi((g_\phi, g_\phi)) = g_\phi \coprod R_\nu g_\phi = f_\phi$$

since for $x \in \nu G^+$, we have $R_\nu g_\phi(x) = g_\phi(x\nu) = f_\phi(x\nu) = f_\phi(x)$. If $\pi \cong \pi_\nu$, we have

$$\Psi(g_\phi) = g_\phi \coprod R_\nu A g_\phi = f_\phi$$

since we have $A g_\phi = g_\phi$ and as before $R_\nu g_\phi = f_\phi$ on νG^+. Since for $x \in \nu G^+$, we have $R_\nu g_\phi(x) = g_\phi(x\nu) = f_\phi(x\nu) = f_\phi(x)$ Both for $\pi \cong \pi_\nu$ and $\pi \ncong \pi_\nu$, S respectively $S \oplus S$ are irreducible representations of G with nontrivial H-invariants. Hence the representation is generated by the subspace of H-invariants. The same then holds for the image under Ψ.

Complexification. In the above, we have given a construction of the invariants in the case of the complex orthogonal group

$$\mathrm{O}(n, \mathbb{C}) = \left\{Q \in \mathbb{C}^{n\times n} \mid Q^\mathsf{T} Q = 1\right\},$$

whereas we are interested in the real orthogonal group $\mathrm{O}(n)$. One passes between the two by complexifying. There is a natural inclusion $\mathrm{O}(n) \subseteq \mathrm{O}(n, \mathbb{C})$ and $\mathrm{O}(n, \mathbb{C})$ is the complexification of $\mathrm{O}(n)$, which means that for any smooth homomorphism α from $\mathrm{O}(n)$ to a complex Lie group G, there is a unique holomorphic homomorphism $\alpha_\mathbb{C}$ from $\mathrm{O}(n, \mathbb{C})$ to G with $\alpha(A) = \alpha_\mathbb{C}(A)$ for all $A \in \mathrm{O}(n)$ [**60**, Chapter 15].

Let V be a finite dimensional, complex vector space. We consider a representation of $\mathrm{O}(n)$ on V to be a smooth group homomorphism from $\mathrm{O}(n)$ to $\mathrm{GL}(V)$ and a representation of $\mathrm{O}(n,\mathbb{C})$ on V to be a holomorphic group homomorphism from $\mathrm{O}(n,\mathbb{C})$ to $\mathrm{GL}(V)$. Holomorphic maps are in particular smooth and $\mathrm{O}(n)$ is a smooth submanifold of $\mathrm{O}(n,\mathbb{C})$. Hence the restriction of a representation of $\mathrm{O}(n,\mathbb{C})$ to $\mathrm{O}(n)$ is a representation of $\mathrm{O}(n)$. By the definition of the complexification and setting $G = \mathrm{GL}(V)$, we see that any representation π of $\mathrm{O}(n)$ is the restriction of a unique representation $\pi_{\mathbb{C}}$ of $\mathrm{O}(n,\mathbb{C})$.

We now show that complexification interacts well with invariant subspaces. Since $\mathrm{O}(n-t) \subseteq \mathrm{O}(n-t,\mathbb{C})$ we have

$$V^{\mathrm{O}(n-t,\mathbb{C})} \subseteq V^{\mathrm{O}(n-t)}.$$

For the other direction, we use polar decomposition. Any matrix $A \in \mathrm{O}(n,\mathbb{C})$ can be written uniquely as

$$A = Ue^{iX}$$

with U in $\mathrm{O}(n)$ and X in the Lie algebra $\mathfrak{so}(n)$ of $\mathrm{O}(n)$ consisting of the skew-symmetric matrices of size n [**60**, Proposition 15.2.1]. Since $\pi_{\mathbb{C}}$ is a homomorphism we have

$$\pi_{\mathbb{C}}(Ue^{iX}) = \pi_{\mathbb{C}}(U)\pi_{\mathbb{C}}(e^{iX}) = \pi_{\mathbb{C}}(U)e^{d\pi_{\mathbb{C}}(iX)} = \pi_{\mathbb{C}}(U)e^{id\pi_{\mathbb{C}}(X)} = \pi(U)e^{id\pi(X)},$$

where $d\pi_{\mathbb{C}} \colon \mathfrak{so}(n,\mathbb{C}) \to \mathfrak{gl}(n)$ and $d\pi \colon \mathfrak{so}(n) \to \mathfrak{gl}(n)$ are the differentials of $\pi_{\mathbb{C}}$ and π. Here we used that $d\pi_{\mathbb{C}}$ is complex linear since $\pi_{\mathbb{C}}$ is holomorphic. Now let v be a vector in V invariant under $\mathrm{O}(n-t)$.

Then $d\pi(X)v = 0$ for any X in the Lie algebra $\mathfrak{so}(n-t)$. By the above, for $A \in \mathrm{O}(n-t,\mathbb{C})$ there are $U \in \mathrm{O}(n-t)$ and $X \in \mathfrak{so}(n-t)$ such that $A = Ue^{iX}$. Hence we have

$$\pi_{\mathbb{C}}(A)v = \pi(U)e^{id\pi(X)}v = \pi(U)(I + id\pi(X) + \frac{1}{2}(id\pi(X))^2 + \ldots)v = \pi(U)v = v,$$

which shows

$$V^{\mathrm{O}(n-t)} \subseteq V^{\mathrm{O}(n-t,\mathbb{C})}.$$

This shows the invariant subspaces agree in the real and complex case.

Realness. We now show that in the semistandard tableaux basis, the matrix coefficients of π are real. This allows us to restrict to real matrices in the semidefinite program. To do this calculation, we will use the description which appears in the summary of Section 2.5 of this chapter and we use the realisation of the polynomial representations of $\mathrm{GL}(t)$ given by Section 3.1. Let T_1 and T_2 be semistandard tableaux.

PROPOSITION 2.21. *The numbers $\langle T(e_{T_1}), \pi(y)T(e_{T_2})\rangle$ are real for all $y \in \mathrm{O}(n)$.*

PROOF. We may define a conjugation $\overline{(\cdot)}$ on W by conjugating the components of a vector in the semistandard tableaux basis. Let η be the orthogonal matrix $\mathrm{diag}(I_t, -I_{n-t})$. We then have $\omega\eta = (I_t \; -iI_t \, 0)$. Given the fact that the matrix coefficients of the representation λ in the semistandard tableaux basis are polynomials with real coefficients, we then have

$$\lambda(\omega\eta xy\epsilon)\overline{v} = \overline{\lambda(\omega xy\epsilon)v}$$

for all $x, y \in \mathrm{O}(n)$ and all $v \in W$. Hence we have

$$\begin{aligned}
&\langle T(e_{T_1}), \pi(y)T(e_{T_2})\rangle \\
&= \int_{\mathrm{O}(n)} \langle \lambda(\omega x \epsilon)e_{T_1}, \lambda(\omega x y \epsilon)e_{T_2}\rangle \, dx \\
&= \int_{\mathrm{O}(n)} \langle \lambda(\omega \eta x \epsilon)e_{T_1}, \lambda(\omega \eta x y \epsilon)e_{T_2}\rangle \, dx \\
&= \int_{\mathrm{O}(n)} \langle \overline{\lambda(\omega x \epsilon)e_{T_1}}, \overline{\lambda(\omega x y \epsilon)e_{T_2}}\rangle \, dx \\
&= \overline{\langle T(e_{T_1}), \pi(y)T(e_{T_2})\rangle}.
\end{aligned}$$

□

2.5. Summary

Let $n \geq 2t$. Let U be the subspace spanned by $e_1, \ldots, e_t$ and consider the hyperbolic resolution given by $\alpha_1, \ldots, \alpha_t = e_1 + ie_1, \ldots, e_t + ie_t$ and $\beta_1, \ldots, \beta_t = e_1 - ie_1, \ldots, e_t - ie_t$. Let G be the complex orthogonal group of $\mathbb{C}^n$ and let H the subgroup of G which leaves U point-wise fixed. Let (λ, W_λ) be an irreducible, polynomial representation of $\mathrm{GL}(t)$. As before, let

$$F(\lambda) = \{f \colon G \to W_\lambda \mid f(n_3 d x) = \lambda(d) f(x)\},$$

where f is assumed to be regular and the equation should hold for all $d \in D, n_3 \in N_3$ and $x \in G$. Let T be the map from W_λ to $F(\lambda)$, which maps ϕ to

$$f_\phi(x) = \lambda(x_{11} + x_{13} e_{31})\phi.$$

The image $T(W_\lambda)$ generates an irreducible representation (π, V_π) of G and T defines a linear bijection onto V_π^H. Furthermore, every irreducible representation of G with nontrivial H-invariants is of this form for a unique irreducible, polynomial representation of $\mathrm{GL}(t)$. By Section 2.4, the restriction of these representations to the real orthogonal group gives a description of all irreducible representations of the real orthogonal group with nontrivial invariants. By Section 2.4, for $\phi_1 = e_{T_1}$ and $\phi_2 = e_{T_2}$, with T_1 and T_2 semistandard tableaux, the matrix coefficients

$$\langle f_{\phi_1}, \pi(g) f_{\phi_2}\rangle = \int_{\mathrm{O}(n)} \langle f_{\phi_1}(x), f_{\phi_2}(xg)\rangle \, dx$$

are real-valued. Finally, let us express f_ϕ if the orthogonal matrix x is expressed in the standard basis. Let ω be the complex $t \times n$ matrix

$$\omega = \begin{bmatrix} I_t & iI_t & 0 \end{bmatrix},$$

and ϵ the $n \times t$ matrix

$$\epsilon = \begin{bmatrix} I_t \\ 0 \end{bmatrix}.$$

We then have

$$\langle \alpha_i, (x_{11} + x_{13} e_{31})\alpha_j\rangle = \langle e_i, (\omega x \epsilon) e_j\rangle$$

and hence we have

$$f_\phi(x) = \lambda(\omega x \epsilon)\phi.$$

Provided one has a way to calculate matrix coefficients of representations of the general linear group, and provided one has a reasonable formula for exact integration of polynomials on the orthogonal group, this gives a concrete way to calculate the matrix coefficients for the H-invariants. To use method I efficiently is somewhat involved and additional calculations are required to bring it up to speed for higher degrees. This is done in the paper [**40**], where a full algorithm is given.

CHAPTER 3

Method II

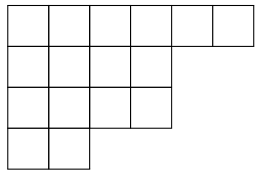
Again, recall that by "method" we shall mean a construction of the space of invariants (3) and an algorithm to compute the zonal Stiefel harmonics. We will first work out some of the details of the representation theory of the general linear group, so that method I can be used in practice. This is done using Weyl's construction for the general linear group. Then, based on this, we will introduce Weyl's construction for the orthogonal group. This forms the starting point for method II.

The main contribution of this chapter is given by the development of method II, for which two ingredients were necessary. The first is given by Theorem 3.5, which yields a new construction of the spaces of invariants in expression (3). The second is given by a practical algorithm for the calculation of the corresponding zonal Stiefel harmonics, and by extension the zonal matrix in Theorem 1.16. What is crucial to make method II practical, is a recent new formula for the traceless projection of a tensor from [**22**] and the use of an auxiliary space. This auxiliary space is described in terms of contraction tableaux, a term which is introduced in this thesis.

The structure of this chapter in more detail is as follows. In Section 3.1 we explain Weyl's construction for the general linear group $\mathrm{GL}(n)$ and how to calculate the matrix coefficients. To do so, we introduce Young diagrams, the calculus of tableaux and we calculate the Gram matrix of the semistandard tableaux basis. The case $\mathrm{GL}(2)$ is treated in more detail. In Section 3.2, we explain Weyl's construction for the orthogonal group. In Section 3.3, we explain how to compute the invariants in expression (3) and we prove Theorem 3.5. In Section 3.4, we give the algorithm to calculate the zonal Stiefel harmonics and introduce the calculus of contraction tableaux. In Section 3.5, we work out some examples. In particular, we draw the connection to the classical theory of spherical harmonics and we work out the zonal Stiefel harmonics for a particular case.

3.1. Weyl's construction for the general linear group

Young diagrams. Let us recall the definition of a Young diagram, for which we follow [**51**]. A Young diagram is a collection of boxes, or cells, arranged in left-justified rows, with a weakly decreasing number of boxes in each row. Listing the number of boxes in each row gives a partition of the integer d that is the total number of boxes. Conversely, every partition of d corresponds to a Young diagram. For example, here is the Young diagram which corresponds to the partition of 16 into $6 + 4 + 4 + 2$.



We usually denote a partition by λ. It is given by a sequence of weakly decreasing positive integers, sometimes written $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_m)$; it is often convenient to allow one or more zeros to occur at the end, and to identify sequences that differ only by such zeros.

With Young diagrams, we may write down the polynomial representations of $\mathrm{GL}(n)$. Let V be a vector space over $\mathbb{C}$ of dimension n and let $\mathrm{GL}(n)$ be the general linear group, which is the group of invertible complex-linear endomorphisms of V. Consider the d-fold tensor product $V^{\otimes d}$. The general linear group $\mathrm{GL}(n)$ acts on $V^{\otimes d}$ by acting on each factor simultaneously and the symmetric group $\mathfrak{S}_d$ on d elements acts on $V^{\otimes d}$ by permuting factors. We will adopt the convention that the general linear group acts on the left of $V^{\otimes d}$ and the symmetric group on the right. For $v \in V^{\otimes d}$, expressed as equations, this reads

$$\otimes_{i=1}^{d} v_i \cdot \sigma = \otimes_{i=1}^{d} v_{\sigma(i)} \tag{43}$$

and

$$A \cdot \otimes_{i=1}^{d} v_i = \otimes_{i=1}^{d} A v_i.$$

These actions are commutative: for $v \in V^{\otimes d}$, we have $(A \cdot v) \cdot \sigma = A \cdot (v \cdot \sigma)$. We now define the Young symmetriser associated to λ. For a fixed λ, we may fill the Young diagram of λ with the numbers 1 up to d by going down the columns first and then moving to the right. This provides a bijection between the boxes of the Young diagram and the set $\{1, \ldots, d\}$. We let $\mathfrak{S}_d$ act on the boxes of the Young diagram via this bijection. Let P denote the subgroup of $\mathfrak{S}_d$ which preserves the rows of the Young diagram of λ and let Q denote the subgroup of $\mathfrak{S}_d$ which preserves the columns of the Young diagram. We then define elements of the group algebra $\mathbb{C}\mathfrak{S}_d$

$$a_\lambda = \sum_{p \in P} p, \quad b_\lambda = \sum_{q \in Q} \mathrm{sign}(q) q$$

and the Young symmetriser $c_\lambda = a_\lambda b_\lambda$. By [**51**, Lemma 4.26], a rational multiple of c_λ is idempotent. We will use c_λ to signify this idempotent multiple. We then define $\mathbb{S}_\lambda V = V^{\otimes d} \cdot c_\lambda$. By commutativity of the actions of $\mathrm{GL}(n)$ and $\mathfrak{S}_d$, $\mathbb{S}_\lambda V$ is a representation of $\mathrm{GL}(n)$.

Theorem 3.1 ([**52**, Proposition 15.47]). *The representation $\mathbb{S}_\lambda V$ is an irreducible representation of* $\mathrm{GL}(n)$. *Every polynomial representation of* $\mathrm{GL}(n)$ *is of this form for a unique λ.*

The calculus of tableaux. We will now explain how to use tableaux to write down a basis for $\mathbb{S}_\lambda V$. Any way of putting a positive integer in each box of a Young diagram will be called a tableau. When we say that a tableau is filled using integers between 1 and n, this means every box contains an integer between 1 and n. In particular, there may be repeats and we do not have to use all integers between 1 and n. Entries of tableaux can just as well be taken from any totally ordered set, which we will consider in Section 3.4. For now, we will consider positive integers. Given a tableau T, we will denote by $\mu_k(T)$ the number of occurrences of the number

k in the tableau T. The vector $\mu(T) \in \mathbb{Z}^n$ with components equal to $\mu_k(T)$ is called the weight of T. A semistandard tableau is defined as a tableau such that each row is weakly increasing and each column is strictly increasing. Here is an example of a semistandard tableau for the partition $(6, 4, 4, 2)$ of 16.

$$\mathrm{T} = \begin{array}{cccccc} 1 & 2 & 2 & 3 & 3 & 5 \\ 2 & 3 & 5 & 5 & & \\ 4 & 4 & 6 & 6 & & \\ 5 & 6 & & & & \end{array}$$

The weight of this tableau is then $\mu(T) = (1, 3, 3, 2, 4, 3)$.

Cave. The names for these concepts differ accross the literature and we follow [**52**]. In [**51**], what we call a tableau is called a filling or numbering, and what we call a semistandard tableau is called a tableau.

With the semistandard tableaux, we can write down a basis for $\mathbb{S}_\lambda V$. We first need to introduce some concepts, which we take from Fulton's book [**51**, Chapter 8]. Consider maps

$$\varphi \colon V^d \to F$$

where V^d is mapped to a $\mathbb{C}$-vector space F, satisfying the three properties:

(i) that φ is $\mathbb{C}$-multilinear;

(ii) that φ is alternating in the entries of any column of λ;

(iii) that for any $v \in V^d$, for any two columns, and for any subset of boxes in the right column, we have

$$\varphi(v) = \sum_w \varphi(w),$$

where the sum is over all w obtained from v by an exchange between the two given columns using the given subset of the right column.

An exchange is defined as follows [**51**, Part II, Introduction]. It depends on a choice of two columns of a Young diagram λ, and a choice of a set of the same number of boxes in each column. For any filling T of λ (with entries in any set), the corresponding exchange is the filling S obtained from T by interchanging the entries in the two chosen sets of boxes, maintaining the vertical order in each; the entries outside these chosen boxes are unchanged. For example, if $\lambda = (4, 3, 3, 2)$, and the chosen boxes are the top two in the third column, and the second and fourth box in the second column, here is the exchange which takes T to S.

$$\mathrm{T} = \begin{array}{cccc} 1 & 5 & 2 & 1 \\ 1 & 3 & 4 & \\ 2 & 4 & 5 & \\ 3 & 5 & & \end{array} \quad \to \quad \mathrm{S} = \begin{array}{cccc} 1 & 5 & 3 & 1 \\ 1 & 2 & 5 & \\ 2 & 4 & 5 & \\ 3 & 4 & & \end{array}$$

We define the Schur module V^λ to be the universal solution to this problem. By this, we mean the following. We have a $\mathbb{C}$-vector space V^λ and a map

$$V \to V^\lambda$$

that we denote by $v \mapsto v^\lambda$, satisfying properties (i)–(iii). Moreover, for any map

$$\varphi \colon V^d \to F$$

satisfying (i)–(iii), there exists a unique homomorphism

$$\tilde{\varphi} \colon V^\lambda \to F$$

of $\mathbb{C}$-vector spaces such that

$$\tilde{\varphi}(v^\lambda) = \varphi(v)$$

for all $v \in V^d$. It may be shown that a Schur module always exists. It is given by Weyl's construction [**51**, §8.1]. We also have

Proposition 3.2. *The space* $\mathbb{S}_\lambda V$ *with the canonical map* $V^d \to \mathbb{S}_\lambda V$ *is a Schur module in the above sense.*

Proof. This follows from naturality of the isomorphism in [**51**, Chapter 8, Proposition 1] and the realization of the irreducible representation of $\mathfrak{S}_n$ as the left-ideal in $\mathbb{C}[\mathfrak{S}_n]$ generated by the young symmetrizer c_λ. □

Given a tableau T on the Young diagram λ, we denote by $T(i)$ the entry at position i, where the position is defined using the bijection with $\{1, \dots, d\}$ corresponding to the Young diagram. Suppose that $e_1, \dots, e_n$ are the standard basis elements of V. For a tableau T filled with integers which lie between 1 and n, we define the element e_T of $V^{\otimes d}$ by tensoring the vectors $e_{T(i)}$ where i goes from 1 to d, i.e.

$$e_T = \bigotimes_{i=1}^{d} e_{T(i)}.$$

Now, finally, we can write down the basis. By [**51**, Theorem 8.1] and Proposition 3.2, a basis of $\mathbb{S}_\lambda V$ is given by the set of $e_T c_\lambda$, where T is semistandard. The dimension of $\mathbb{S}_\lambda V$ is given by [**52**, Theorem 6.3]

$$\prod_{1 \le i < j \le n} \frac{\lambda_i - \lambda_j + j - i}{j - i}.$$

Furthermore, we may apply the calculus of tableaux to the elements $e_T c_\lambda$. By this we mean that we may apply the relations which arise from (i)–(iii).

To calculate with tableaux, we give a useful algorithm. With this, one may decompose $e_T c_\lambda$ with a general tableau T as a sum of such tensors with semistandard tableaux. We order the tableaux using the reverse lexicographical ordering, i.e. $T' > T$ if the last entry in the last column where T' differs from T is larger. For an integer $1 \le s \le \lambda_1$, let $(a_1, \dots, a_p)$ be the s-th column of T and $(b_1, \dots, b_q)$ be the $(s+1)$-th column of T. For $1 \le r \le q$ and integers $1 \le i_1 < \cdots < i_r \le p$, let $\Phi(T, s, r, i_1, \dots, i_r)$ be the tableau obtained from T where we replace the first r entries in column $s+1$ by $a_{i_1}, \dots, a_{i_r}$ and replace the $i_1, \dots, i_r$ entries in column s by $b_1, \dots, b_r$. Suppose the set of all semistandard tableaux is given by $\{T_1, \dots, T_m\}$. The algorithm below returns a vector with the coordinates of $e_T c_\lambda$ in the basis $e_{T_1} c_\lambda, \dots, e_{T_m} c_\lambda$. The algorithm is recursive and terminates since at every call we increase the position of the tableau in the reverse lexicographic order. The last step uses properties (ii) and (iii).

This provides a way to calculate the matrix coefficients. We have

$$A \cdot e_T c_\lambda = \sum_S A_{k_1,j_1} \cdots A_{k_d,j_d} \, e_S c_\lambda \tag{44}$$

Algorithm 1 Algorithm to decompose a tableau into semistandard tableaux

procedure SSDECOMP(T)

If there is a column in T with two identical entries, return 0.

Else, let σ be the permutation of T which orders each column to become strictly increasing and does not exchange elements between different columns.

Replace T by $\sigma(T)$.

If T is semistandard, return a vector with sign(σ) at the appropriate entry and zeros otherwise.

Else, find r and s such that $T(r,s) > T(r,s+1)$.

Return sign$(\sigma) \sum_{1\le i_1<\cdots<i_r\le p}$ SSDECOMP$(\Phi(T,s,r,i_1,\dots,i_r))$.

end procedure

where the sum is over all n^d tableaux S filled with $k_1,\dots,k_d$ between 1 and n. Let T be semistandard and bring each term on the right-hand side into semistandard shape with the algorithm. Provided we can compute the Gram matrix $\langle e_T c_\lambda, e_S c_\lambda\rangle$, for semistandard tableaux S and T, this gives a way to compute the matrix coefficients in the semistandard tableaux basis. We compute the Gram matrix in the next section.

The Gram matrix for the semistandard tableaux basis. The space $V^{\otimes d}$ may be given the inner product $\prod_{i=1}^d \langle v_i, w_i\rangle$, where each factor is the inner product $\sum_{i=1}^n \overline{v_i} w_i$. We denote this inner product by $\langle\cdot,\cdot\rangle$. This is an inner product such that, when restricted to the unitary group, the representation is unitary. The space $\mathbb{S}_\lambda V$ then inherits this inner product. We are interested in the Gram matrix of the semistandard tableaux basis for this inner product

$$\langle e_T c_\lambda, e_S c_\lambda\rangle,$$

which is not even necessarily diagonal. Let us describe how to calculate this Gram matrix. We also denote by λ the representation

$$\lambda\colon \mathrm{GL}(n) \to \mathrm{GL}(\mathbb{S}_\lambda V). \tag{45}$$

Let us define an inner product $\langle\cdot,\cdot\rangle_{ss}$ on $\mathbb{S}_\lambda V$ by declaring the semistandard tableaux basis to be orthonormal. Restricting the representation $\mathbb{S}_\lambda V$ to the unitary group $\mathrm{U}(n)$ gives an irreducible representation of $\mathrm{U}(n)$. By compactness of $\mathrm{U}(n)$, there is a unique inner product on $\mathbb{S}_\lambda V$, up to multiplication by a positive real number, such that the representation of $\mathrm{U}(n)$ is unitary. Representing this inner product as a matrix, there is a unique, up to multiplication by a positive real number, Hermitian positive definite matrix M, such that

$$\lambda(k)^* M \lambda(k) = M \tag{46}$$

is satisfied for all $k \in \mathrm{U}(n)$. However, we already know what M is: it is the inner product $\langle\cdot,\cdot\rangle$ on $V^{\otimes d}$ described earlier. Therefore, possibly replacing M by a positive real multiple of itself, we have

$$\langle e_T c_\lambda, M e_S c_\lambda\rangle_{ss} = \langle e_T c_\lambda, e_S c_\lambda\rangle.$$

We see that we may compute the Gram matrix by solving (46) for M using the inner product such that the semistandard tableaux basis is orthonormal.

To solve this system, we turn to Lie algebras. The differential of the map (45)

$$d\lambda : \mathfrak{gl}(n) \to \mathrm{End}(\mathbb{S}^a V)$$

is a representation of Lie algebras [**52**, Chapter 8]. Here $\mathfrak{gl}(n)$ denotes the Lie algebra of $\mathrm{GL}(n)$, which consists of all complex-linear endomorphisms of V. Furthermore, we denote by $\mathfrak{u}(n)$ the Lie algebra of skew-hermitian matrices, which is the Lie algebra of the unitary group. We now give the matrix coefficients of the associated representation of the Lie algebra $\mathfrak{gl}(n)$. This follows from the product rule [**52**, §8.1] Let us work it out explicitly. Because a representation of a Lie algebra is linear, it suffices to compute the matrix coefficients on a basis of $\mathfrak{gl}(n)$. Let E_{kl} be the matrix with a 1 as k, l entry and zeroes elsewhere. We have $E_{kl}^{\mathsf{T}} e_{l_3} = E_{lk} e_{l_3} = \delta_{kl_3} e_l$ and hence

$$d\lambda(E_{kl})e_T = \sum_S e_S$$

where the sum ranges over all tableaux S which may be obtained from T by changing one and only one k to an l. The matrix coefficients of the representation is then given by

$$\langle e_{T_1}, d\lambda(E_{kl})e_{T_2}\rangle_{ss} = \sum_S \delta_{T_1,S}, \tag{47}$$

where the sum is the same as before, but for T_2. By differentiating, (46) implies

$$M d\lambda(X) = -d\lambda(X)^* M \tag{48}$$

for all $X \in \mathfrak{u}(n)$. By using the exponential map and connectedness of the unitary group, the converse is obtained. Hence we may equivalently demand (48) for all $X \in \mathfrak{u}(n)$. By real linearity in X, it is equivalent to demand this for a real basis of $\mathfrak{u}(n)$, which is given by $E_{kl} - E_{lk}$ and $i(E_{kl} + E_{lk})$ where k and l range between 1 and t and $k \neq l$. Therefore, M is the unique, up to a positive real number, positive semidefinite matrix which solves the linear system

$$M(d\lambda(E_{kl}) - d\lambda(E_{lk})) = -(d\lambda(E_{kl}) - d\lambda(E_{lk}))^{\mathsf{T}} M$$
$$M(d\lambda(E_{kl}) + d\lambda(E_{lk})) = (d\lambda(E_{kl}) + d\lambda(E_{lk}))^{\mathsf{T}} M$$

Furthermore, we would now like to show that this forces M to have only real entries. This will ensure that the resulting semidefinite program, which depends on M, only real numbers occur. Observe that the matrices $d\lambda(E_{kl}) - d\lambda(E_{lk})$ and $d\lambda(E_{kl}) + d\lambda(E_{lk})$ have integral, and therefore real, coefficients. Hence M solves this system if and only the complex conjugate, without transpose, of M also solves the system. Because such M are unique up to multiplication by a positive real number, we deduce that M is a positive real multiple of its complex conjugate. This is true if and only if M has real entries, which is what we wanted to show.

For $t = 1$, $\mathrm{GL}(1)$ is abelian and hence all irreducible representations are one-dimensional, so the question of inner products on the irreducible representations is somewhat trivial. For $t = 2$, we will see that the linear constraints already determine M up multiplication by a real number. For $t = 3$ and the degrees $d \leq 4$ which we computed, we saw that this also was the case. Therefore, we did not have to worry about solving a semidefinite program exactly. Perhaps there also exists a combinatorial formula for this Gram matrix, which the author of this thesis would welcome.

GL(2). Let us work out the case for $\mathrm{GL}(2)$. In this case, we have $V = \mathbb{C}^2$ with basis e_1, e_2, the weight $\lambda = (\lambda_1, \lambda_2)$ satisfies $\lambda_1 \geq \lambda_2 \geq 0$, and we define $m = \lambda_1 - \lambda_2$. A semistandard tableau for such λ is uniquely determined by the number of occurrences of the number 2. Recall $\mu_2(T)$ is the number of occurrences of 2 in the tableau T. A basis is given by T_k with $\mu_2(T_k) = \lambda_2 + k$, where $0 \leq k \leq m$. Let us show that we have $\langle e_{T_k} c_\lambda, e_{T_l} c_\lambda \rangle = \binom{m}{k} \delta_{k,l}$. Consider the skew-hermitian matrices $X = \left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right]$ and $Y = \left[\begin{smallmatrix} 0 & i \\ i & 0 \end{smallmatrix}\right]$. By (47), and using (i)–(iii), we obtain

$$d\lambda(X) e_{T_k} c_\lambda = -(m-k) e_{T_{k+1}} c_\lambda + k e_{T_{k-1}} c_\lambda$$

and hence, in the inner product such that the semistandard tableaux basis is orthonormal, we have $d\lambda(X)_{l,k} = -(m-k)\delta_{k+1,l} + k\delta_{k-1,l}$, with $0 \leq k, l \leq m$. As an ansatz, suppose M is diagonal and $M_{00} = 1$. We then have

$$M_{kk}(k+1) = (M d\lambda(X))_{k,k+1} = (-d\lambda(X)^* M)_{k,k+1} = (m-k) M_{k+1,k+1},$$

which gives a recursive formula for the diagonal entries of M. Together with $M_{00} = 1$, this implies $M_{kk} = \binom{m}{k}^{-1}$. One may verify that with this M, equation (48) is also satisfied for the matrix Y. Furthermore, M is positive semidefinite. The matrices X and Y are a real basis of $\mathfrak{u}(2)$ and therefore we have obtained the desired M.

We now explicitly compute the matrix coefficients from equation (44). We have

$$A \cdot e_{T_k} c_\lambda = \sum_S A_{k_1,j_1} \cdots A_{k_d,j_d}\, e_S c_\lambda$$

where the sum is over all 2^d tableaux S filled with $k_1, \ldots, k_d$ between 1 and 2. We have

$$\langle e_{T_k} c_\lambda, A \cdot e_{T_l} c_\lambda \rangle = \det(A)^{\lambda_2} \langle e_{T_k} c_{\lambda'}, A \cdot e_{T_l} c_{\lambda'} \rangle,$$

where $\lambda' = (m, 0)$ and e_{T_k}, respectively e_{T_l}, on the right-hand side is meant to signify the semistandard tableau on λ' with k, respectively l, 2s. This follows from the fact that the Young symmetrizer antisymmetrises over columns of length 2. Therefore, it suffices to give an explicit formula for λ with $\lambda_2 = 0$. In that case, we are dealing with totally symmetric tensors and a counting argument reveals

$$A \cdot e_{T_l} c_\lambda = \sum_{i=0}^{m-l} \sum_{j=0}^{l} \binom{m-l}{i} \binom{l}{j} A_{11}^{m-l-i} A_{21}^{i} A_{12}^{l-j} A_{22}^{j} e_{T_{i+j}} c_\lambda.$$

The explicit formula for the Gram matrix then gives us the matrix coefficients in the semistandard tableaux basis. We have

$$\langle e_{T_k} c_\lambda, A \cdot e_{T_l} c_\lambda \rangle = \binom{m}{k}^{-1} \sum_j \binom{m-l}{k-j} \binom{l}{j} A_{11}^{m-l-k+j} A_{21}^{k-j} A_{12}^{l-j} A_{22}^{j},$$

where the sum is over all integers j such that the exponents are nonnegative integers.

3.2. Weyl's construction for the orthogonal group

We now turn our attention to the orthogonal group, for which we will require the general definition. Let M be an invertible symmetric matrix. An element g of $\mathrm{GL}(n)$ is an orthogonal transformation or an isometry for M if $g^{\mathsf{T}} M g = M$. A different choice of M will lead to a different, but conjugate, subgroup of $\mathrm{GL}(n)$. One may then ask why to bother with this general definition, since we are chiefly concerned with the orthogonal group with respect to the identity matrix I. The reason is that for convencience of calculations, the choice of M does matter. We now give a convenient choice of M, with which we may apply weight theory as in [**52**, Chapter 18]. Define

$$M = \begin{cases} \begin{bmatrix} 0 & I_m \\ I_m & 0 \end{bmatrix} & \text{if } n = 2m, \\ \begin{bmatrix} 0 & I_m & 0 \\ I_m & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} & \text{if } n = 2m+1. \end{cases}$$

To pass between the orthogonal groups with respect to M and I, we will have to compute a square root N of M. Let ξ be a complex number such that $\xi^2 = \frac{1}{2i}$. One may verify that a square root N of M is given by to

$$N = \begin{cases} \begin{bmatrix} \xi I_m & i\xi I_m \\ i\xi I_m & \xi I_m \end{bmatrix} & \text{if } n = 2m, \\ \begin{bmatrix} \xi I_m & i\xi I_m & \\ i\xi I_m & \xi I_m & \\ 0 & 0 & 1 \end{bmatrix} & \text{if } n = 2m+1. \end{cases} \tag{49}$$

We then have that the map g is orthogonal for I if and only if $N^{-1}gN$ is orthogonal for M. So we see that the orthogonal groups for different forms are conjugate. To define irreducible representations of $\mathrm{O}(n)$ we introduce contractions, acting on the right of a tensor. For a pair i, j, define the contraction d_{ij} by

$$v_1 \otimes \cdots \otimes v_d \cdot d_{ij} = v_i^{\mathsf{T}} M v_j \sum_{k,l}^{n} (M^{-1})_{kl} v_1 \otimes \cdots \otimes e_k \otimes \cdots \otimes e_l \otimes \cdots \otimes v_d, \tag{50}$$

where the factors are inserted at positions i and j. Strictly speaking, this is a contraction followed by insertion of the tensor M^{-1}, but we shall nevertheless refer to this as a contraction. In this way, a contraction is an endomorphism of $V^{\otimes d}$. These endomorphisms are related to the Brauer algebra and the Schur-Weyl duality for the orthogonal group, cf. [**113**, Chapter V.5]. We will not elaborate on this here, but give the results which are important to us. The action of the orthogonal group and that of a contraction is commutative: for $v \in V^{\otimes d}$, we have $(g \cdot v) \cdot d_{ij} = g \cdot (v \cdot d_{ij})$. Define $V^{[d]}$ to be the vector space consisting of those tensors in $V^{\otimes d}$ which go to zero for all such contractions. By the above commutativity, the space $V^{[d]}$ is a representation of the orthogonal group. The representation $\mathbb{S}_\lambda V$ is a representation of the orthogonal group by restriction. We now consider the representation $\mathbb{S}_{[\lambda]} V = \mathbb{S}_\lambda V \cap V^{[d]}$. Recall the conjugate partition λ' of a partition λ, obtained by transposing the Young diagram. The following theorem is also known as Weyl's construction.

Theorem 3.3 ([**52**, Theorem 19.5]). *The representation $\mathbb{S}_{[\lambda]} V$ of $\mathrm{O}(n)$ is nonzero if and only if $\lambda'_1 + \lambda'_2 \leq n$, in which case it is an irreducible representation.*

3.3. Invariants

Let U be the subspace of V spanned by $e_1, \ldots, e_t$. We define $\mathrm{O}(n-t)$ as the subgroup of $\mathrm{O}(n)$ which fixes U pointwise. As before, we are interested in a description of the space of $\mathrm{O}(n-t)$-invariants. Let $n \geq 2t$.

Theorem 3.4. *The representation* $\mathbb{S}_{[\lambda]}V$ *with* $\lambda = (\lambda_1, \ldots, \lambda_t, 0, \ldots, 0)$ *and* $\lambda_t \geq 0$ *has nontrivial* $\mathrm{O}(n-t)$*-invariants and every irreducible representation of* $\mathrm{O}(n)$ *with nontrivial* $\mathrm{O}(n-t)$*-invariants is of this form for a unique such* λ*. For such* λ*, we have* $\dim(\mathbb{S}_{[\lambda]}V)^{\mathrm{O}(n-t)} = \dim \mathbb{S}_\lambda U$*.*

This was shown by Gelbart [**54**] for $n > 2t$ and the proof is based on branching rules. The result for $n = 2t$ may be found, for instance, in [**57**]. Though not necessary logically, let us derive this results with the methods of Chapter 2 for $n \geq 2t$.

Proof. Recall some of the notation from Chapter 2. The space U has a hyperbolic resolution given by $\alpha_k = e_k + ie_{t+k}$ and $\beta_k = e_k - ie_{t+k}$. The space V_1 is the subspace of V spanned by $\alpha_1, \ldots, \alpha_t$. The orthogonal group $G = \mathrm{O}(n)$, or $G = \mathrm{SO}(n)$ for the case $n = 2t$, has a bitriangular structure (N_1, D, N_3) arising from the hyperbolic resolution of U. We have a natural inclusion $\mathbb{S}_\lambda V_1 \subseteq \mathbb{S}_{[\lambda]}V^{N_1}$. Since $\mathbb{S}_\lambda V_1$ is an irreducible representation of D and $\mathbb{S}_{[\lambda]}V$ is an irreducible representation of G, the inclusion is an equality. Hence the highest D-type of $\mathbb{S}_{[\lambda]}V$ is $\mathbb{S}_\lambda V_1$. The representation $\mathbb{S}_\lambda V_1$ is trivial on D_2 and polynomial on D_1. Furthermore, every polynomial representation of D which is trivial on D_2 and polynomial on D_1 is isomorphic to such a $\mathbb{S}_\lambda V_1$. The result follows from Theorem 2.15 for $n > 2t$ and from Section 2.4 and [**52**, Theorem 19.22] for $n = 2t$. □

Equidimensionality implies an abstract isomorphism, but a construction is required to actually know the value of a zonal Stiefel harmonic at a given point. The purpose of the work of Gross and Kunze [**57**] and Chapter 2 is to give a construction using induced representations. We will now give a new construction using Weyl's construction. For our purposes, this approach has certain computational advantages. Recall that we give the space V the standard inner product $\langle v, w\rangle = \sum_{i=1}^n \overline{v_i} w_i$ and define the inner product on $V^{\otimes d}$ accordingly via a product. With respect to this inner product, we may consider adjoints. We denote by $\mathfrak{P}_M$ the projection operator from $V^{\otimes d}$ to $V^{[d]}$, where $V^{[d]}$ depends on M. This is defined to be the unique self-adjoint idempotent linear endomorphism of $V^{\otimes d}$ with image $V^{[d]}$. Note that the space $V^{[d]}$ is invariant under the action of the orthogonal group. Therefore, the projection $\mathfrak{P}_M$ is a morphism of representations of the orthogonal group.

Theorem 3.5. *For* $n \geq 2t$*, the restriction* $\mathfrak{P}_I : \mathbb{S}_\lambda U \to (\mathbb{S}_{[\lambda]}V)^{\mathrm{O}(n-t)}$ *is a linear bijection.*

Let us first show that the projection map, when restricted to $\mathbb{S}_\lambda U \subseteq V^{\otimes d}$, has the correct codomain. Firstly, the space $V^{[d]}$ is invariant under the action of the symmetric group. This may be seen by considering equations (43) and (50), from which

$$d_{ij} \cdot \sigma = \sigma \cdot d_{\sigma^{-1}(i)\sigma^{-1}(j)} \tag{51}$$

follows. For the inner product on $V^{\otimes d}$ that we chose, the orthogonal complement of $V^{[d]}$ is invariant under the symmetric group too. Therefore, the projection $\mathfrak{P}_I$ commutes with the action of the symmetric group. Hence we may write $\mathfrak{P}_I\colon \mathbb{S}_\lambda U \to \mathbb{S}_\lambda V$. By definition, the map $\mathfrak{P}_I$ maps into $V^{[d]}$, and we may write $\mathfrak{P}_I\colon \mathbb{S}_\lambda U \to \mathbb{S}_\lambda V \cap V^{[d]} = \mathbb{S}_{[\lambda]}V$. Since the map $\mathfrak{P}_I$ also commutes with the action of the orthogonal group, and since the subspace $U^{\otimes d}$ is fixed pointwise under $\mathrm{O}(n-t)$, we may write $\mathfrak{P}_I\colon \mathbb{S}_\lambda U \to (\mathbb{S}_{[\lambda]}V)^{\mathrm{O}(n-t)}$. By Theorem 3.4, the spaces are equidimensional. Therefore, it suffices to show injectivity. The restriction of an injective function is injective and, therefore, it suffices to show

Proposition 3.6. *For $n \geq 2t$, the restriction $\mathfrak{P}_I : U^{\otimes d} \to V^{\otimes d}$ is injective.*

We start with a lemma.

Lemma 3.7. *We have $N^{-1} \cdot \ker \mathfrak{P}_I = \ker \mathfrak{P}_M$.*

Proof. Let us simplify notation and denote by W_I the space of traceless tensors for I and by W_M the space of traceless tensors for M. We then have $\ker \mathfrak{P}_I = W_I^{\perp}$, respectively $\ker \mathfrak{P}_M = W_M^{\perp}$. We have $N^* = N^{-1}$ and therefore, $N^{-1} \cdot W_I^{\perp} = W_M^{\perp}$ holds if and only if $N^{-1} \cdot W_I = W_M$ holds. For any $1 \leq i, j \leq d$, denote by d_{ij}^I, respectively d_{ij}^M, the contraction for the matrix I, respectively M. From the definition of the contraction, we obtain $N \cdot d_{ij}^M \cdot N^{-1} = d_{ij}^I$. Therefore, we have $N^{-1} \cdot W_I = W_M$ and the result follows. □

Proof of Proposition 3.6. The idea of the proof is to conjugate with N from equation (49) to obtain the corresponding statement for the symmetric matrix M and then apply weight theory. We have to show $\ker \mathfrak{P}_I \cap U^{\otimes d} = \{0\}$. By Lemma 3.7, we have $N^{-1} \cdot \ker \mathfrak{P}_I = \ker \mathfrak{P}_M$, and hence it is equivalent to show $\ker \mathfrak{P}_M \cap \left(N^{-1} U\right)^{\otimes d} = \{0\}$.

For a natural number a, denote by $[a]$ the set $\{1, \ldots, a\}$. Let $\alpha_k = e_k - i e_{m+k}$ with $k \in [t]$. Recall $n = 2m$ if n is even and $n = 2m+1$ if n is odd. Hence $t \leq m$ in both cases. Using equation (49) for N; $N^{-1} = N^*$; and $t \leq m$, a basis of $N^{-1}U$ is given by the set of α_k with $k \in [t]$. A basis of the space $\left(N^{-1}U\right)^{\otimes d}$ is therefore given by $\otimes_{j=1}^d \alpha_{k_j}$ with $(k_1, \ldots, k_d) \in [t]^d$. We will now consider the weight decomposition of such a tensor.

The space $V^{\otimes d}$ is a representation of the special orthogonal group and therefore of the special orthogonal Lie algebra. Therefore, the space $V^{\otimes d}$ decomposes into weight spaces. The Cartan subalgebra, weights and direction are chosen as in [**52**, Chapter 18]. For both $n = 2m$ and $n = 2m+1$, a basis of the Cartan subalgebra is given by H_k for $k \in [m]$, where H_k is the $n \times n$ diagonal matrix such that for $k, l \in [m]$, we have $H_k e_l = \delta_{kl} e_l$ and $H_k e_{l+m} = -\delta_{kl} e_{l+m}$. For the missing case, if $n = 2m+1$ and $l = 2m+1$, we have $H_k e_l = 0$. The direction is given by a functional $\sum_{k=1}^m c_k H_k$ with $c_1 > \cdots > c_m > 0$ and the weights L_k are dual to H_l satisfying $L_k(H_l) = \delta_{kl}$. Thus, for any H in the Cartan subalgebra and for $k \in [t]$, we have $H e_k = L_k(H) e_k$ and $H e_{m+k} = -L_k(H) e_k$. Therefore, for any $(k_1, \ldots, k_d) \in [n]^d$, we have, by the definition of the action of the Lie algebra [**52**, 8.12],

$$H \cdot \otimes_{j=1}^d e_{k_j} = \Big(\sum_{k_j \leq m} L_{k_j} - \sum_{2m \geq k_j > m} L_{k_j} \Big)(H) \otimes_{j=1}^d e_{k_j}, \tag{52}$$

and hence such tensors are weight vectors. Let us now consider the tensors $\otimes_{j=1}^d \alpha_{k_j}$ with $(k_1, \ldots, k_d) \in [m]^d$. To obtain the weight decomposition, we may: substitute $\alpha_k = e_k - i e_{m+k}$; work out the brackets; and then group according to weight. By equation (52) and the choice of direction, we see that the highest weight component of $\otimes_{j=1}^d \alpha_{k_j}$ is given by $\otimes_{j=1}^d e_{k_j}$. Furthermore, we observe:

(i) that for any $(k_1, \ldots, k_d) \in [t]^d$, the highest weight component of $\otimes_{j=1}^d \alpha_{k_j}$ is an element of $U^{\otimes d}$;

(ii) that the highest weight component of $\otimes_{j=1}^d \alpha_{k_j}$ uniquely determines the indices $(k_1, \ldots, k_d)$;

(iii) that the set, containing the highest weight components of $\otimes_{j=1}^{d}\alpha_{k_j}$ for all $(k_1,\dots,k_d)\in[t]^d$, is a linearly independent set.

Suppose $v \in \left(N^{-1}U\right)^{\otimes d}$ and suppose $v \neq 0$. Then we may consider the component u of v with highest weight. If two vectors have a highest weight component which is an element of $U^{\otimes d}$, then the sum of these two vectors again have a highest weight component in $U^{\otimes d}$, provided the sum of the highest weight components is not zero. Since v is a linear combination of elements of the form $\otimes_{j=1}^{d}\alpha_{k_j}$ and because of the observations (i)–(iii), u must be an element of $U^{\otimes d}$. Since every element of $U^{\otimes d}$ goes to zero under all contractions for M, we have $\mathfrak{P}_M u = u$. Since the projection $\mathfrak{P}_M$ is a morphism of representations, it preserves weight decomposition, and hence we have $\mathfrak{P}_M v \neq 0$. Hence the projection $\mathfrak{P}_M$ restricted to $\left(N^{-1}U\right)^{\otimes d}$ is injective. □

3.4. Algorithm for the zonal Stiefel harmonics

In this section, the bilinear form is fixed and we denote by $\mathfrak{P} = \mathfrak{P}_I$ the projection onto $V^{[d]}$ for the identity matrix I. By Theorem 3.5, a basis of the space of invariants is given by $\mathfrak{P}e_T c_\lambda$ with T semistandard and filled with the numbers $1,\dots,t$. So, we need to compute the traceless projection of an element of $\mathbb{S}_\lambda U$ in practice. This may be done with a new explicit formula for the projection operator [**22**], which we describe now. Consider the linear operator A_d, written on the left, but defined by acting on the right of $V^{\otimes d}$ by

$$\sum_{1\le i<j\le d} d_{ij}.$$

The operator A_d commutes with the action of the symmetric group, i.e. $(A_d\cdot v)\cdot\sigma = A_d\cdot(v\cdot\sigma)$, which may be seen by considering equation (51). Furthermore, the kernel of A_d is the space of traceless tensors $V^{[d]}$ by [**22**, Lemma 3.1]. A formula for the traceless projection is therefore given by

$$\mathfrak{P} = \prod_{\alpha}\left(1-\frac{1}{\alpha}A_d\right) \tag{53}$$

where the product ranges over α in the set $\mathrm{Spec}^{\times}(A_d)$, which is an explicit set containing the nonzero eigenvalues of A_d. This set can be calculated using representation theory of the Brauer algebra and no diagonalisation is necessary. For the projection $\mathfrak{P} : \mathbb{S}_\lambda V \to \mathbb{S}_{[\lambda]}V$ restricted to $\mathbb{S}_\lambda V$, fewer eigenvalues are necessary and one may restrict the product in equation (53) to the set $\mathrm{Spec}^{\times}_{\lambda}(A_d)$. These results and the explicit description of these sets containing the eigenvalues may be found in [**22**].

Before we start working out this formula, we first note an immediate consequence. By [**22**, Proposition 3.4], each eigenvalue of A_d is a nonconstant linear function in n. Hence the limit of $\mathfrak{P}$ as n goes to infinity is the identity operator. Hence the limit of the zonal matrix is equal to the matrix of coefficients of the representation $\mathbb{S}_\lambda U$, which answers [**41**, Conjecture 8.1]. One may compare this to the familiar fact that the limit of the Gegenbauer polynomials yield the monomials.

Direct calculation with a basis of $V^{\otimes d}$, which is of size n^d, is computationally undesirable. Therefore, to calculate the traceless projection, we introduce an auxiliary space, which consists of the vectors $e_T c_\lambda$, where T is a tableaux filled with $1,\dots,t$ and the tensors obtained from these under iterated contractions. Let us make this more precise. Consider all tableaux filled with the numbers $1, 2, \dots, t$ and indices $i_1, i_2, \dots$. Recall $T(i)$ denotes the element of the tableau in box i, where the boxes are ordered as before, starting from the left, going down columns and moving to the right. To such a tableau T, we may associate the tensor

$$e_T = \sum_{i_1, i_2, \dots} \bigotimes_{i=1}^{d} e_{T(i)},$$

where we sum every index $i_1, i_2, \dots$ which occurs in the tableau T from 1 to n. Here is an example:

$$T = \begin{array}{|c|c|} \hline 1 & i_1 \\ \hline i_1 & 2 \\ \hline \end{array} \quad \text{gives} \quad e_T = \sum_{i_1=1}^{n} e_1 \otimes e_{i_1} \otimes e_{i_1} \otimes e_2.$$

Recall the weight $\mu(T)$ of T is the vector such that $\mu_i(T)$ is the number of times the symbol i appears in the tableau T. We define a contraction tableau to be a tableau T such that:

(i) T is filled with integers $1, \dots, t$ and indices $i_1, i_2, \dots$;
(ii) for every natural number k, we have $\mu_{i_k}(T) \in \{0, 2\}$;
(iii) for every natural numbers k_1 and k_2 with $k_1 < k_2$, we have $\mu_{i_{k_1}} > \mu_{i_{k_2}}$.

Condition (iii) ensures that we always pick the lowest set of indices possible. One may verify that for any contraction tableau T and any positions i and j, we have that $e_T d_{ij}$ is an integral multiple of a tensor which is associated to a contraction tableau. Ordering the indices $1 < 2 < \dots < t < i_1 < i_2 < \dots$, we may consider the list X of all semistandard contraction tableaux. This list may be made smaller by keeping only one contraction tableau if there are several which correspond to the same tensor. We also define the space W to be the linear span in $V^{\otimes d}$ of $e_T c_\lambda$ with $T \in X$. Since the calculus of tableaux, i.e. properties (i)–(iii) from Section 3.1, is linear, we may perform exchanges simultaneously for the entire sum. Thus, for any contraction tableau T, we may, using Algorithm 1, write $e_T c_\lambda$ as a linear combination of $e_S c_\lambda$, where S is a semistandard contraction tableau. For $T \in X$, we have $e_T d_{ij} c_\lambda \in W$, using the Algorithm 1 to obtain the precise linear combination. Therefore, $e_T c_\lambda A_d = e_T A_d c_\lambda$ is a linear operator on W. Therefore we calculate the projection of an element of W in terms of the spanning set $e_T c_\lambda$ with $T \in X$. We may say the following about the size of the spanning set. For a fixed λ, we have a finite list Y of all possible weights of contraction tableaux. For each weight μ, the number of semistandard tableaux of shape λ and weight μ is known as the Kostka number $K_{\lambda\mu}$. For the Kostka number, an upper bound is given by removing the semistandard condition,

$$K_{\lambda\mu} \le \frac{|\lambda|!}{\mu_1! \, \mu_2! \cdots \mu_m!}$$

where we the product is over all components of μ. This is simply the number of ways to divide $|\lambda|$ objects into m groups of specified sizes. The size of the spanning set is given by $\sum_{\mu \in Y} K_{\lambda\mu}$. The fact that we may work with this spanning set instead of a basis of $V^{\otimes d}$, is what makes this calculation feasible.

Let d_{ij} be any contraction, T a contraction tableau, and S the tableau such that e_S is an integral multiple of $e_T d_{ij}$ What is also useful for calculation is the observation that for any symbol k, we have an equality $\mu_k(T) = \mu_k(S)$ modulo 2. In other words, contractions preserve weight modulo 2. We may define an equivalence relation on the set X if the weights agree modulo 2. Grouping the elements of X according to this equivalence relation, we see that W splits into 2^t subspaces, which are the options for the first t components of the weight vectors modulo 2. Since contractions preserve weight modulo 2, so does A_d, and we see that A_d preserves this splitting of W.

We now wish to compute the matrix coefficients $\langle \mathfrak{P} e_{T_1} c_\lambda, g \cdot \mathfrak{P} e_{T_2} c_\lambda \rangle$, where T_1 and T_2 are semistandard tableaux filled using integers between $1, \ldots, t$. Using the fact that $\mathfrak{P}$ is self-adjoint, we have

$$\langle \mathfrak{P} e_{T_1} c_\lambda, g \cdot \mathfrak{P} e_{T_2} c_\lambda \rangle = \langle e_{T_1} c_\lambda, g \cdot \mathfrak{P} e_{T_2} c_\lambda \rangle. \tag{54}$$

We have $\mathfrak{P} e_{T_2} c_\lambda = \sum_{T_3 \in X} v_{T_3} e_{T_3} c_\lambda$, and therefore expression (54) reduces to calculating $\langle e_{T_1} c_\lambda, g \cdot e_{T_3} c_\lambda \rangle$, with T_1 a semistandard tableau filled with $1, \ldots, t$ and T_3 a semistandard contraction tableau. Formula (44) gives us

$$g \cdot e_{T_3} c_\lambda = \sum_{T_4} \sum_{i_1, i_2, \ldots}^{n} g_{k_1, j_1} \cdots g_{k_d, j_d} \, e_{T_4} c_\lambda$$

where the sum is over all n^d tableaux T_4 filled using integers $k_1, \ldots, k_d$ between 1 and n. This sum may be restricted. Since we are taking the inner product with T_1, we may restrict the sum to such tableau T_4 with $\mu(T_1) = \mu(T_4)$. Furthermore, the symmetriser c_λ allows us to restrict the sum even more, e.g. entries in columns of T_4 have to differ. Because the rows of an orthogonal matrix are orthonormal, the sum over $i_1, i_2, \ldots$ allows us to replace certain terms, e.g. $\sum_{i_1=1}^{n} g_{k_1, i_1} g_{k_2, i_1} = \delta_{k_1, k_2}$. This also has the effect that the only entries of g which occur are of the form g_{ij} with i such that $\mu_i(T_1) \neq 0$ and j such that $\mu_j(T_2) \neq 0$. We will later see that this ensures that the zonal matrix is a polynomial in the desired block of g. Finally, the $e_{T_4} c_\lambda$ have to be brought into semistandard form using Algorithm 1. The inner product $\langle e_{T_1} c_\lambda, e_{T_4} c_\lambda \rangle$ is computed in Section 3.1. Finally, note that for this choice of basis, the zonal Stiefel harmonics in (54) are real-valued.

3.5. Examples

t = 1. Let us mention the connection to the classical theory of spherical harmonics, which in our notation is the case with $t = 1$. The orthogonal group $\mathrm{O}(n)$ acts smoothly and transitively on $\mathbb{S}^n$, and so conditions (i)–(iii) from Section 1.1 are fulfilled. There is only one orbit, of which we choose as representative the vector e_1. That is, the function R sends the single point to e_1. The stabiliser subgroup is then $\mathrm{O}(n-1)$. In this case, the irreducible repesentations with nontrivial invariants are given by $\mathbb{S}_{[d]} V$, which denotes the representation with $\lambda = (d)$ and d not strictly negative, i.e. the space of totally symmetric tensors. The space of totally symmetric tensors may be identified with the space of homogeneous polynomials of degree d and under this identification the operator A_d is the Laplacian. So we see that the irreducible representation of the orthogonal group $\mathbb{S}_{[d]} V$ is the space of harmonic polynomials of degree d, i.e. the homogeneous polynomials which are annihilated by the Laplacian. The spherical harmonics are then given by $\langle v, \pi(g) w \rangle$ with $v \in \mathbb{S}_{[d]} V$ and $w \in (\mathbb{S}_{[d]} V)^{\mathrm{O}(n-1)}$. In this case, the space U is generated by the first basis element e_1 and $\mathbb{S}_d U$ is therefore generated by e_1^d. Thus, by Theorem 3.5, the space $(\mathbb{S}_{[d]} V)^{\mathrm{O}(n-1)}$ is generated by $\mathfrak{P} e_1^d$. By Section 1.4, for every invariant positive kernel

$K \in C(\mathbb{S}^{n-1} \times \mathbb{S}^{n-1})$, we have absolute uniform convergence of

$$K(x,y) = \sum_{d=0}^{\infty} \widehat{K}_d Z_d(x,y),$$

where we have:

$$\widehat{K}_d = \int_{\mathrm{O}(n)} K(e_1, ge_1)\langle \mathfrak{P}e_1^d, g \cdot \mathfrak{P}e_1^d \rangle dg;$$

$$Z_d(x,y) = \langle s(x)\mathfrak{P}e_1^d, s(y)\mathfrak{P}e_1^d \rangle;$$

s is a choice of section; and $\widehat{K}_d \geq 0$. A section s is given by assigning to x any orthogonal matrix $s(x)$, such that the first column equals to x. The representation is unitary and $\mathfrak{P}$ is self-adjoint, so we have $Z_d(x,y) = \langle e_1^d, s(x)^\mathsf{T} s(y)\mathfrak{P}e_1^d \rangle$. By the observation at the end of Section 3.4, this is a polynomial in the top-left block of $s(x)^\mathsf{T} s(y)$, and therefore a polynomial in the inner product of x and y. This proves part of a theorem by Schoenberg. He proved more, since he also showed that the polynomials in question are the Gegenbauer polynomials. It would be interesting to find a direct proof for this fact in our framework. Let us verify it for a particular case. Let $d = 2$. The operation $\frac{1}{n}d_{12}$ is self-adjoint and idempotent, i.e. a projection operator, and hence traceless tensors are given by the orthogonal complement of the space spanned by $\psi = \sum_{k=1}^{n} e_k \otimes e_k$. Hence the projection onto the traceless part of a tensor is given by $\mathfrak{P} = 1 - \frac{1}{n}d_{12}$. The Young symmetriser in this case is given by $c_\lambda = \frac{1}{2}(() + (12))$. We then have

$$\begin{aligned}
&\langle \mathfrak{P}(e_1 \otimes e_1) \cdot c_\lambda, g \cdot \mathfrak{P}(e_1 \otimes e_1) \cdot c_\lambda \rangle \\
&= \quad \langle e_1 \otimes e_1, g \cdot (e_1 \otimes e_1 - \frac{1}{n}\psi) \rangle \\
&= \quad g_{11}^2 - \frac{1}{n}
\end{aligned}$$

which is the second Gegenbauer polynomial.

t = 2. We proceed as before, but now for the Stiefel manifold. In particular, let us consider the space $\mathrm{O}(n)/\mathrm{O}(n-2)$, which may be identified with the space of ordered pairs of orthonormal vectors. There is only one orbit, of which we choose as representative the pair (e_1, e_2). The orthogonal group $\mathrm{O}(n)$ acts smoothly and transitively on $\mathrm{O}(n)/\mathrm{O}(n-2)$, and so conditions (i)–(iii) from Section 1.1 are fulfilled. The stabiliser subgroup is now $\mathrm{O}(n-2)$. In this case, U is the vector subspace of V generated by e_1 and e_2. In this case, the irreducible repesentations with nontrivial invariants are given by $\mathbb{S}_{[\lambda]}V$ with $\lambda = (\lambda_1, \lambda_2)$ with $\lambda_1 \geq \lambda_2 \geq 0$ and an explicit bijection with $\mathbb{S}_\lambda U$ is given by considering the traceless projection. Again, we have absolute uniform convergence of the Fourier series, but now the Fourier coefficients are positive semidefinite matrices, since the dimension of $\mathbb{S}_\lambda U$ can be larger than 1. Let us work out a zonal matrix. For simplicity of the exposition, let us assume $\lambda = (2,0)$. A basis of the invariants is given by $\mathfrak{P}e_1^{2-j}e_2^j$ where $j = 0,1,2$. Let $x, y \in \mathrm{O}(n)/\mathrm{O}(n-2)$. A section for $x = (x_1, x_2)$ is given by an orthogonal matrix of which the first column is equal to x_1 and the second column is equal to x_2. Similarly for y. Again, by the remark at the end of Section 3.4, the zonal matrix is a polynomial only in the inner products of x_i and y_j, with $1 \leq i,j \leq 2$. For example, for the case with $\lambda = (2, 0)$, we now obtain a zonal matrix

$$\begin{bmatrix} g_{11}^2 - \frac{1}{n} & g_{11}g_{12} & g_{12}^2 - \frac{1}{n} \\ g_{11}g_{21} & \frac{1}{2}(g_{11}g_{22} + g_{21}g_{12}) & g_{12}g_{22} \\ g_{21}^2 - \frac{1}{n} & g_{21}g_{22} & g_{22}^2 - \frac{1}{n} \end{bmatrix}$$

where the matrix $s(x)^{\mathsf{T}} s(y)$ is to be substituted for g.

CHAPTER 4

Equiangular lines

This chapter is based on a paper by De Laat, Machado and the author of this thesis [**41**]. We compute the second and third levels of the Lasserre hierarchy for certain projective and spherical finite distance problems. With this, we give new linear bounds on the maximum number of equiangular lines in dimension n with common angle $\arccos\alpha$. These are obtained through asymptotic analysis in n of the semidefinite programming bound given by the second level. We differ from that paper by using method II, since the original paper used method I. This simplifies certain calculations considerably.

4.1. Introduction

In discrete geometry, linear programming bounds are important for bounding the quality of geometric configurations [**47, 115, 28, 4, 29**]. These bounds have been used to show that constructions are optimal, for example the sphere packings coming from the E_8 and Leech lattices [**111, 30**]. Moreover, the best known asymptotic bounds for binary codes [**84**], spherical codes and sphere packing densities [**62, 33**], and certain problems in Euclidean Ramsey theory [**5, 24**] are derived from the linear programming bounds.

However, for many instances the linear programming bounds are not sharp and research is being done into semidefinite programming bounds. Initiated by Schrijver for binary codes, and Bachoc and Vallentin for the kissing number problem, three-point semidefinite programming bounds have been developed which take into account interactions between triples of points, as opposed to pairs of points for the linear programming bounds [**107, 6, 32, 27**]. Various three-point bounds exist in other contexts, but we focus on semidefinite programming bounds in the geometric setting. For the equiangular lines problem this has been generalized to a hierarchy of k-point bounds [**42**]. For many problems, these higher-order bounds lead to significant improvements, including new optimality proofs via sharp bounds; see, e.g., [**7, 32, 48**]. However, until now no new asymptotic results in the dimension have been derived from these bounds.

The Lasserre hierarchy [**70**] and the dual sum-of-squares approach by Parrilo [**99**] are important for obtaining bounds for hard problems in combinatorial optimization [**73, 55, 78**]. De Laat and Vallentin have extended the Lasserre hierarchy for the independent set problem to a continuous setting so that it can be applied to problems in discrete geometry [**44**]. The first level of the hierarchy reduces to the linear programming bound. The second level, however, is a 4-point bound from which the k-point with $k = 4$ mentioned above can be derived by removing many of the constraints. Hence the second level of the Lasserre hierarchy, although more difficult to compute, is a promising approach to improve bounds. The second level of this hierarchy has only been computed for an energy minimization problem in dimension 3 [**39**]. We would also like to mention that an adaptation of this hierarchy for the sphere packing problem was given recently [**31**]. In summary, computing the higher levels of this hierarchy is a promising approach for various problems in discrete geometry.

In this chapter, we compute the second and third level of the Lasserre hierarchy for the equiangular lines problem with a fixed angle $\arccos \alpha$. This problem asks to determine the maximum number $N_\alpha(n)$ of lines through the origin in $\mathbb{R}^n$ such that the angle between any pair of lines is $\arccos \alpha$. Recently, there have been several breakthroughs for this problem, starting with the result by Bukh in 2016 that $N_\alpha(n)$ is at most linear in n for any fixed α [**21**]. In 2018 Balla, Dräxler, Keevash, and Sudakov showed $\limsup_{n\to\infty} N_\alpha(n)/n$ is at most 1.93 unless $\alpha = 1/3$, in which case it is 2 [**9**]. In 2021 Jiang, Tidor, Yao, Zhang, and Zhao showed

$$N_\alpha(n) = \lfloor (a+1)(n-1)/(a-1) \rfloor \tag{55}$$

for $\alpha = 1/a$ with a an odd integer $a \geq 3$ and all sufficiently large n [**61**]. The significance of these particular inner products $\alpha = 1/a$ lies in the fact that the equiangular lines problem without fixed angle can be solved in any dimension by computing $N_\alpha(n)$ for a given finite list of such α; see [**69**]. The linear bound by Bukh holds for all dimensions, but the slope is huge. The results from [**9**] and [**61**] hold only for $n \geq n_\alpha$ for a very large n_α. In these results, the parameters are so large because the proofs rely on Ramsey theory.

Asymptotically linear bounds not relying on Ramsey theory have also been given [**56, 8**]. The best current bound was given by Balla in 2021. He proved (Theorem 1 in [**8**]) for all dimensions n and for $\alpha \in (0,1)$ the bound

$$N_\alpha(n) \leq \frac{\sqrt{n}}{2\alpha^3} + \frac{(1+\alpha)n}{2\alpha}. \tag{56}$$

Our main result is the following conjecture, which we prove for $\alpha = 1/a$ with $a = 3, 5, 7, 9, 11$.

Conjecture 4.1. Let $\alpha \in (0,1)$. The optimal objective of the second level $\mathrm{las}_2(n)$ of the Lasserre hierarchy for bounding $N_\alpha(n)$ satisfies

$$\mathrm{las}_2(n) \leq c_\alpha + \frac{1+\alpha}{2\alpha} n \tag{57}$$

for $n \geq n_\alpha$, where c_α does not depend on the dimension.

For the values of α mentioned, we provide both an explicit small c_α and an explicit small n_α, so we give new bounds in many dimensions not covered by (55). Furthermore, because of the $\sqrt{n}$ term, we also improve on (56) for these α. Our explicit linear bounds are listed in Table 1. These are the first asymptotic bounds in the dimension coming from semidefinite programming. We have also computed the third level of the Lasserre hierarchy, with which we obtain new bounds for fixed dimensions. More detailed results are given in Section 5.5. The third level also provides numerical evidence for the existence of linear bounds for all dimensions, of which the asymptotic slopes improve on (56) and our bound (57).

We would like to reflect briefly on how surprising Conjecture 4.1 is for a semidefinite programming bound. For fixed n, finite convergence of the Lasserre hierarchy is guaranteed, so in principle this hierarchy can be used to solve any equiangular lines problem. However, for a fixed level of the hierarchy, it could have been that the bound on $N_\alpha(n)$ becomes very bad for large n. Indeed, this is the behavior we see for the Delsarte and the k-point bounds from [**42**], where for any fixed α and k, the bound on $N_\alpha(n)$ grows rapidly as a function of n. This is a testament to the strength of the Lasserre hierarchy.

The first level of the hierarchy is equal to the Lovász theta prime number [**39**], and this can be reduced to the Delsarte, Goethals, Seidel linear programming bound using Schoenberg's characterization [**106, 4**]. In this chapter, we compute the second and third level of the Lassere hierarchy 1 using the parametrisation of the kernels in Theorem 1.16. To use this parametrisation, a complete system of the space $\mathrm{Hom}_{\mathrm{O}(n)}(\mathcal{I}_t, V_\lambda)$ of continuous equivariant maps is required for every irreducible representation V_λ of $\mathrm{O}(n)$. In 4.2, we describe the spaces $\mathcal{I}_t$ and construct such a complete system. In particular, we will construct functions R and s as described in Sections 1.1 and 1.2. We then describe how method II may be used to calculate the zonal matrix. The original paper used method I. In Section 5.5 we give the explicit program and discuss results. We first give improved bounds on $N_\alpha(n)$ in fixed dimensions, as shown in Figures 1 and 2, and then consider bounds for more general spherical finite distance problems. In Section 4.5 an asymptotic analysis of the bounds is given, which leads to the proof of Conjecture 4.1 for the values of α mentioned.

4.2. A complete system

The space $\mathcal{I}_t$. Let $D \subseteq [-1, 1]$ be a finite subset such that $x \in D$ if and only if $-x \in D$. Consider a graph of which the vertex set is given by the $(n-1)$-dimensional real projective space $\mathbb{P}^{n-1}$ and the edge set is given as follows. Two different elements of projective space have an edge if the inner product between two norm 1 vectors spanning the lines does not lie in D. Because $D = -D$, this does not depend on the choice of these vectors. An independent set then corresponds to a configuration of lines with prescribed inner products, and hence prescribed angles. Recall from the introductory chapter the space $\mathcal{I}_t$ of independent sets of size t and also the space $\mathcal{I}_{=t}$ of independent sets of size t precisely. The action of the orthogonal group on $\mathbb{P}^{n-1}$ preserves edges and therefore, it also acts on $\mathcal{I}_t$ in the natural way. Let us show that the space $\mathcal{I}_{=t}$ has finitely many orbits, so that we are in the situation of Section 1.4. Indeed, we may enumerate them as follows. Consider the set Y of matrices of size t that are positive semidefinite and have rank at most n with 1s on the diagonal and elements of D elsewhere. On the set Y we may define an equivalence relation by declaring $y_1 \sim y_2$ if y_1 may be

α	c_α	n_α
1/3	4	13
1/5	30	87
1/7	116	261
1/9	316	166018
1/11	699	751307

TABLE 1. We prove $N_\alpha(n) \leq c_\alpha + \frac{1+\alpha}{2\alpha} n$ for all $n \geq n_\alpha$. The constants $n_{1/9}$ and $n_{1/11}$ can also be made smaller by solving finitely many semidefinite programs.

obtained from y_2 by performing simultaneous permutation of rows and columns and by simultaneous multiplication of a subset of the rows and columns by -1. On the space $\mathcal{I}_{=t}$, we may then define a map into $Y/\sim$ by assigning to an independent set the Gram matrix. A couple of choices have to be made, because an element of projective space is defined up to a sign and an independent set is defined up to an ordering. However, because of the equivalence relation, the map into $Y/\sim$ is well-defined. Furthermore, if two elements of $\mathcal{I}_{=t}$ differ by an element of $\mathrm{O}(n)$, then they are assigned to the same element of $Y/\sim$. Therefore, we obtain a factorisation $\mathcal{I}_t/\mathrm{O}(n) \to Y/\sim$. The space $Y/\sim$ is a quotient of a finite space and is therefore finite itself. An inverse to this factorisation is given by choosing a representative of an element of $Y/\sim$, computing a Cholesky factorisation and assembling the columns in a set. Therefore, the factorisation is a bijection and there are finitely many orbits. Hence the space $\mathcal{I}_t$, being a disjoint union of such spaces, is also a space with finitely many orbits. For notation, we will write $\mathcal{I}_t/\mathrm{O}(n) = \{1, \ldots, N\}$. Since this is a finite set, the conditions (i)–(iii) of Chapter 1 are fulfilled. By Section 1.4, we have absolute uniform convergence of the Fourier series, though we shall not use this fact.

We will use the kernels from Theorem 1.16 to write the program (1) explicitly for the equiangular lines problem with a fixed angle. A couple of jobs are left to do to use Theorem 1.16. Namely, we have to construct a complete system for the space $\mathrm{Hom}_{\mathrm{O}(n)}(\mathcal{I}_t, V_\pi)$ of continuous equivariant maps for each irreducible representation (π, V_π) of the orthogonal group. Firstly, we need to choose a function R which assigns to the orbit $i \in \mathcal{I}_t/\mathrm{O}(n)$ a representative $R(i)$ in $\mathcal{I}_t$. Secondly, we need to describe the stabiliser subgroups $H(i)$ and the irreducible representations V_λ of $\mathrm{O}(n)$ with nontrivial $H(i)$-invariants. Having done so, suppose that for each $i \in \mathcal{I}_t/\mathrm{O}(n)$, we have a basis $v_{\lambda,i,j}$ of $V_\lambda^{H(i)}$ with $1 \leq j \leq k_{\lambda,i}$, with $k_{\lambda,i} = \dim V_\lambda^{H(i)}$. By the description at the start of Section 1.4 and Proposition 1.8, a complete system of $\mathrm{Hom}_{\mathrm{O}(n)}(X_i, V_\lambda)$ is given by the functions $\psi_{\lambda,i,j}(x) = s(x) \cdot v_{\lambda,i,j}$, where s is a section as in Section 1.2. These are then combined, extending by zero, to form a complete system of $\mathrm{Hom}_{\mathrm{O}(n)}(\mathcal{I}_t, V_\lambda)$. Thirdly, we need to calculate the zonal matrix

$$Z_{\lambda,(i_1,j_1),(i_2,j_2)}(J_1, J_2) = \langle \psi_{\lambda,i_1,j_1}(J_1), \psi_{\lambda,i_1,j_1}(J_2) \rangle$$

for which we will use method II.

Invariants. For every $i \in \mathcal{I}_t/\mathrm{O}(n)$, we can choose the representatives $R(i)$ to lie in the span of the first $t_i = |R(i)|$ basis vectors. We assume for notational simplicity that the vectors in $R(i)$ are linearly independent, which is true for all applications considered in this paper. Let $\mathrm{O}(n - t_i)$ be the subgroup of $\mathrm{O}(n)$ of all orthogonal matrices which fix the first t_i basis vectors pointwise. Every permutation of the set $R(i)$ can be achieved with an orthogonal matrix in $\mathrm{O}(n)$ which fixes the final $n - t_i$ basis vectors pointwise. We will denote by $P(i)$ the subgroup of $\mathrm{O}(n)$ which permutes the elements of $R(i)$. Finally, denote by $-I$ the identity matrix I times -1. One readily verifies that $H(i)$ is the subgroup generated by $\mathrm{O}(n - t_i), P(i)$ and $-I$. Furthermore, these subgroups commute, and so the invariants under $H(i)$ can be calculated as the invariants under $P(i)$ and $-I$ inside $V_\lambda^{\mathrm{O}(n-t_i)}$.

The representations V_λ with nontrivial invariants $V_\lambda^{\mathrm{O}(n-t_i)}$ are described by Theorem 3.5. A basis of $V_\lambda^{\mathrm{O}(n-t_i)}$ is given by the set of tensors $v_T = \mathfrak{P} e_T c_\lambda$, where T ranges over semistandard tableaux using numbers between 1 and t_i. The dimension m_i of the space $V_\lambda^{\mathrm{O}(n-t_i)}$ is given by equation 3.1. We enumerate the tableaux in such a way that the first m_i semistandard tableaux give a basis for $V_\lambda^{\mathrm{O}(n-t_i)}$ and the bases for the spaces $V_\lambda^{\mathrm{O}(n)} \subseteq V_\lambda^{\mathrm{O}(n-1)} \subseteq \cdots \subseteq V_\lambda^{\mathrm{O}(n-t)}$ are nested.

To use the basis of $V_\lambda^{\mathrm{O}(n-t_i)}$ to construct a basis for $V_\lambda^{H(i)}$ we use the following procedure. First, we construct the matrices generating the groups $P(i)$. For this we fix an ordering of the vectors in $R(i)$. We will then abuse notation and denote also by $R(i)$ the $n \times t_i$ matrix with these vectors as columns. The Gram matrix $A(i) = R(i)^{\mathsf{T}} R(i)$ is a matrix with 1s in the diagonal and elements from D elsewhere. Given a permutation σ of the columns, denote by P_σ the corresponding $t_i \times t_i$ permutation matrix. If $P_\sigma^{\mathsf{T}} A(i) P_\sigma = A(i)$, then there exists a corresponding $r_\sigma \in P(i)$ given by

$$r_\sigma = R(i) P_\sigma A(i)^{-1} R(i)^{\mathsf{T}}.$$

and we observe that r_σ satisfies $r_\sigma R(i) = R(i) P_\sigma$. To obtain the generators for the group $P(i)$, we take the generators σ of the symmetric group on t_i elements which satisfy $P_\sigma^{\mathsf{T}} A(i) P_\sigma = A(i)$ and take the corresponding matrices r_σ.

To obtain a basis for the space $V_\lambda^{H(i)}$ we compute a basis for the solution space of the linear system

$$r_\sigma \cdot \sum_j a_j v_{T_j} = \sum_j a_j v_{T_j} \tag{58}$$

where a_j are complex numbers with $1 \leq j \leq m_i$. We use method II to obtain the explicit linear system. Finally, we impose the constraint $v_T = -I \cdot v_T = (-1)^{|\lambda|} v_T$. For $|\lambda|$ odd, this annihilates $V_\lambda^{H(i)}$ and for $|\lambda|$ even this has no effect. The solutions will be denoted by $v_{\lambda,i,j}$ with $1 \leq i \leq N$ and $1 \leq j \leq k_{\lambda,i}$, where N is the number of orbits and $k_{\lambda,i} = \dim V_\lambda^{H(i)}$.

Let us look at an example. Let $t = 2$ and consider an orbit X such that the elements of X have cardinality two. Let r be the $n \times n$ orthogonal matrix which maps e_2 to $-e_2$ and fixes the orthogonal complement of e_2. We may choose a representative $R = \{v_1, v_2\}$ of X such that $rv_1 = v_2$ and $rv_2 = v_1$. Then the group P is the group of two elements $\{I, r\}$. Using the definition of the representation, we then have $r \cdot v_T = v_T$ if there is an even number of 2s in the tableau T and $r \cdot v_T = -v_T$ if there is an odd number of 2s in T. We see that the space $V_\lambda^{H(i)}$ vanishes if $|\lambda|$ is odd. For $|\lambda|$ even, a basis of V_λ^H is given by the set of v_T with T semistandard and filled with 1s and 2s, and an even number of 2s.

The sections. Suppose $J_1 \in X_{i_1}$ and $J_2 \in X_{i_2}$. We want to construct sections for J_1 and J_2 and compute the zonal matrix. Let us first compute $s(J_1)$. Fix an ordering of the vectors in $R(i_1)$ and J_1, and denote also by $R(i_1)$ and J_1 the matrices with these vectors as their columns. Let $A(i_1) = R(i_1)^{\mathsf{T}} R(i_1)$ and let P be a permutation matrix for which $A(i_1) = P^{\mathsf{T}} J_1^{\mathsf{T}} J_1 P$. Let Q be an orthogonal matrix with the first t_{i_1} columns given by the corresponding columns of $J_1 P A^{-1} R(i_1)^{\mathsf{T}}$. The representative $R(i_1)$ is chosen to be supported in the first t_{i_1} coordinates, so we have $QR(i_1) = J_1 P$, and we can define $s(J_1) = Q$. The matrix $s(J_2)$ is computed similarly. Then the top-left $t_{i_1} \times t_{i_2}$ block of $s(J_1)^{\mathsf{T}} s(J_2)$ is given by the corresponding block of

$$(J_1 P(i_1) A(i_1)^{-1} R(i_1)^{\mathsf{T}})^{\mathsf{T}} J_2 P(i_2) A_{i_2}^{-1} R(i_2)^{\mathsf{T}}. \tag{59}$$

Hence the zonal matrix

$$\begin{aligned}
&Z_{\lambda,(i_1,j_1),(i_2,j_2)}(J_1,J_2)\\
&=\langle \psi_{\lambda,i_1,j_1}(J_1),\psi_{\lambda,i_1,j_1}(J_2)\rangle\\
&=\langle s(J_1)\cdot v_{\lambda,i_1,j_1}, s(J_2)\cdot v_{\lambda,i_2,j_2}\rangle\\
&=\langle v_{\lambda,i_1,j_1}, s(J_1)^{\mathsf{T}}s(J_2)\cdot v_{\lambda,i_2,j_2}\rangle
\end{aligned}$$

may be computed with method I. The result is a polynomial in the correct block of $s(J_1)^{\mathsf{T}}s(J_2)$ and hence in the correct block of (59) by Section 3.4. The coefficients lie in $\mathbb{Q}(n)$.

4.3. New bounds in fixed dimensions

Let us now give program (1) explicitly for the equiangular lines problem with a fixed angle. Recall from the introductory chapter that any feasible solution to this program gives an upper bound to the maximal size of a configuration of equiangular lines with a fixed angle. We have

$$\begin{aligned}
&\text{minimize} && K(\emptyset,\emptyset) && \\
&\text{subject to} && A_t K(R(i)) \le -1_{\mathcal{I}_{=1}}(R(i)), && i\in\mathcal{I}_{2t}/\mathrm{O}(n),\\
& && \widehat{K}_\lambda \succeq 0, && |\lambda|\le d.
\end{aligned}\qquad (60)$$

For $J_1, J_2 \in \mathcal{I}_t$, the evaluation of the kernel is given by

$$K(J_1,J_2)=\sum_\lambda \langle Z_\lambda(J_1,J_2),\widehat{K}_\lambda\rangle$$

where $\lambda=(\lambda_1,\dots,\lambda_t)$ satisfies $\lambda_1\ge\cdots\ge\lambda_t\ge 0$ and $|\lambda|=\sum_{i=1}^t\lambda_i\le d$. Here we have used the notation from Theorem 1.16. The zonal matrix is computed as described in Section 4.2. The operator A_t is as described in (1). The entries of the constraint matrices are explicitly computed rational functions in the dimensions n over the ground field of the algebraic numbers. To bound $N_\alpha(n)$ we consider the projective finite distance problem with $D=\{\pm\alpha\}$. In the paper [**41**], this program is computed using method I for $t=2,3$, both with $d\le 5$. The results in this chapter are obtained in this way. More information on that implementation can be found in that paper.

Let us now discuss the results. There has been extensive research into the determination of $N_\alpha(n)$. As mentioned in the introduction, usually only inner products $\alpha=1/a$ with a an odd natural number are considered, since these are the only cases for which there may exist equiangular line configurations of size larger than $2n$ [**76**], and the determination of $N_\alpha(n)$ for these values of α solves the equiangular lines problem without fixed angle in dimension n [**69**]. In [**76, 94, 23**] the equations

$$N_{1/3}(n)=\begin{cases}28 & \text{for } 7\le n\le 14, \text{ and}\\ 2(n-1) & \text{for } n\ge 15\end{cases}$$

and

$$N_{1/5}(n)=\begin{cases}276 & \text{for } 23\le n\le 185, \text{ and}\\ \lfloor \frac{3}{2}(n-1)\rfloor & \text{for } n\ge 185,\end{cases}$$

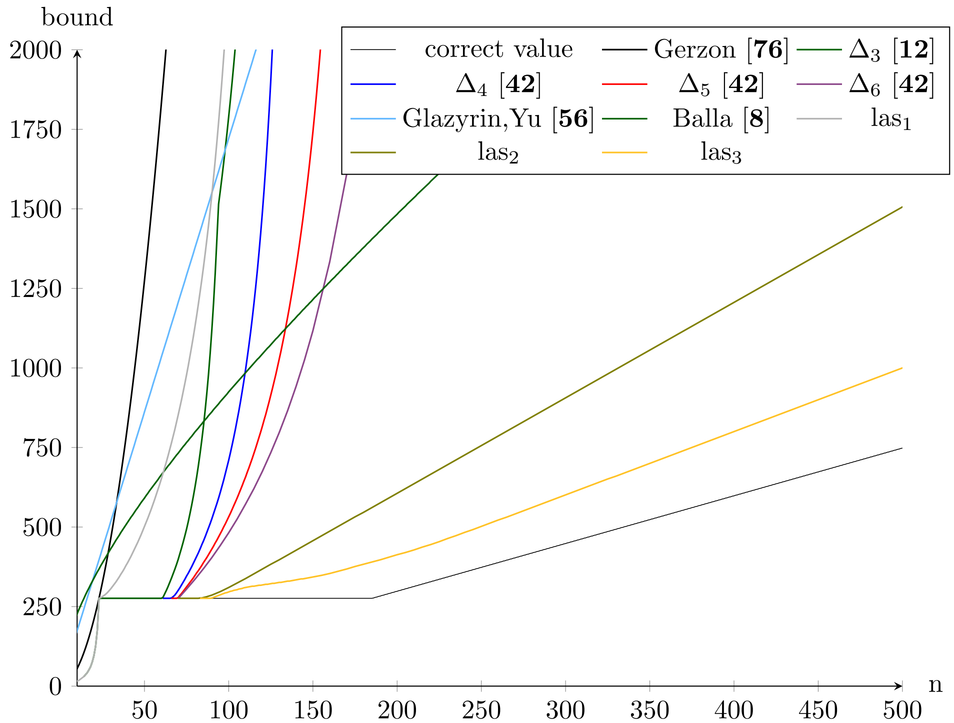


FIGURE 1. Bounds for $N_{1/5}(n)$.

are shown, but for $a \geq 7$ less is known; see [**64**, Appendix A]. As mentioned in the introduction, the correct values are known for very large dimensions and there exist general upper and lower bounds.

A fundamental result in the linear/semidefinite programming approach is the Delsarte, Goethals, and Seidel [**47**] linear programming bound. Since this bound takes into account constraints between pairs of points, it is called a 2-point bound which we denote by Δ_2. In [**6, 12**] this is generalized to a 3-point bound Δ_3 and computed for the equiangular lines problem, and in [**90, 42**] this is generalized to a k-point bound Δ_k and computed for $k = 4, 5, 6$. As mentioned in the introduction we have $\Delta_2 = \text{las}_1$. The bounds las_2 and las_3 considered in this paper thus provide an alternative generalization of the linear programming bound. As shown in Figure 2, for $a = 7$ and for many dimensions the bounds las_2 and las_3 are much stronger than any of the previous bounds coming from semidefinite programming or elsewhere. Similar results hold for larger values of a, but we do not include the plots because they look qualitatively similar. One common feature of Δ_k for $k = 3, 4, 5, 6$ is that starting at $n = a^2 - 2$ they stabilize and produce the constant bound

$$\frac{(a^2-2)(a^2-1)}{2} \tag{61}$$

on $N_{1/a}(n)$ until a certain dimension $D_k(a)$. For $a = 5$ there is an exceptional configuration related to the Leech lattice of $(a^2-2)(a^2-1)/2 = 276$ points in dimension $a^2 - 2$ [**34, 76**]. This configuration stays optimal until a construction of

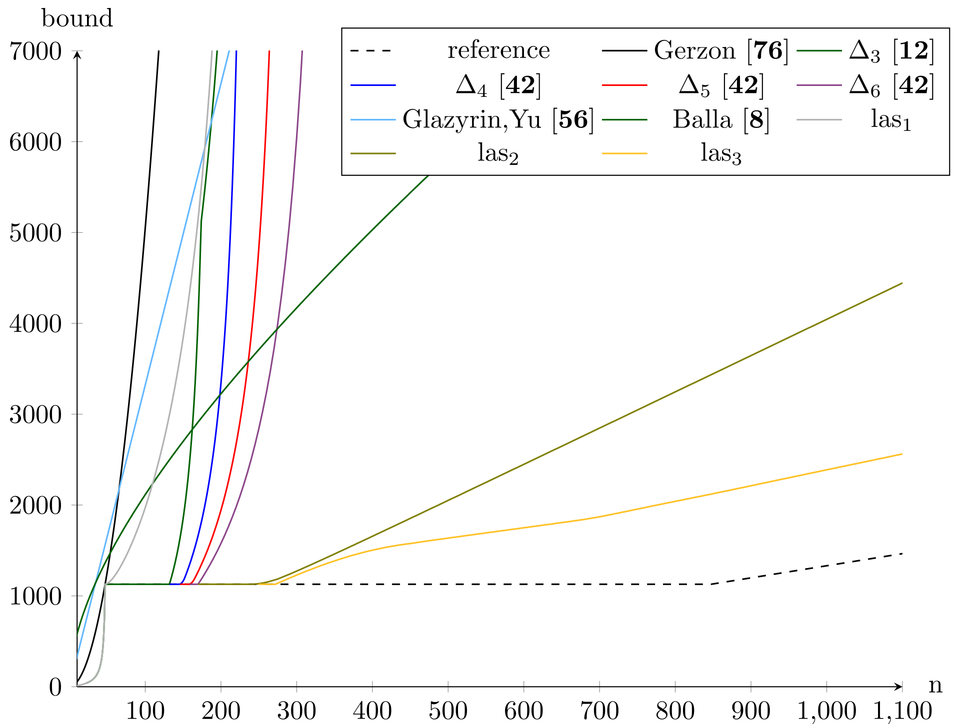


FIGURE 2. Bounds for $N_{1/7}(n)$. The dashed line extends (61) until dimension (62), from which it continues with the construction of $\lfloor (n-1)(a+1)/(a-1) \rfloor$ lines.

$\lfloor (n-1)(a+1)/(a-1) \rfloor$ equiangular lines in dimension n (see [**21**]) matches (61), which happens in dimension

$$\frac{(a^2-2)(a-1)^2}{2} + 1. \tag{62}$$

The general situation is different, however, since it is known that a configuration of $(a^2-2)(a^2-1)/2$ lines in dimension a^2-2 cannot exist for a number of values of a starting at $a=7$ [**10, 93**]. In fact, in [**64**] it is shown that for those values of a there is no configuration of $(a^2-2)(a^2-1)/2$ equiangular lines in dimensions $a^2-2 \le n \le D_4(a)$. It is therefore of interest to find better semidefinite programming bounds on $N_{1/a}(a^2-2)$ and to increase the range of dimensions for which we know that (61) gives an upper bound on $N_{1/a}(n)$. As can be seen in Table 2, the bounds las_2 and las_3 are equal to (61) for a significantly larger range of dimensions. Furthermore, we have obtained an example where las_3 improves over las_2 and las_1 and hence the linear programming bound for a dimension lower than a^2-2. For $a=7$ and $n=13$ the bound improves from 17 to 16. In [**114, 64**] explicit quadratic expressions are given for $D_3(a)$ and $D_4(a)$. Based on the data in Table 2 we conjecture that for las_2 and las_3 the corresponding expressions are cubic instead of quadratic. Recall that (62) is quartic in a.

4.4. More general distance sets

We may also consider a non-projective version, in which case the graph is the sphere $\mathbb{S}^{n-1}$. This allows for distance sets D which are not necessarily symmetric under change of sign. Since the projective space is equal to the quotient $\mathbb{P}^{n-1} \cong \mathbb{S}^{n-1}/-I$, the only change is invariance under $-I$. This implies that the invariant space $V_\lambda^{H_i}$ is unchanged if $|\lambda|$ is even, but we now have also have to consider representations with $|\lambda|$ odd. Furthermore, there are more orbits, since now we only consider two Gram matrices as representatives of the same orbit only if they are equal up to simultaneous permutations of rows and columns, but no longer equal if they differ by simultaneous multiplication by -1 of a subset of rows and columns. Both of these changes lead to a larger semidefinite program. In this section we discuss some applications of las_2 to problems where the allowed distance set D is not of the form $\{\pm\alpha\}$. Furthermore, for some of these computations the cardinality of D is 3 as opposed to 2. Here nothing changes in the formulation of the bounds, but the number of orbits to consider increases greatly and las_3 becomes too hard to compute. For instance, with inner products $\{1/7, -1/7\}$ there are 156 orbits with sets of size 6, while with inner products $\{1/7, -1/7, 0\}$ there are 25506 such orbits.

The first application we considered is to a problem with sets of matrices having orthogonal rows. Following [**1, 63**], a Hadamard matrix of order n is a $(+1,-1)$-valued $n \times n$ matrix H such that $HH^{\mathsf{T}} = nI$, and a weighing matrix of order n and weight k is a $(+1,-1,0)$-valued $n \times n$ matrix such that $WW^{\mathsf{T}} = kI$. Two Hadamard matrices H_1 and H_2 of order n are said to be quasi-unbiased for parameters (l, a) if $a^{-1/2}H_1H_2^{\mathsf{T}}$ is a weighing matrix of weight l. Note that necessarily $l = n^2/a$. Hadamard matrices $H_1, \ldots, H_f$ of order n are said to be quasi-unbiased for parameters (l, a) if they are pairwise quasi-unbiased for those parameters. Table 1 of Araya, Harada, and Suda [**1**] has a list of the possible

a	$\Delta_2 = \mathrm{las}_1$	Δ_3	Δ_4	Δ_5	Δ_6	las_2	las_3	Intersection
5	23	60	65	69	70	82 (80)	90 (89)	185
7	47	131	145	158	169	243 (239)	272 (271)	847
9	79	227	251	273	300	535 (530)	610 (610)	2529
11	119	347	381	413	448	1000 (993)	1152 (1152)	5951
13	167					1676 (1668)	1946 (1946)	12025
15	223					2604 (2595)	3040 (3040)	21855
17	287					3823 (3813)	4483 (4483)	36737
19	359					5374 (5362)	6321 (6321)	58159
21	439					7294 (7281)	8603 (8603)	87801
23	527					9626 (9611)	11377 (11377)	127535
25	623					12407 (12391)	14692 (14692)	179425

TABLE 2. The largest dimension n for which the respective bounds can be used to show (61) holds. In parentheses we list the largest dimension for which the bound is exactly equal to $(a^2-2)(a^2-1)/2$. The bound Δ_3 is computed in [**12, 65**] and the bounds Δ_4, Δ_5, Δ_6 are computed in [**42**]. The column labeled 'Intersection' shows the dimension from (62) for reference.

parameters for quasi-unbiased Hadamard matrices of order up to 48 together with bounds for the maximum size of these sets. Kao, Suda, and Yu [**63**] applied the semidefinite programming bound Δ_3 to derive bounds based on an observation that normalizing the rows of a set of f quasi-unbiased Hadamard matrices for parameters (l, a) gives a spherical 3-distance set in S^{n-1} with $|X| = nf$ and inner products $\{\pm l^{-1/2}, 0\}$. We apply las_2 using polynomial representations of degree $|\lambda| \leq 8$ to give the bounds as listed in Table 3.

For completeness we also mention applications we tried where we did not get new results. We applied our bound to a problem involving "Q-antipodal Q-polynomial schemes with 3 classes" as described by Martin, Muzychuk, Williford [**83**], but we observed that las_2 produces the same results as listed in the table in [**63**].

Another application of bounds for 3-distance sets is to the maximum size of a 3-distance set in S^{n-1} for any possible choice of angles [**92, 110**]. Here a theorem by Nozaki [**96**] is used so that for each inner product d_3 only finitely many other inner products d_1 and d_2 need to be considered. By using sums-of-squares techniques the bounds $\Delta_2 = \mathrm{las}_1$ and Δ_3 can be applied [**92, 110, 79**]. We applied las_2 to this problem, and did get improvements for some parameters, but overall could not get new results because like Δ_2 and Δ_3, las_2 becomes unbounded as $d_3 \to 1$. Finally, we tried to disprove the existence of certain strongly regular graphs; see Cameron [**14**, Chapter 8] for an introduction to these graphs and also the more complete monograph by Brouwer and Van Maldeghem [**20**]. The existence of a strongly regular graph with a given set of parameters implies the existence of a spherical 2-distance set in a certain dimension and with certain inner products; see Theorem 5.1 in [**14**, Chapter 8]. We applied las_3 with $|\lambda| \leq 5$ to all sets of parameters listed as open in [**20**, Chapter 12] with at most 200 vertices, without getting a new result.

4.5. Asymptotic analysis of the bounds

In this section we explain how we obtain a computer generated and verified proof of Conjecture 4.1 for $a = 3, 5, 7, 9, 11$. First we observe empirically that the degree of

n	l	a	Lower bound from [**1**]	Upper bound from [**1**]	Δ_3 [**63**]	las_2
16	4	64	8	35	15	15
24	4	144	2	85	25	23
24	9	64	16	85	95	95
32	4	256	8	155	47	31
36	9	144	-	199	79	67
40	4	400	-	247	101	39
40	25	64	-	28	30	30
48	4	576	2	361	276	47
48	9	256	16	361	104	96
48	16	144	-	361	316	316
48	36	64	2	28	30	30

TABLE 3. Improved bounds on the maximum number of quasi-unbiased Hadamard matrices of order n with parameters (l, a).

the required representations does not grow. In fact, for large dimensions, we only use the representations with $\lambda = (0,0), (3,1), (4,0)$. Though it is not necessary for our proof, we have the following conjecture:

CONJECTURE 4.2. The optimal value of las_2 for bounding $N_\alpha(n)$ can be obtained by using only the representations with $\lambda = (0,0), (2,0), (3,1), (4,0)$. Moreover, for dimensions beyond the stable range the representation with $\lambda = (2,0)$ is not needed.

As numerical evidence for Conjecture 4.1 we observed that the function $\mathrm{las}_2(n)$ can be expanded in terms of $n, 1, n^{-1}, n^{-2}, \ldots$, and through interpolation we find the first few coefficients in this expansions for many values of α. We found that the first expansion coefficient satisfies the formula $(1+\alpha)/(2\alpha)$. For $\alpha = 1/5$, the expansion of $\mathrm{las}_2(n)$ seems to be particularly well-behaved having rational coefficients:

$$3n + 6 + \frac{120}{n} + \frac{5530}{n^2} + \frac{1449485}{3n^3} + \frac{2961283225}{72n^4} + O\left(\frac{1}{n^5}\right). \tag{63}$$

To prove Conjecture 4.1 for a given value of α we construct, for each sufficiently large n, a feasible solution to the semidefinite program $\mathrm{las}_2(n)$ such that the corresponding sequence of objective values is linear in n with slope $(1+\alpha)/(2\alpha)$. For this we consider the perturbed hierarchy $\mathrm{las}_{2,4}(n)$, where we subtract $1/n^4$ from the right hand side of each inequality constraint in (60) and force each eigenvalue of each block matrix to be at least $1/n^4$. Let $\{F^\lambda(n)\}_\lambda$ be the optimal solution of $\mathrm{las}_{2,4}(n)$ lying on the central path of the interior-point method. We now make the ansatz that there exist matrices $A^{\lambda,k}$, whose entries are algebraic numbers of low degree and reasonable bitsize, such that

$$F^\lambda(n)_{(i_1,j_1),(i_2,j_2)} = \sum_{k=0}^{\infty} A^{\lambda,k}_{(i_1,j_1),(i_2,j_2)} n^{1+\lambda_1+2\lambda_2-t_{i_1}-t_{i_2}-k}, \tag{64}$$

where as before t_i is the cardinality of the orbit representative R_i. Then we use the interior-point solver to numerically compute a near optimal solution approximately on the central path of $\mathrm{las}_{2,4}(n)$ for dimensions $N, N+1, \ldots, N+L$, and we use this to compute approximations of the coefficient matrices $A^{\lambda,0}, \ldots, A^{\lambda,l-1}$ via interpolation. We then use the LLL algorithm to find the entries of the coefficient matrices exactly as algebraic numbers, and denote by $\mathrm{sol}(n)$ the solution whose matrices are given by the truncation of (64) using these l rounded coefficient matrices. We found good values for the parameters l, L, and N through experimentation. If the dimension N_α, beyond which the solutions are feasible, is to be made small, the number of terms l in the truncation should not be too small and not too large. Perhaps this is due to Runge's phenomenon. After that, N and L should be chosen such that we find $A^{\lambda,0}, \ldots, A^{\lambda,l-1}$ in sufficiently high precision so that we can round them correctly. For the results presented in this paper we use $N = 10^{100}$ and the parameters l and L listed in Table 4.

Next, we verify that $\mathrm{sol}(n)$ is a solution for $\mathrm{las}_2(n)$. Since the entries of both $\mathrm{las}_2(n)$ and $\mathrm{sol}(n)$ are exact rational functions in n, we can compute the slack in the inequality constraints of the solution sol(n) to $\mathrm{las}_2(n)$ as exact rational functions in n (where a positive slack means the inequality constraint is satisfied strictly). We then fix an integer n_α and evaluate these rational functions at $n_\alpha + n$. We then verify that the coefficients of the numerator and denominator polynomials are all positive, which proves the slacks are positive for $n \geq n_\alpha$, and hence the inequality constraints are satisfied for all $n \geq n_\alpha$. Then we compute the determinants of the leading principal submatrices, evaluate these rational functions in $n_\alpha + n$, and check that all coefficients of the numerator and denominator polynomials are positive, which proves the solution matrices are positive semidefinite for all $n \geq n_\alpha$. Finally we check that the objective function is linear in n with slope $(\alpha+1)/(2\alpha)$, which gives a computer verified proof of Conjecture 4.1 for this value of α. Note that although floating point computations are used to obtain the proofs, the verification procedure is implemented entirely in exact arithmetic. To make the value n_α, beyond which we can prove our bound holds, as small as possible we solve finitely many semidefinite programs in fixed dimensions. We only do this for the values $a = 3, 5, 7$, but in principle it could be done for $a = 9, 11$ too. First, we solve $\mathrm{las}_{2,4}(n)$ or $\mathrm{las}_{2,5}(n)$. Then, we approximate the floating point solution by a rational solution and we check in exact arithmetic whether the rounded solution is feasible for $\mathrm{las}_2(n)$ and has objective below $f_\alpha(n)$. The reason we use two different perturbations is that $\mathrm{las}_{2,4}(n)$ does not give good enough bounds in low dimensions and it is too difficult to find a feasible solution for $\mathrm{las}_{2,5}(n)$ in high dimensions. We use $\mathrm{las}_{2,4}(n)$ for $N_{\alpha,4} \leq n < N_\alpha$ and $\mathrm{las}_{2,5}(n)$ for $N_{\alpha,5} \leq n \leq N_{\alpha,4}$. For $\alpha = 1/7$, for example, the interpolation procedure shows that

$$\mathrm{las}_2(n) \leq 4n + a_1 + a_2 n^{-1} + \cdots + a_8 n^{-7} \quad \text{for all} \quad n \geq 13739,$$

for certain explicitly given $a_1, \ldots, a_8 \in \mathbb{Q}[\sqrt{2}]$. From this we can then derive that $N_{1/7}(n) \leq 4n + 116$ for all $n \geq 13739$. Next we solve finitely many semidefinite programs to decrease the dimension $N_\alpha = 13739$ to $n_\alpha = 261$. In Table 1 we list the bounds obtained with this approach. Note that the same approach works, in principle, for other values of α not listed in the table, but we did not perform these computations. For $t = 3$ we seem to get asymptotically linear bounds with a better slope than with $t = 2$. However, since computing the third level of the hierarchy for $d > 5$ is currently too computationally demanding we do not have the equivalent of Conjecture 4.2. The bounds might very well improve as we increase d beyond 5, and we do not know the slope of the asymptotically linear behavior as the degree d goes to infinity. In Table 5 we give the numerically computed slopes for $d = 4$ and $d = 5$.

α	$f_\alpha(n)$	N_α	l	L	$N_{\alpha,4}$	$N_{\alpha,5}$
1/3	$2n+4$	500	9	12	17	12
1/5	$3n+30$	2235	10	15	253	87
1/7	$4n+116$	13739	9	11	4638	261
1/9	$5n+316$	166018	9	12		
1/11	$6n+699$	751307	9	12		

Table 4. Parameters used to obtain the interpolations.

a	$\frac{a+1}{2}$	$d=4$	$d=5$	$\frac{a+1}{a-1}$	a	$\frac{a+1}{2}$	$d=4$	$d=5$	$\frac{a+1}{a-1}$
5	3	2.000	2.000	1.500	19	10	6.948	4.156	1.111
7	4	2.003	2.003	1.333	21	11	7.975	4.773	1.100
9	5	2.428	2.065	1.250	23	12	9.018	5.428	1.091
11	6	3.171	2.268	1.200	25	13	10.071	6.117	1.083
13	7	4.038	2.617	1.167	27	14	11.130	6.836	1.077
15	8	4.968	3.066	1.143	29	15	12.193	7.583	1.071
17	9	5.943	3.585	1.125	31	16	13.258	8.354	1.067

TABLE 5. Approximate slopes of las_3 for degrees $d = 4$ and $d = 5$ and inner products $\alpha = 1/a$ together with the slope $(a+1)/2$ given by las_2 and the correct asymptotic slope $(a+1)/(a-1)$ proven by [**61**].

CHAPTER 5

Kissing configurations

This chapter is based on a paper by De Laat, Leijenhorst and the author of this thesis [**40**]. We prove that the D_4 root system is the unique optimal kissing configuration in $\mathbb{R}^4$, and is an optimal spherical code. This chapter diverges slightly from the paper, since we have written this chapter in terms of method II, whereas the paper used method I. We also give a different proof of polynomiality. Furthermore, we will deduce a density claim made in that paper using the results in Chapters 1–3. This density claim is not necessary for the main result, but is of independent interest.

5.1. Introduction

A kissing configuration in dimension n is a collection of nonoverlapping, equal-size spheres in $\mathbb{R}^n$ that touch (or "kiss") a central sphere of the same size. We will assume the spheres have unit radius, and we identify a kissing configuration with the set C of contact points with the central sphere. Such a set C is a spherical code with minimal angle at least $\pi/3$. The kissing number $k(n)$ in dimension n is the maximum size of such a set C.

In dimension four, a kissing configuration is given by the D_4 root system. This root system may be constructed as the set of all 24 vectors in $\mathbb{R}^4$ with integer coordinates and length $\sqrt{2}$, referred to as the roots. In this paper we normalize the roots to have unit length. Viewed geometrically, the roots form the vertices of the 24-cell, which is one of the six regular polytopes in dimension four. The possible inner products between distinct roots are 0, $\pm 1/2$, and -1. Hence D_4 is a kissing configuration in dimension 4 of size 24; that is, $k(4) \geq 24$. In 2008, Musin showed $k(4) = 24$; the D_4 root system is an optimal kissing configuration [**89**].

In this chapter, we show it is unique. More precisely, we show that the D_4 root system is the only optimal kissing configuration in dimension four up to isometry. This implies it satisfies the stronger geometric condition of being an optimal spherical code: it minimizes

$$t_{\max}(C) = \max_{\substack{x,y \in C \\ x \neq y}} \langle x, y \rangle$$

over all sets C consisting of 24 points in the unit sphere $S^3 = \{x \in \mathbb{R}^4 \mid \langle x, x \rangle = 1\}$. This contrasts with the result by Cohn, Conway, Elkies, and Kumar [**25**] that the D_4 root system is not universally optimal, meaning that there exists an absolutely monotonic function f (a smooth function with all derivatives nonnegative on $[-1, 1]$) for which D_4 does not minimize

$$\sum_{\substack{x,y \in C \\ x \neq y}} f(\langle x, y \rangle)$$

over all $C \subseteq S^3$ of size 24. In their paper, they conjecture that no universally optimal spherical code of 24 points exists in S^3. The combination of the D_4 root system being the unique optimal spherical code, but not a universally optimal spherical code, proves this conjecture.

The kissing number problem has a rich history, going back to a discussion between Newton and Gregory in 1694 on the correct value of $k(3)$, which was resolved in 1953 by Schütte and Van der Waerden [**108**]. Currently, the value of $k(n)$ is known for $n = 1, 2, 3, 4, 8$, and 24. For background on the kissing number problem, we refer to [**101**].

In 1973, Delsarte introduced the linear programming bound, which can be used to bound the sizes of codes over finite alphabets [**46**]. Delsarte, Goethals, and Seidel adapted this to the sphere so that it can be used to compute upper bounds on $k(n)$ [**47**]. Remarkably, this bound is sharp in dimensions 8 and 24, where by a sharp bound we mean that the optimal objective value is exactly equal to the kissing number, without having to take the integer part. The optimal objective value is 240 in dimension 8 and 196560 in dimension 24, which coincides with the sizes of the kissing configurations obtained by taking the shortest nonzero vectors in the E_8 root lattice and the Leech lattice Λ_{24} [**98, 77**]. This proves optimality of those configurations, and since the bound is sharp, complementary slackness holds, which was used to prove uniqueness [**11**].

In dimension four, the Delsarte bound was used to show $k(4) \leq 25$, which was the first improvement over Coxeter's upper bound of 26 from 1964 [**97, 35**]. In [**2**] it was shown that the Delsarte bound cannot be used to prove $k(4) = 24$, and Musin's optimality proof for the D_4 root system uses a strengthening of the Delsarte bound. However, this strengthening does not lead to a sharp bound.

The Delsarte bound is called a two-point bound since it considers constraints between pairs of points on the sphere. Bachoc and Vallentin developed the three-point semidefinite programming bound for spherical codes, adapted from Schrijver's three-point bound for binary codes [**6, 107**]. The three-point bound recovers the optimality results in dimensions 3 and 4 and improves the best-known upper bound for the kissing number problem in many other dimensions. To compute the three-point bound it is first reduced to a finite-dimensional problem by truncating an inverse Fourier transform, and since its introduction in 2008, all improvements to upper bounds on $k(n)$ have come from increasing this truncation degree [**85, 81, 74**].

The numerical data (see [**74**, Table 6.1] for the newest results), however, suggests that the three-point bound for the kissing number problem is not sharp in any dimension $3 \leq n \leq 24$ and any truncation degree, except for the cases $n = 8$ and $n = 24$ where the Delsarte bound is already sharp. There has been considerable work on k-point bound generalizations of the three-point bound, but this has not yet resulted in sharp, or even improved, bounds for the kissing number problem (or spherical code problems in general) [**90, 67, 91, 42, 88, 15**].

Over the last decades, the moment/sums-of-squares approach by Lasserre and Parrilo (see [**70, 71, 99**]) has become an important tool in mathematical optimization and theoretical computer science. Applying the Lasserre hierarchy to the independent set problem in a finite graph gives a converging hierarchy of increasingly large semidefinite programs giving successively stronger upper bounds on the independence number. We can think of the kissing number problem as the independent set problem in the graph on the unit sphere S^{n-1}, where two distinct vertices $x, y \in S^{n-1}$ are adjacent if $\langle x, y\rangle > 1/2$. In [**44**], De Laat and Vallentin extended this hierarchy to infinite graphs such as these, giving a hierarchy of $2t$-point bounds, where t is the level of the hierarchy. In principle, this solves the kissing number problem in any dimension, since this hierarchy converges in finitely many steps. In practice, computing the levels of this hierarchy beyond the first level (which reduces to the Delsarte linear programming bound) is challenging.

In this paper, we compute the second level of this hierarchy for spherical code problems. We show the second level of the hierarchy is sharp for the kissing number problem in dimension four (the upper bound is exactly 24) by computing an exact optimal solution. We then use complementary slackness to extract a uniqueness proof for the D_4 root system from the optimal solution.

This is the first time the second level of the Lasserre hierarchy has been computed for a spherical code problem and the first improvement over the three-point bounds for spherical codes. The second level of the Lasserre hierarchy has been computed for two problems on infinite graphs. These problems concerned energy minimization on the two-dimensional sphere [**39**]. The techniques used there, however, become too expensive when going to higher dimensional spheres or higher truncation degree of the Fourier transform, and computing a sharp bound for the kissing number problem in dimension four would be prohibitively expensive with the techniques from that paper.

In Chapter 4, we computed the second and third levels of the hierarchy for the equiangular lines problem with a fixed angle θ. Recall the corresponding graph on $\mathbb{P}^{n-1}$ has an edge between distinct points x and y if $\langle x, y\rangle \neq \pm\cos\theta$. Although this is an infinite graph, the quotient space $\mathcal{I}_t/\mathrm{O}(n)$, where $\mathcal{I}_t$ is the set of independent sets of size at most t and $\mathrm{O}(n)$ is the orthogonal group, is finite. For the kissing number problem, the quotient space $\mathcal{I}_t/\mathrm{O}(n)$ is infinite. Because of this, computing the hierarchy for the kissing number problem is more involved, and in this chapter, we extend the techniques from Chapter 4 to do so.

Consider the graph with vertex set $\mathbb{S}^{n-1}$ and with an edge between distinct points x and y if $\langle x, y\rangle \notin D$, where $D = [-1, 1-\alpha]$ with $\alpha > 0$. An independent set of this graph then corresponds to a kissing configuration. We will compute the second step of the Lasserre hierarchy (1) using the kernels from Theorem 1.16. To do so, we will construct a complete system of

$$\mathrm{Hom}_{\mathrm{O}(n)}(\mathcal{I}_2, V_\lambda).$$

for every irreducible representation V_λ of $\mathrm{O}(n)$.

This chapter contains two main technical contributions. In Chapter 4, the zonal matrices Z_λ are constructed for the equiangular lines problem, where the set of independent sets has finitely many orbits and where there are only finitely many pointwise constraints. In this Chapter, we extend this to infinitely many orbits for the case $t = 2$, and we give a rescaling so that the entries of $Z_\lambda(J_1, J_2)$ become polynomials in the inner products between the vectors in $J_1 \cup J_2$. This allows us to reduce (1) to a finite-dimensional problem by truncating the Fourier series, and to write the constraints using sums-of-squares characterizations, which means we can use semidefinite programming to compute bounds.

The second technical contribution of this chapter is the use of method II. To obtain a sharp bound for the kissing number problem in $\mathbb{R}^4$ we need the zonal matrices Z_λ with $|\lambda| \leq 14$. As an anecdote, we remark that setting up the semidefinite program takes two hours with an implementation of method II, and with method I it took two days. A more careful implementation of method II should bring it down further.

Cohn and Elkies [**28**] gave a noncompact adaptation of the Delsarte linear programming bound, and conjectured it gives the optimal sphere packing density in dimensions 8 and 24. Note that for noncompact problems, such as the sphere packing problem, one needs a sharp bound to prove optimality. In [**111**], Viazovska proved the groundbreaking result that the E_8 root lattice gives an optimal sphere packing in $\mathbb{R}^8$ by constructing an optimal solution to the Cohn-Elkies bound, after which optimality of the Leech lattice Λ_{24} was shown similarly in [**30**]. Currently, the sphere packing problem has been solved in dimensions 1, 2, 3, 8, and 24, where the proof for the three-dimensional case used a completely different approach [**58**].

It is conjectured that the D_4 lattice gives the optimal sphere packing in dimension four, where optimality among lattice packings has been known since 1873 [**66**]. A numerically sharp three-point bound for the lattice sphere packing problem in $\mathbb{R}^4$ has recently been computed in [**27**], but a (numerically) sharp bound for the general sphere packing problem is not known in dimension four. Since we show the second level of the Lasserre hierarchy is sharp for the kissing number problem in dimension four (just as the Delsarte bound is sharp in dimension 8 and 24), one might expect a noncompact adaptation (see also [**31**]) might be sharp for the sphere packing problem in dimension four (as is the Cohn-Elkies bound in dimensions 8 and 24). We therefore suspect the second level of the Lasserre hierarchy gives a viable approach to solving the sphere packing problem in dimension four.

In this chapter, we focus on the four-dimensional case. The reason for this is that computing the zonal matrices and solving the semidefinite programs is computationally expensive, and we have only performed computations for $|\lambda| \leq 16$. In the same way as for the three-point bounds, this is the truncation degree around which the bounds start to improve on the Delsarte bound. For the four-dimensional case of the kissing number problem, this results in a sharp bound, but it seems that in most other dimensions the degree is not yet high enough to obtain improved bounds. For the six-dimensional case, we report a small improvement in the upper bound from 78 to 77, which is the first improvement since the introduction of the three-point bound. We shall not dwell on this here and refer to the paper [**40**] for that result.

The chapter is organised as follows. In Section 5.2, we construct a complete system. In Section 5.3, we show that the corresponding zonal matrices consist of polynomials in the inner products. In Section 5.4 we discuss the semidefinite programming formulation, and in Section 5.5 we discuss optimality and uniqueness of the D_4 root system.

5.2. A complete system

The space $\mathcal{I}_t$. The description of the space $\mathcal{I}_t$ shares similarities with the case of equiangular lines in Section 4.2, but now the quotient space $\mathcal{I}_t/\mathrm{O}(n)$ is no longer discrete and we have to take topology into account. Let us recall the definition of the topology. Let $\mathbb{S}^{n-1}$ be the $(n-1)$-dimensional real sphere. We define

$$X_t = \left\{(x_1, \ldots, x_t) \in \mathbb{S}^{n-1} \mid \langle x_i, x_j \rangle \leq 1 - \alpha \text{ if } i \neq j \right\}. \tag{65}$$

and the map

$$\Xi : X_t \to \mathcal{I}_{=t}$$
$$(x_1, \dots, x_t) \mapsto \{x_1, \dots, x_t\}$$

This map provides a continuous bijection from $X_t/\mathfrak{S}_t$ to $\mathcal{I}_{=t}$ [**38**]. Since the domain is compact and the target is Hausdorff, this is a homeomorphism. This map preserves the action of the orthogonal group and the actions of $\mathfrak{S}_t$ and $\mathrm{O}(n)$ commute.

Let Y be the set of Gram matrices of size t, i.e. the set of positive semidefinite matrices with 1s on the diagonal and elements of $D = [-1, 1-\alpha]$ elsewhere. The map from X_t to Y which sends an element of X_t to its Gram matrix has the property that two elements in the same orbit are sent to the same Gram matrix. Furthermore, this map is continuous. Hence we have a continuous factorisation through the quotient space $X_t/\mathrm{O}(n) \to Y$, which is a continuous bijection. The domain is compact and the target is Hausdorff, and therefore, the factorisation is a homeomorphism. An inverse to the map $X_t \to X_t/\mathrm{O}(n)$ is therefore given by sending the corresponding Gram matrix to its principal square root, which is a continuous function. Therefore, we see that condition (ii) from Section 1.1 is fulfilled. It may be also shown that, for this choice of R, condition (iii) is fulfilled.

Similarly to Section 4.2, we define an equivalence relation between elements of Y by declaring $y_1 \sim y_2$ if they differ by a simultaneous permutation of the rows and columns. The actions of $\mathfrak{S}_t$ and $\mathrm{O}(n)$ commute and therefore, the induced maps between the quotients gives a continuous bijection between $\mathcal{I}_{=t}/\mathrm{O}(n)$ and $Y/\sim$. Being an induced map between quotients, we see that $R/\sim$ is continuous and therefore condition (ii) is fulfilled. We suspect that, with this choice, condition (iii) is fulfilled. However, we will not prove these statements at this level of generality and focus on the case $t = 2$. Furthermore, we will use a different choice of R. This choice will be particularly suitable for the problem of polynomiality, which we will explain later.

Invariants. We will now describe a complete system for $\mathrm{Hom}(\mathcal{I}_2, V_\lambda)$. By Proposition 1.8, it is equivalent to do so for the space $E(\mathcal{I}_2, V_\lambda)$. Recall that $E(\mathcal{I}_2, V_\lambda)$ is the subspace of the space of continuous functions $C(\mathcal{I}_2/\mathrm{O}(n), V_\lambda)$ with values in V_λ satisfying the invariance condition

$$\phi(u) \in V_\lambda^{H(u)} \tag{66}$$

for all $u \in \mathcal{I}_2/\mathrm{O}(n)$. Also recall that $H(u)$ is the subgroup of $\mathrm{O}(n)$ which stabilises the representative $R(u)$ of $u \in \mathcal{I}_2/\mathrm{O}(n)$. We first have to define a continuous choice of representative R, which will be done piecewise for each connected component of the quotient space. The quotient space $Y = \mathcal{I}_2/\mathrm{O}(n)$ consists of three connected components: two singletons $Y_0 = \mathcal{I}_{=0}/\mathrm{O}(n)$ and $Y_1 = \mathcal{I}_{=1}/\mathrm{O}(n)$ and a closed interval $Y_2 = \mathcal{I}_{=2}/\mathrm{O}(n) \cong [-1, 1-\alpha]$. The isomorphism from Y_2 to the interval may be seen by sending $\{x_1, x_2\}$ to the inner product $x_1 \cdot x_2$. To define R in the case Y_2, we first define the auxiliary functions

$$q_1(u) = \sqrt{2(1+u)}, \quad q_2(u) = \sqrt{2(1-u)}.$$

for $u \in [-1, 1-\alpha]$ and define vectors

$$R_1(u) = \frac{q_1(u)}{2} e_1 + \frac{q_2(u)}{2} e_2, \quad R_2(u) = \frac{q_1(u)}{2} e_1 - \frac{q_2(u)}{2} e_2.$$

We then define

$$R(u) = \begin{cases} \emptyset & \text{if } u \in Y_0 \\ \{e_1\} & \text{if } u \in Y_1 \\ \{R_1(u), R_2(u)\} & \text{if } u \in Y_2 \end{cases}$$

and note that this is continuous and hence condition (ii) from Chapter 1 is fulfilled. We now describe the subgroups $H(u) = \mathrm{Stab}(R(u))$ for this choice of R. We use the convention that $\mathrm{O}(n-i)$ denotes the subgroup of $\mathrm{O}(n)$ which fixes the basis vectors $e_1, \ldots, e_i$. Furthermore, denote by $\mathrm{Stab}(e_2)$ the subgroup of $\mathrm{O}(n)$ which fixes the basis vector e_2. Let r be the reflection through the hyperplane orthogonal to e_2, denote by I the identity matrix and let $S_2 = \{I, r\}$. We then have

$$H(u) = \begin{cases} \mathrm{O}(n) & \text{if } u \in Y_0 \\ \mathrm{O}(n-1) & \text{if } u \in Y_1 \\ \langle S_2, \mathrm{O}(n-2)\rangle & \text{if } u \in Y_2 \backslash \{-1\} \\ \langle S_2, \mathrm{Stab}(e_2)\rangle & \text{if } u \in Y_2 \text{ and } t = -1. \end{cases}$$

The brackets denote the smallest subgroup generated by a subset. Note that $H(u)$ fulfils condition (iii). Also note that the subgroups S_2 and $\mathrm{O}(n-2)$ commute and that the subgroups S_2 and $\mathrm{Stab}(e_2)$ commute. Therefore, for $u \neq 1$, the $H(u)$-invariants may be computed as the S_2-invariants inside the $\mathrm{O}(n-2)$-invariants, and a similar statement holds for $u = -1$.

We now describe a complete system of $E(\mathcal{I}_t, V_\lambda)$. First of all, for all $u \in Y$, we have $\mathrm{O}(n-2) \subseteq H(u)$ and hence a function in $C(Y, V_\lambda)$ satisfying (66) always takes values in $V_\lambda^{\mathrm{O}(n-2)}$. As we have seen in Chapter 4, the representations V_λ with nontrivial invariants $V_\lambda^{\mathrm{O}(n-2)}$ are described by and Theorem 3.3 and Theorem 3.5. Hence (λ_1, λ_2) satisfies $\lambda_1 \geq \lambda_2 \geq 0$. A basis of $V_\lambda^{\mathrm{O}(n-2)}$ is given by the set of tensors $v_T = \mathfrak{P} e_T c_\lambda$, where T ranges over semistandard tableaux filled with numbers from 1 to 2. Every function $\phi \in E(\mathcal{I}_t, V_\lambda)$ can then be written in components as

$$\phi(u) = \sum_T \phi_T(u) v_T \tag{67}$$

where ϕ_T takes real values and every summand $\phi_T v_T$ must satisfy (66). Therefore, it suffices to write down a complete system for all functions in $E(\mathcal{I}_t, V_\lambda)$ of the form $g(u)v_T$ satisfying condition (66). Furthermore, we may do so separately for each each connected component of $\mathcal{I}_t$, which are given by $\mathcal{I}_{=t}$ with $t = 0, 1, 2$. The complete systems are then combined, extending by zero, to give a complete system of $E(\mathcal{I}_t, V_\lambda)$.

Firstly, let us consider $E(\mathcal{I}_{=0}, V_\lambda)$. Recall $\mathcal{I}_{=0} = \{\emptyset\}$ and therefore Y_0 only has one element. Let u be the one element of Y_0. As described in Section 1.4, a complete system is then given by a basis of $V_\lambda^{H(u)}$. For $u \in Y_0$, we have $H(u) = \mathrm{O}(n)$. Therefore, by Theorem 3.5, we have $V_\lambda^{\mathrm{O}(n)} \neq 0$ if and only $\lambda = (0, 0)$. Recall that the case $\lambda = (0, 0)$ corresponds to the trivial representation acting on $\mathbb{C}$ sending every element of $\mathrm{O}(n)$ to 1. To speak of all cases uniformly, we will make the convention that this corresponds of a Young diagram with zero boxes and the basis element is given by the empty tableau.

Now consider $E(\mathcal{I}_{=1}, V_\lambda)$. Recall $\mathcal{I}_{=1} \cong \mathbb{S}^{n-1}$ and therefore Y_1 only has one element. Let u be the one element of Y_1. As described earlier, a complete system is then given by a basis of $V^{H(u)}$. For $u \in Y_0$, we have $H(u) = \mathrm{O}(n-1)$. Therefore, by Theorem 3.5, we have $V_\lambda^{\mathrm{O}(n-1)} \neq 0$ if and only $\lambda = (\lambda_1, 0)$. A basis is given by the tableau filled only with 1s.

Finally, consider $E(\mathcal{I}_{=2}, V_\lambda)$. Recall $Y_2 \cong [-1, 1-\alpha]$. As mentioned, the function $g(u)v_T$ already takes value in $V_\lambda^{\mathrm{O}(n-2)}$, but we have to satisfy satisfy the additional requirements $g(-1)v_T \in V_\lambda^{\mathrm{Stab}(e_2)}$ and $g(u)v_T \in V_\lambda^{S_2}$ for $u \in Y_2$ and $u \neq -1$. We may assume $g(u)v_T$ does not vanish identically on Y_2. Let u_0 be such that $g(u_0) \neq 0$. Let's look at the effect of r. We have $re_2 = -e_2$ and r fixes the other basis elements. Hence $r \cdot e_T$ is equal to $(-1)^k e_T$, where k is the number of 2s in T. Hence the same is true for v_T. This was also calculated in Section 4.2. Evaluation at u_0 then gives us that we have invariance under S_2 if and only if the number of 2s in T is even. Finally, to take care of the condition at $u = -1$, one of the following must be true:

(i) that $g(-1) = 0$;
(ii) that T has only 2s.

With the above, we will index a complete system of $E(\mathcal{I}_2, V_\lambda)$ by so-called admissible tuples, which we define now. We consider certain tuples of the form (λ, i, j, k), where $\lambda = (\lambda_1, \lambda_2)$ is a pair of integers satisfying $\lambda_2 \geq \lambda_2 \geq 0$, i and k are integers greater than or equal to zero and T is a semistandard tableau. If $i = 0$, we call the tuple (λ, i, j, T) admissible if $\lambda = (0, 0)$, T is the empty tableau and $j = 0$. We define an associated function on Y_0 by

$$\phi_{(0,0),0,0,T}(u) = v_T$$

For every λ, the set of admissible tuples, with that lambda fixed, defines a complete system for $E(\mathcal{I}_{i=0}, V_\lambda)$. If $i = 1$, we call the tuple admissible if $\lambda_2 = 0$, T is a semistandard tableau filled with only 1s and $j = 0$. We define an associated function on Y_1 by

$$\phi_{(\lambda_1,0),0,0,T}(u) = v_T$$

Similarly, for every λ, the set of admissible tuples, with that λ fixed, defines a complete system for $E(\mathcal{I}_{i=1}, V_\lambda)$.

Finally, if $i = 2$, we call the tuple admissible if j is any natural number and T is a semistandard tableau filled with an even number of 2s. On Y_2, we define an auxiliary function by $Q_T(u) = q_1(u)^{\mu_1(T)} q_2(u)^{\mu_2(T)}$ where q_1 and q_2 are as defined earlier. We define an associated function on Y_2 by

$$\phi_{\lambda,i,j,T}(u) = u^j Q_T(u) v_T$$

For an admissible tuple, the function $\phi_{\lambda,i,j,T}$ satisfies condition 66 by the above description. We will now show that for every λ, the set of admissible tuples, with that λ fixed, defines a complete system for $E(\mathcal{I}_{=2}, V_\lambda)$. By decomposition (67), it suffices to prove density for functions of the form $g(u)v_T$ with g a continuous real-valued function on Y_2. We make a case distinction.

Firstly, suppose $\mu_1(T) > 0$. Then $g(-1) = 0$ by the above description. Let $I(\{-1\})$ denote the ideal of functions in $C([-1, 1-\alpha], \mathbb{R})$ which vanish at -1. We have to show that the vector subspace generated by functions

$$u^j Q_T(u)$$

where $j \geq 0$ is a dense subspace of $I(\{-1\})$. This follows from the following lemma.

Lemma 5.1. *The subset $\langle Q_T \rangle \subseteq I(\{-1\})$ is dense.*

PROOF. The subset $\{c + gQ_T \mid c \in \mathbb{R},\, g \in C(Y_2, \mathbb{R})\}$ is closed under multiplication and separates points. Hence it is a dense subset of $C(Y_2, \mathbb{R})$ by the Stone-Weierstraß theorem. Let $f \in I(\{-1\})$ and let $a_k + g_k(u)Q_T(u)$ approach f as $k \to \infty$. Since $\mu_1(T) > 0$, we have $Q_T(-1) = 0$. Hence we have $a_k \to f(-1) = 0$ and we may assume $a_k = 0$ without loss of convergence. We may then approximate the function g with polynomials u^j to obtain the result. □

Secondly, suppose $\mu_1(T) = 0$. Then Q_T does not vanish anywhere on Y_2. For any g, one may approximate g/Q_T with polynomials to obtain the result.

The above functions combined form a complete system of $E(\mathcal{I}_2, V_\lambda)$. By Proposition 1.8, we have

PROPOSITION 5.2. *For every λ, the functions*

$$\psi_{\lambda,i,j,T}(J) = s(J) \cdot \phi_{\lambda,i,j,T}(p(J))$$

for admissible (λ, i, j, T) define a complete system of $\mathrm{Hom}_{\mathrm{O}(n)}(\mathcal{I}_2, V_\lambda)$.

5.3. Polynomiality

What does it mean to be a polynomial on $\mathcal{I}_{=t}$? The space $(\mathbb{S}^n)^t$ has a natural structure of an affine variety and therefore a notion of what it means to be a polynomial on it. The ring of polynomials on $(\mathbb{S}^n)^t$ is denoted by $\mathcal{O}((\mathbb{S}^n)^t)$. We say that a function on X_t, as defined by equation (65) is polynomial if it is the restriction of a polynomial on $(\mathbb{S}^n)^t$, and we denote by $\mathcal{O}(X_t)$ the ring of polynomial functions on X_t. We define a polynomial function on $X_t/\mathfrak{S}_t$ to be a polynomial on X_t which is symmetric under permutation of the components, also denoted by $\mathcal{O}(X_t/\mathfrak{S}_t)$. By definition, we have $\mathcal{O}(X_t/\mathfrak{S}_t) \cong \mathcal{O}(X_t)^{\mathfrak{S}_t}$. By the above homeomorphism, we have an isomorphism between the spaces $X_t/\mathfrak{S}_t$ and $\mathcal{I}_{=t}$, and therefore, by definition, we have $\mathcal{O}(\mathcal{I}_{=t}) \cong \mathcal{O}(X_t)^{\mathfrak{S}_t}$.

The ring of polynomials $\mathcal{O}(X_t)$ is then defined as the ring of functions which are restrictions of polynomials on $(\mathbb{R}^n)^t$. We identify the ring of polynomials $\mathcal{O}(\mathcal{I}_{=t})$ on $\mathcal{I}_{=t}$ with the ring of symmetric polynomial $\mathcal{O}(X_t)^{\mathfrak{S}_t}$ on X_t. We now give a description of $\mathcal{O}(X_t)$. We have $X_t \subseteq (\mathbb{S}^{n-1})^t$ and by [**17**, Proposition 2.8.14], their algebraic dimensions agree. Since the variety $(\mathbb{S}^{n-1})^t$ is irreducible, the Zariski closure of X_t must equal $(\mathbb{S}^{n-1})^t$. Hence, any polynomial which vanishes on X_t, must vanish on $(\mathbb{S}^{n-1})^t$. Thus, the restriction map from $\mathrm{O}((\mathbb{S}^n)^t)$ to $\mathrm{O}(X_t)$ is an isomorphism of rings. Thus, we have a bijection

$$\mathcal{O}(\mathcal{I}_{=t}) \cong \mathcal{O}((\mathbb{S}^{n-1})^t)^{\mathfrak{S}_t}. \tag{68}$$

In words, a polynomial on $\mathcal{I}_{=t}$ is a symmetric polynomial on a t-fold copy of the sphere. We now show that the complete system is polynomial in this sense.

LEMMA 5.3. *Let (λ, i, j, T) be admissible. For any $v \in V_\lambda$, the function*

$$\langle v, \psi_{\lambda,i,j,T}(J)\rangle \tag{69}$$

is polynomial on $\mathcal{I}_2$.

PROOF. By the above, we have to show that the function given by precomposition with Ξ is a symmetric polynomial. We prove this for each i separately. For a vector x_i, Denote by x_{ij} the j-component. For $i = 0$, the function is a constant. Let $i = 1$ and $J = \{x_1\}$. A section is given by any orthogonal matrix $s(\Xi(x_1))$, of which the first column is equal to x_1. Recall that T in this case is a semistandard tableau filled with 1s. By equation (44), we have

$$s(\Xi(x_1)) \cdot e_T = \sum x_{j_1 1} \cdots x_{j_d 1} e_{T'},$$

where the sum is over all tableau T' filled with $j_1, \ldots, j_d$. By equation (44) and the fact that T is filled with 1s and 2s, the function (69) is a polynomial in the components of x_1. Therefore, the inner product is a polynomial in x_{1j}. Now let $i = 2$ and let $u = x_1 \cdot x_2 \neq -1$. Since the function $\psi_{\lambda,i,j,k}(J)$ does not depend on the choice of section, we may assume without loss of generality that the first column of $s(\Xi(x_1, x_2))$ equals $(x_1 + x_2)/q_1(u)$ and the second equals $(x_1 - x_2)/q_2(u)$. Recall that T is filled with 1s and 2s and an even number of 2s. We then have

$$s(\Xi(x_1, x_2))e_T = Q_T(u)^{-1}[x_1 + x_2, x_1 - x_2, \ldots]e_T,$$

and therefore

$$\begin{aligned} &s(\Xi(x_1, x_2))Q_T(u)v_T \\ &= \mathfrak{P}s(\Xi(x_1, x_2))Q_T(u)e_T c_\lambda \\ &= \mathfrak{P}[x_1 + x_2, x_1 - x_2, \ldots]e_T c_\lambda. \end{aligned}$$

By equation (44) and the fact that T is filled with 1s and 2s, we see that function (69) must be a polynomial in the components of x_1 and x_2. Recall that we made the assumption that $u \neq -1$. The set where $u \neq -1$ holds defines a non-empty subset, which is open in the analytic topology. Therefore, by the discussion at the start of this section, it is a symmetric polynomial on the entirety of $\mathcal{I}_{=2}$. $\square$

Corollary 5.4. *The function*

$$\langle \psi_{\lambda,i_1,j_1,T_1}(J_1), \psi_{\lambda,i_2,j_2,T_2}(J_2) \rangle$$

where the tuples are both admissible, is a symmetric polynomial in the inner products of the vectors of J_1 and J_2.

Proof. The inner product is unitary. Therefore, abstractly, the statement follows from the previous lemma together with the fundamental theorem of invariant theory. Concretely, this polynomial is obtained with method II or with method I as described in [**40**]. For method II, this follows from: the equation

$$\langle \psi_{\lambda,i_1,j_1,T_1}(J_1), \psi_{\lambda,i_2,j_2,T_2}(J_2) \rangle = \langle \phi_{\lambda,i_1,j_1,T}, s(J_1)^{\mathsf{T}} s(J_2) \phi_{\lambda,i_2,j_2,T_2} \rangle;$$

the fact that method II produces a polynomial which depends explicitly on the appropriate block of $s(J_1)^{\mathsf{T}} s(J_2)$; and the scaling. $\square$

5.4. Semidefinite programming formulation

Let $d_1 \leq d_2 \leq \delta$ be positive integers with δ even. In our application to the D_4 root system, we use $d_1 = 14$ and $d_2 = \delta = 16$.

In the semidefinite program, we optimize over positive semidefinite matrices $\widehat{K}_\lambda$. Here the rows and columns are indexed by tuples (i, j, T) for which (λ, i, j, T) is admissible and $|\lambda| + 2j \leq d_2$, and we similarly restrict the rows and columns of Z_λ. Let

$$K(J_1, J_2) = \sum_{|\lambda| \leq d_1} \langle Z_\lambda(J_1, J_2), \widehat{K}_\lambda \rangle,$$

where we have used the notation from Theorem 1.16. It follows from Proposition 5.4 that $A_2K(Q)$ is a polynomial in the inner products between the vectors in Q. With the results from Section 5.2, we can find polynomials $p_1, \ldots, p_4$ in 0, 1, 3, and 6 variables, such that

$$\begin{aligned} p_1 &= A_2K(\{x_1\}), \\ p_2(\langle x_1, x_2\rangle) &= A_2K(\{x_1, x_2\}), \\ p_3(\langle x_1, x_2\rangle, \langle x_1, x_3\rangle, \langle x_2, x_3\rangle) &= A_2K(\{x_1, x_2, x_3\}), \\ p_4(\langle x_1, x_2\rangle, \langle x_1, x_3\rangle, \ldots, \langle x_3, x_4\rangle) &= A_2K(\{x_1, \ldots, x_4\}). \end{aligned}$$

Here p_3 is S_3-invariant and p_4 is S_4-invariant, where S_3 acts by permuting variables and the action of S_4 is such that

$$\begin{aligned} &p_4(\langle x_{\sigma(1)}, x_{\sigma(2)}\rangle, \langle x_{\sigma(1)}, x_{\sigma(3)}\rangle, \ldots, \langle x_{\sigma(3)}, x_{\sigma(4)}\rangle) \\ &\quad = p_4(\langle x_1, x_2\rangle, \langle x_1, x_3\rangle, \ldots, \langle x_3, x_4\rangle). \end{aligned}$$

for all $\sigma \in S_4$. Note that the polynomials $p_1, \ldots, p_4$ are of degree at most d_2, and their coefficients depend linearly on the entries of the matrices $\widehat{K}_\lambda$.

The Fourier truncated version of (1) can be formulated as the following semidefinite program with polynomial inequality constraints:

$$\begin{array}{lll} \text{minimize} & (\widehat{K}_0)_{(0,0,0),(0,0,0)} & \\ \text{subject to} & \widehat{K}_\lambda \succeq 0, & |\lambda| \le d_1, \\ & p_1 \le -1, & \\ & p_2(u) \le 0, & u \in [-1, \cos\theta], \\ & p_3(u_1, u_2, u_3) \le 0, & (u_1, u_2, u_3) \in \Delta_3, \\ & p_4(u_1, \ldots, u_6) \le 0, & (u_1, \ldots, u_6) \in \Delta_4. \end{array} \tag{70}$$

Let

$$G_3 = \begin{bmatrix} 1 & u_1 & u_2 \\ u_1 & 1 & u_3 \\ u_2 & u_3 & 1 \end{bmatrix} \quad \text{and} \quad G_4 = \begin{bmatrix} 1 & u_1 & u_2 & u_3 \\ u_1 & 1 & u_4 & u_5 \\ u_2 & u_4 & 1 & u_6 \\ u_3 & u_5 & u_6 & 1 \end{bmatrix}.$$

The semialgebraic set Δ_i consists of all $u \in \mathbb{R}^{\binom{i}{2}}$ with $(u_j + 1)(\cos\theta - u_j) \ge 0$ for all $1 \le j \le \binom{i}{2}$ and the Gram matrix must be positive definite. In this case, this is equivalent to asking that the determinants of all principal submatrices of size at least 3 of G_i are nonnegative.

We can now use sum-of-squares polynomials to relax this further to a semidefinite program. For the two-point constraint, for instance, we can use Lukács result (see, e.g., [**102**]) to replace the condition $p_2(u) \le 0$ for $u \in [-1, \cos\theta]$ by

$$p_2(u) + s_0(u) + (u+1)(\cos\theta - u)s_1(u) \equiv 0, \tag{71}$$

where s_0 and s_1 are sum-of-squares polynomials of degree δ and $\delta - 2$, respectively. Let $m_l(u)$ be a vector whose entries form a basis for the polynomials up to degree l. We can write

$$s_k(u) = \langle m_{\delta/2-k}(u) m_{\delta/2-k}(u)^{\mathsf{T}}, M_k\rangle,$$

where M_k is a positive semidefinite matrix. In this way, we can replace the two-point polynomial inequality constraint by two positive semidefinite matrices and several linear constraints that enforce the polynomial identity (71).

We can do something similar for the three-point and four-point constraints. Suppose $\Delta_i = \{u : g_k(u) \geq 0,\, k = 1, \ldots, l\}$, then we relax the polynomial inequality constraint to the identity

$$p_i(u) + \sum_{k=0}^{l} r_k(u) g_k(u) \equiv 0,$$

where we set $g_0(u) = 1$ and $r_k(u)$ is a sum-of-squares polynomial of degree at most $\delta - \deg(g_k)$. By Putinar's theorem [**103**] (see also [**82**, Chapter 13]), this relaxation converges to the original polynomial constraint when $\delta \to \infty$.

In the resulting semidefinite program, the positive semidefinite matrix variables for the four-point constraint will be far larger than any other matrix in the program. For this reason, exploiting the symmetries in the polynomials is essential.

If a semialgebraic set is invariant under the action of a group, then there exists a description in terms of invariant polynomials [**19**]. Let

$$\{q_1, \ldots, q_l\}$$

be an orbit of the polynomials describing Δ_i under the action of S_i. Then we can replace the polynomials in this orbit by the S_i-invariant polynomials

$$\sum_{\substack{B \subseteq \{1,\ldots,l\} \\ |B| = b}} \prod_{k \in B} q_k$$

for $b = 1, \ldots, l$ [**81, 74**].

We may now assume the sum-of-squares polynomials for the three-point and four-point constraints are also invariant under the given action of the symmetric groups S_3 and S_4. This means that instead of using one large positive semidefinite matrix, we can use several smaller positive semidefinite matrices to model each sum-of-squares polynomial [**53**]. To do this explicitly we follow [**74**, Section 4].

This symmetry reduction involves the irreducible, unitary representations of S_3 and S_4. Although the irreducible, unitary representations we use involve irrational numbers, the irrationalities cancel in the final formulation, and the semidefinite program we obtain is rational whenever $\cos\theta$ is rational.

5.5. Uniqueness in dimension four

In this section, we prove that the D_4 root system is the unique optimal kissing configuration in dimension four and is an optimal spherical code. For this, we first compute a numerically optimal solution to (70) with $n = 4$ and $\theta = \pi/3$. To get a sharp bound, we use $d_1 = 14$ and $d_2 = \delta = 16$ for the truncation of the inverse Fourier transform and the sums-of-squares degrees. The resulting semidefinite program is large, and to solve it the use of the semidefinite programming solver from [**74**] is essential. This solver supports arbitrary precision floating-point arithmetic and exploits the low-rank structure of the constraint matrices arising from enforcing the polynomial constraints through sampling at a unisolvent set [**80**]. We compute the optimal solution to 40 digits of precision using 256-bit floating-point arithmetic. This takes about two weeks on 8 cores of a modern computer equipped with 128GB of working memory.

The next step is to round the numerical solution to an exact optimal solution. Since the dimension of the optimal face is lower than the dimension of the space given by the affine constraints, simply projecting the numerically optimal solution into the affine space does not work: the resulting matrix variables will generally not be positive semidefinite. Instead, we use a recently developed rounding heuristic [**26**]. This method is faster than a previous one [**48**], which is crucial for the size of the semidefinite program we consider here.

Although a semidefinite program defined over the rationals does not necessarily admit a rational optimal solution [**95**] this is the case here, and the rounding procedure finds a rational optimal solution within 4 hours. This gives an exact feasible solution K with objective value $K(\emptyset, \emptyset) = 24$.

To verify that the exact solution is indeed feasible we check that the affine constraints hold, which can be done in rational arithmetic, and we check that the solution matrices are positive semidefinite. To be able to check positive semidefiniteness, the rounding procedure writes each solution matrix in the form BXB^{T}, where B is a rectangular, rational matrix, and X is a positive definite, rational matrix. We check that X is indeed positive definite by computing the Cholesky decomposition in rigorous ball arithmetic. As part of the verification procedure, the zonal matrices Z_λ need to be constructed, which takes less than two days on a modern computer with method I, and with an implementation of method II it takes two hours. The remainder of the verification procedure takes less than two hours.

Using Sturm sequences we verify that the polynomial p_2 corresponding to $A_2K|_{I=2}$ has roots -1, $\pm 1/2$, and 0 in the interval $[-1, 1/2]$. That is, for distinct $x, y \in S^3$ with $\langle x, y\rangle \leq 1/2$, $A_2K(\{x, y\}) = 0$ if and only if $\langle x, y\rangle \in \{-1, \pm 1/2, 0\}$. In the remainder of this section, we use this fact to show the D_4 root system is an optimal spherical code and is the unique optimal kissing configuration up to isometry.

The script and data files to perform this verification procedure are available at [**36**]. There we also make available the implementation we used for generating the proofs. Our scripts are written in Julia [**16**] and use the Nemo computer algebra system [**49**].

Lemma 5.5. *If $C \subseteq S^3$ is a subset of size 24 with minimal angle at least $\pi/3$, then*

$$\langle x, y\rangle \in \{-1, -1/2, 0, 1/2\}$$

for all distinct $x, y \in C$.

Proof. Let K be the exact solution discussed above. By positivity of K and by the linear constraints

$$A_2K(Q) \leq -1_{\mathcal{I}_{=1}}(Q), \qquad Q \in \mathcal{I}_4 \setminus \{\emptyset\},$$

we have

$$0 \leq \sum_{\substack{J_1, J_2 \in \mathcal{I}_2 \\ J_1, J_2 \subseteq C}} K(J_1, J_2) = \sum_{\substack{Q \in \mathcal{I}_4 \\ Q \subseteq C}} A_2K(Q) \leq K(\emptyset, \emptyset) - |C|.$$

Since $|C| = K(\emptyset, \emptyset) = 24$, equality holds throughout, so in particular, $A_2K(Q) = 0$ for all $Q \subseteq C$ with $|Q| \leq 4$. As mentioned above, for distinct $x, y \in S^3$, we have $A_2K(\{x, y\}) = 0$ if and only if $\langle x, y\rangle \in \{-1, \pm 1/2, 0\}$, which proves the lemma. □

This shows the D_4 root system corresponds to an optimal spherical code: among the 24-point subsets of S^3, the minimal distance between distinct points is as large as possible.

Theorem 5.6. *The D_4 root system is an optimal spherical code.*

Proof. If there were a spherical code C of cardinality 24 with smallest angle strictly larger than $\pi/3$, then any small enough perturbation of C would correspond to a kissing configuration of size 24, which contradicts with Lemma 5.5. $\square$

Note that for cases where the Bachoc-Vallentin three-point bound is sharp, optimality of the corresponding spherical code follows immediately, because in that case sharpness directly implies that there are only finitely many possible inner products [**95**]. We do not know whether the same is always true for a truncation of the Lasserre hierarchy, since it is not clear whether the polynomial p_2 can be identically zero when the bound is sharp.

Theorem 5.7. *The D_4 root system is the unique optimal kissing configuration in $\mathbb{R}^4$ up to isometry.*

Proof. Let $C \subseteq S^3$ be an optimal kissing configuration in $\mathbb{R}^4$. We first verify that C is a root system.

(i) The vectors in C must span $\mathbb{R}^4$, since otherwise C would give a kissing configuration in $\mathbb{R}^3$ of size 24.

(ii) Since C is a subset of the unit sphere, the only real multiples of $\alpha \in C$ can be α and $-\alpha$.

(iii) Let $\alpha, \beta \in C$ and consider the reflection $\beta' = \beta - 2\langle \alpha, \beta\rangle \alpha$ of β through the hyperplane orthogonal to α. By Lemma 5.5, it follows that
$$\langle \beta', \gamma\rangle \in \{\pm 1, \pm 1/2, 0\}$$
for every $\gamma \in C$. So, β' must be in C by optimality of C.

(iv) By Lemma 5.5, for $\alpha, \beta \in C$, the value $2\langle \alpha, \beta\rangle$ is an integer. In other words, the reflection of β through the hyperplane orthogonal to α is obtained by subtracting an integer multiple of α from β.

Hence, the set C is a root system in $\mathbb{R}^4$. The irreducible root systems have been classified, and the only irreducible root systems where all vectors have the same length are A_j, D_j, E_6, E_7, and E_8 [**109**, Table 4.1]. Since all roots in C have the same length, it must be a direct sum of these irreducible root systems. In other words,
$$C = \bigoplus_{i=1}^{k} \Phi_i$$
for some k and root systems $\Phi_1, \ldots, \Phi_k$, where each Φ_k is isomorphic to A_j, D_j, E_6, E_7, or E_8.

Let us assume that D_4 does not occur in the decomposition. By considering the dimensions, the summands must be isomorphic to A_j with $1 \leq j \leq 4$ and D_j with $1 \leq j \leq 3$. We denote by r the total number of roots occurring in C, by r_i the number of roots of Φ_i, and by d_i the rank of Φ_i. For A_j we have $r_j/d_j = j+1$ and for D_j we have $r_j/d_j = 2(j-1)$. Hence, we have $r_i/d_i < 6$ for the root systems which occur in the decomposition. Furthermore, since the span of C is $\mathbb{R}^4$, we have $\sum_{i=1} d_i = 4$. We then have
$$r = \sum_{i=1}^{k} r_i = \sum_{i=1}^{k} \frac{r_i}{d_i} d_i < 6 \sum_{i=1} d_i = 24.$$
Since the number of roots in C is equal to 24, this gives a contradiction. Hence, C is D_4 up to isometry. $\square$

Conclusions

We have developed a harmonic analytic framework for describing invariant positive definite kernels on spaces of independent sets in the context of discrete geometry. To use this, we also developed two methods with which to calculate the zonal Stiefel harmonics. With these tools, we studied the equiangular lines problem with a fixed angle and the kissing number problem by calculating steps of the Lasserre hierarchy. The results demonstrate that this is a powerful tool for tackling problems in discrete geometry. For both problems, it provided information not only on the maximal size of configurations, but also on other properties.

In the case of the equiangular lines problem, we deduce sublinear growth in terms of the dimension n using an asymptotic analysis of the semidefinite program. The connection to other techniques used to obtain this result, which are mentioned in the introduction of Chapter 4, remains unclear.

The asymptotic analysis of solutions of a semidefinite programs depending on a parameter is of more general interest. An alternative approach to the interpolation method from Chapter 4 may proceed as follows. First, the semidefinite programme is reformulated as a polynomial optimisation problem. Using Lagrange multipliers, this may be expressed as a polynomial system with the same number as variables as constraints. Generically, such a system has finitely many solutions. Although these systems are often not generic, a small perturbation of the system may still give a valid bound, depending on the situation. One may then use Gröbner basis techniques to solve this system. In principle, a Gröbner basis calculation may be done over any field and therefore the field of rational functions $\mathbb{Q}(n)$, where n is a parameter, may be used. Sturm sequences may then be used to investigate whether the objective value lies within a desired interval. For the second step of the Lasserre hierarchy for the equiangular lines problem with a fixed angle, this leads to a quadratic program with 20 constraints and variables. Discussions with experts from the field of Gröbner basis calculation indicated that this approach would be challenging, but perhaps just within reach.

In the case of the kissing number problem, a uniqueness result is obtained via complementary slackness. It is known that the Lasserre hierarchy converges [**44**]. However, the fact that the second step already yields such rich information for both problems is remarkable. It would be interesting to have a better understanding of this.

In method II, a new formula for the traceless projection of tensors from [**22**] was used. Perhaps a deeper understanding of this work could be beneficial from a theoretical and computational standpoint.

As mentioned, we have developed a general harmonic analytic framework for problems of this kind. To apply it, a continuous choice of orbit satisfying conditions (i)-(iii) from Chapter 1 is required. It seems intuitive that these conditions are relatively mild. For a topological packing graph with the structure of a differentiable manifold, and with a transitive group action by a compact connected group, one could investigate under which circumstances the conditions hold for the spaces $\mathcal{I}_t$ of independent sets, cf. the discussion at the end of Chapter 1.

Further research lies in optimisation of the implementation of method II. One may also attempt to calculate higher steps of the Lasserre hierarchy. The construction of complete systems as in Chapter 5 should be worked out in this case. The choice of R and the scalings to obtain polynomiality as in Chapter 5 would have to be investigated. The work in this thesis should be a good starting point for this.

One may look for other problems to which these techniques may be applied. We will do so in a paper in preparation [**37**], in which we will study: other spherical coding problems; energy miminisation; and codes on the Stiefel manifold.

Finally, we note that the case of the symplectic group appears analogous, and it would be interesting to explore problems symmetric under an action of the symplectic group.

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List of Publications

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D. de Laat, N.M. Leijenhorst, **W.H.H. de Muinck Keizer**, *Optimality and uniqueness of the D_4 root system*, under review, arXiv:2404.18794, 2024.

D. de Laat, N.M. Leijenhorst, **W.H.H. de Muinck Keizer**, *Traceless projection of tensors with applications to hierarchies in discrete geometry*, in preparation.

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