Upper Bounds on the Measure of Distance-Avoiding Sets on the Complex Unit Sphere

by

Finn Dijkstra

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Student number:	4600339	
Masters program	Applied Mathematics	
Specialization:	Discrete Mathematics and Optimization	
Faculty:	Electrical Engineering, Mathematics and Computer Science	
Thesis committee:	Dr. F.M. de Oliveira Filho,	TU Delft, daily supervisor
	Dr. ir. W.G.M. Groenevelt,	TU Delft
	A.J.F. Bekker,	TU Delft, daily co-supervisor
Thesis Advisor:	Prof. dr. D.C. Gijswijt,	TU Delft

Preface

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Contents

CHAPTER 1

Introduction and preliminaries

In this thesis, the primary goal is to find upper bounds for the *t-avoiding-set problem*:

What is the maximum surface measure of a set on the complex n-dimensional unit sphere, such that there exists no pair of points in the set with inner product t?

A *t-avoiding set* is a set that contains no pair of points with inner product t. By conjugate symmetry of the inner product, a t-avoiding set is also $\bar{t}$-avoiding. The problem is of particular interest for $t = 0$ for its use in quantum information theory [11]. Throughout the thesis, we will use concepts from the fields of graph theory and complex analysis to find the upper bounds. In order to apply the concepts, we will primarily work with the graph theory interpretation of the problem.

Construct a graph where every point on the n-dimensional complex sphere is a vertex of the graph, and a pair of vertices form an edge if and only if their inner product is t or $\bar{t}$. On this graph, a set of vertices where no pair of vertices in the set has an edge corresponds to a t-avoiding set on the complex sphere.

By using the appropriate measure on the graph, it is clear that finding the maximum measure of a set of vertices of the graph such that no pair of vertices in the set has an edge is equivalent to the t-avoiding-set problem. The graph theory interpretation of the optimization problem is called the *independence-number problem* and the maximum measure, or optimal value, is called the *independence number*. To find an upper bound for the independence number, we use the *Lovász theta number*. The Lovász theta number is used to refer to both the optimal value and the optimization problem. Additionally, we develop an approach building on the Lovász theta number to further improve the upper bounds for the independence number.

1.1. Outline of Thesis

In this thesis, we will find upper bounds for the t-avoiding-set problem using a formulation for the Lovász theta number. The formulation will be further constrained using the Boolean quadric polytope to improve the bound. In Chapter 2, we will explain the relevant topics using finite graphs and show how the Lovász theta number was used for the t-avoiding-set problem on the real sphere. In Chapter 3, the process of formulating the Lovász theta number for the complex sphere is outlined. In Chapter 4, the Lovász theta number formulation will be extended with the aforementioned Boolean quadric polytope constraint to find the improved bounds.

1.1.1. The Lovász theta number. In Chapter 2, we first introduce useful concepts from graph theory on finite graphs. This includes introducing optimization problems to calculate the independence number and Lovász theta number. We additionally show how symmetry of the graph can be exploited in order to reduce the complexity of the optimization problems. Afterwards, we show how an optimization problem for the Lovász theta number was used to find upper bounds for the t-avoiding-set problem on the real sphere. By exploiting symmetry on the sphere, we show how the *Jacobi polynomials* can be used as a basis for solutions of the optimization problem.

1.1.2. The complex t-avoiding-set problem. Throughout Chapter 3, we explore the basics around the complex t-avoiding-set problem and its upper bound. To start, we introduce the necessary concepts for formulating the problems. The primary concept is *Hilbert-Schmidt kernels* and its properties such as *invariance* and *positive definiteness*. Other concepts include *zonal functions* and *disk polynomials*, which form a basis for invariant, continuous, positive definite Hilbert-Schmidt kernels. After the preliminaries, we show how to construct different Hilbert-Schmidt kernels from set descriptions to show the relation between the two.

The next section constructs an optimization problem for the Lovász theta number used to find an upper bound for the complex t-avoiding-set problem. In this section, we additionally construct real-valued disk polynomials to use as a basis for solutions of the Lovász theta problem. In the penultimate sections, we investigate the 0-avoiding set and $e^{i\phi}$-avoiding set problems. For both cases, we show that we may constrain the problem to sets of a certain structure. Additionally, t-avoiding sets will be constructed that are either conjectured or proven to be of maximal size. To round off the chapter, we will show the results of the Lovász theta problem.

1.1.3. The Boolean quadric polytope. In Chapter 4, we will extend the Lovász theta number by adding the *Boolean quadric polytope* set of constraints. The constraints are induced by a finite subset of points on the sphere and enforce behavior on those points similar to Hilbert-Schmidt kernels constructed from set descriptions. In the first section of the chapter, we show the relation between the constraints and sets on the sphere. In the next part, we construct the extended formulation for Lovász theta number. In addition to adding the Boolean quadric polytope constraint set, we describe a method to reduce the formulation from one with infinitely many variables or constraints to one with finitely many. This method is constructed in order to ensure the optimal value remains an upper bound for the measure of t-avoiding set. After the formulation of the problem, a section is dedicated to methods used to find sets of points to induce the Boolean quadric polytope constraints. We will finish the chapter by discussing the upper bounds obtained from the extended problem.

1.2. Preliminaries

The focus of this thesis is on unit spheres in different spaces, we introduce the notation for the unit sphere in the inner product space D as $S(D) = \{x : x \in D, \langle x, x\rangle = 1\}$. We use the inner product $\langle u, v\rangle = \sum_{i=1}^{n} u_i v_i$ for $\mathbb{R}^n$ and we use the inner product $\langle u, v\rangle = \sum_{i=1}^{n} u_i \overline{v_i}$ for $\mathbb{C}^n$. Those inner product define $S(\mathbb{R}^n)$, the real n-dimensional unit sphere, and $S(\mathbb{C}^n)$, the complex n-dimensional unit sphere. Additionally, we use the notation $\overline{\mathbb{D}}$ for the closed complex unit disk $\{z : z \in \mathbb{C}, |z| \leq 1\}$.

1.2.1. Concepts from graph theory. A *graph* is a pair $G = (V, E)$ where V is a nonempty set and E is a set containing pairs of elements in V. The set V is the *vertex set* of G and its elements are called *vertices*. the set E is the *edge set* and its elements are called an *edges*. All used graphs are *undirected*, that is, the vertex pairs in E are unordered. Additionally, all used graphs are *simple*, which means that there are no loops nor parallel edges. Therefore, for all used graphs, the edge set E is a subset of $\{e : e \subseteq V, |e| = 2\}$. A graph is *finite* if V is finite. Likewise, a graph is *infinite* if V is infinite. Consider the graphs $H = (V_H, E_H)$ and $G = (V_G, E_G)$. H is a *subgraph* of G if $V_H \subseteq V_G$ and $E_H \subseteq E_G \cap \{e : e \subseteq V_H, |e| = 2\}$. H is an *induced subgraph* of G if $V_H \subseteq V_G$ and $E_H = E_G \cap \{e : e \subseteq V_H, |e| = 2\}$.

The set $U \subseteq V$ is *independent* if there is no pair of vertices in U that form an edge. The size of the largest independent set on a graph $G = (V, E)$ is called the *independence number*, denoted by $\alpha(G)$. If $G = (V, E)$ is an infinite graph and V is equipped with a measure, then the independence number is the supremum for the measure of an independent set, also denoted by $\alpha(G)$.

1.2.2. Optimization and semidefinite programming. An optimization problem is the problem of finding the supremum/infimum of an *objective function* for input variables that satisfy a set of *constraints*. In this thesis, all optimization problems are of the form:

$$\begin{aligned} \sup / \inf \; & f(x) \\ & g_i(x) \le \beta_i \quad i \in P, \\ & x \in D. \end{aligned}$$

Here, the function f is the objective function and each inequality $g_i(x) \le \beta_i$ is a constraint. Any assignment for the variable x in the domain D is called a *solution* for the problem. A solution is *feasible* if the assignment satisfies every constraint and a solution is *infeasible* if it does not. The *objective value* for a solution is the value of the objective function for the assignment. The *optimal value* is the supremum/infimum of the objective value for all feasible solutions.

In this work, the domain of a variable is $\mathbb{R}$ if it is not otherwise defined within the optimization problem. If domain of each variable is $\mathbb{R}$ and if the objective function and all constraints are linear, the problem is a *linear program (LP)*. Whenever the domain of each variable is the integers instead, the problem is called an *integer program (IP)*.

Let A and B be optimization problems with the same objective function and with their respective sets of feasible solutions S_A and S_B. If $S_A \subseteq S_B$, then B is called a *relaxation* of A, whereas A is called a *restriction* of B. Whenever we are unable to solve an optimization problem, we often solve an easier relaxations or restrictions to find bounds for the optimal value of the original problem. For example, if B is a relaxation of A and the objective is to maximize the objective function, then the optimal value of B is an upper bound for the optimal value of A.

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is positive semidefinite, if $x^T A x \ge 0$ for every $x \in \mathbb{R}^n$. Similarly, a Hermitian matrix $A \in \mathbb{C}^{n \times n}$ is positive semidefinite, if $x^* A x \ge 0$ for every $x \in \mathbb{C}^n$. If a matrix A is positive semidefinite, it is denoted as $A \succeq 0$. The cone of all positive semidefinite matrices in $\mathbb{R}^{n \times n}$ is denoted as $\mathcal{S}_+^n$. If the only variable in an optimization problem is a positive semidefinite matrix A and if the objective function and all constraints are defined using inner products of A with a symmetric matrix, then the problem is a *semidefinite program (SDP)*.

CHAPTER 2

The Lovász theta number

In order to find upper bounds for the maximal measure of a set that avoids an inner product t, we present the problem using concepts from graph theory. The primary concepts we use are the independence number and its positive semidefinite relaxation, the Lovász theta number. In this chapter we start by looking at finite graphs to show how the optimization problems are formulated and how symmetry of a graph may be used to reduce the complexity of the problem. Afterwards, we shall show how the problem has previously been formulated on the real n-dimensional unit sphere and what bounds were found using the Lovász theta number.

2.1. Finite graphs

In this section, we introduce the independence-number problem and the Lovász theta number on finite graphs. Additionally, we show how symmetry of a graph can be used to reduce the complexity of formulation of the Lovász theta number.

Let $G = (V, E)$ be a graph. An *automorphism* is a bijection $T : V \to V$ such that $(u, v) \in E$ if and only if $(Tu, Tv) \in E$ for all $u, v \in V$. The set of all automorphisms of G forms the group $\mathrm{Aut}(G)$. A graph is *vertex transitive* whenever for any $u, v \in V$ there exists $T \in \mathrm{Aut}(G)$ such that $Tu = v$. Similarly, a graph is *edge transitive* whenever for any $\{u, v\}, \{x, y\} \in E$ there exists $T \in \mathrm{Aut}(G)$ such that $\{Tu, Tv\} = \{x, y\}$. The automorphism group of a graph can be used to simplify the Lovász theta number. To explain the process on finite graphs, we consider *distance-transitive* graphs. Let $d(u, v)$ denote the shortest-path distance between u and v. The graph G is distance transitive whenever for any $u, v, x, y \in V$ there exists $T \in \mathrm{Aut}(G)$ such that $(Tu, Tv) = (x, y)$ if and only if $d(u, v) = d(x, y)$. Any distance-transitive graph is *vertex transitive* and *edge transitive*, as $d(u, u) = 0$ for all $u \in V$ and $d(u, v) = 1$ for all $\{u, v\} \in E$. While the graph used for the t-avoiding-set problem is not distance transitive, its automorphism group may be exploited in the same way.

2.1.1. Optimization problem for the independence number.

To find the independence number, we need to represent subsets of V such that we can verify that a subset is independent. To start, we represent the subset U by its *characteristic vector* χ_U, which has 1 at an index whenever its corresponding vertex is in U and 0 elsewhere. The characteristic vector, however, does not allow us to easily verify that U is independent. To solve this we create a *characteristic matrix*: $\chi_U \chi_U^T$. The subset $U \subseteq V$ is independent if and only if for every edge in E, the corresponding value in the matrix $\chi_U \chi_U^T$ is 0. The size of U can be calculated using its characteristic matrix: the trace of the characteristic matrix is equal to the size of U or, alternatively, the sum of all elements in the matrix is equal to the square of the size of U. By normalizing the characteristic matrix such that its trace is 1, we can set up an optimization problem for the independence number $\alpha(G)$:

$$\begin{aligned}\alpha(G) = \max\ & \textstyle\sum_{u\in V}\sum_{v\in V} A_{u,v}\\ & A_{u,v} = 0 \quad \forall\{u,v\}\in E,\\ & \mathrm{Tr}(A) = 1,\\ & A = \lambda B,\\ & \lambda \geq 0,\\ & B \in \{\chi_U\chi_U^T : U \subseteq V\}.\end{aligned}$$

2.1.2. The semidefinite-programming relaxation. Finding the independence number for a large graph in a realistic amount of time is often not possible as the problem is strongly NP-hard. To still find an upper bound for the independence number, we relax the problem such that we no longer evaluate just the normalized characteristic matrices but all positive semidefinite matrices. This type of relaxation was originally introduced by Lovász [9]. A matrix $A \in \mathbb{R}^{V\times V}$ is positive semidefinite if and only if there exists $\mu_1,\ldots,\mu_{|V|} \in \mathbb{R}^V$, $\lambda_1 \ldots \lambda_{|V|} \geq 0$ such that $A = \sum_{i=1}^{|V|} \lambda_i \mu_i \mu_i^T$. Now we can construct a new problem to find an upper bound for the independence number:

$$\begin{aligned}\vartheta(G) = \max\ & \textstyle\sum_{u\in V}\sum_{v\in V} A_{u,v}\\ & A_{u,v} = 0 \quad \forall\{u,v\}\in E,\\ & \mathrm{Tr}(A) = 1,\\ & A \succeq 0,\\ & A \in \mathbb{R}^{V\times V}.\end{aligned}$$

We use the Lovász theta number to refer to both the optimal value and the optimization problem.

2.1.3. Exploiting symmetry on distance-transitive graphs. To reduce the amount of solutions that are just another with an automorphism applied, we can limit the scope of the problem to invariant solutions. Let $T \in \mathrm{Aut}(G)$, we define the action TA by $(TA)_{u,v} = A_{Tu,Tv}$ for all $u, v \in V$. A matrix A can be made invariant under $\mathrm{Aut}(G)$ by invariant averaging across all transformations:

$$A' = \frac{1}{|\mathrm{Aut}(G)|}\sum_{T\in\mathrm{Aut}(G)} TX.$$

A useful property of matrices constructed as such, is that if A was a feasible solution for the Lovász theta number, then A' is also a feasible solution with the same objective value. Consequently, we can restrict the Lovász theta number to invariant matrices without loss in objective value.

Whenever the graph G is distance transitive, the matrix is especially well structured. Let $d(u,v)$ denote the shortest-path distance between u and v and $D = \{d(u,v) : u,v \in V\} \subseteq \mathbb{N}$. For every $d \in D$, let $E_d = \{(u,v) : u,v \in V, d(u,v) = d\}$. One can easily verify that the amount of automorphisms that map (u,v) to (x,y) is 0 if $d(u,v) \neq d(x,y)$ and $|\mathrm{Aut}(G)|/|E_d|$ if $d(u,v) = d(x,y) = d$. By averaging a matrix A across all automorphisms, the invariant matrix A' is such that for any $u, v \in V$

$$A'_{u,v} = \frac{1}{|\mathrm{Aut}(G)|}\sum_{T\in\mathrm{Aut}(G)} TA_{u,v} = \frac{1}{|E_d|}\sum_{(x,y)\in E_d} A_{x,y},$$

where $d(u,v) = d$. Therefore, any invariant matrix for distance-transitive graphs can be defined by assigning values to each element in D.

We observe two benefits by restricting the Lovász theta number to invariant matrices. First of all, all solutions that had the same average value for each element in D are represented by a single matrix and therefore the set of solutions is significantly smaller. The reduction in size is greater whenever a graph has a large automorphism group, which is the case for distance-transitive graph. The second property requires a graph to be vertex and edge transitive. Both distance-transitive graphs and the graphs used for the t-avoiding-set problem are vertex and edge transitive. Let A be an invariant positive semidefinite matrix. For edge-transitive graphs, it holds that the elements in invariant matrices which corresponding to an edge all have the same value. Therefore, if the constraint $A_{u,v} = 0$ is satisfied for any $\{u, v\} \in E$, then constraint $A_{u,v} = 0$ is satisfied for all $\{u, v\} \in E$. The same holds true for vertex-transitive graph and the diagonal elements of A. By combining these properties, we can fix $\{x, y\} \in E$ and simplify the Lovász theta number to the following without changing the optimal value:

$$\begin{aligned} \vartheta(G) = \max\ & \textstyle\sum_{u\in V} \sum_{v\in V} A_{u,v} \\ & A_{x,y} = 0, \\ & A_{x,x} = \tfrac{1}{|V|}, \\ & A \succeq 0, \\ & A \in \mathbb{R}^{V\times V} \quad \text{is invariant under } \mathrm{Aut}(G). \end{aligned}$$

2.2. Extension to the real sphere

To apply the concepts from graph theory to the t-avoiding-set problem, a suitable graph representation of the problem must be formulated. As this thesis uses the findings of de Oliveira Filho [2] as a basis, a summary of the relevant concepts in that thesis shall be provided.

2.2.1. Problem formulation on $S(\mathbb{R}^n)$. To start, we define a graph representation of the real sphere such that the t-avoiding-set problem is equivalent to the independence-number problem. To achieve this, the infinite graph is defined as $G(S(\mathbb{R}^n), t)$, where every point on the sphere is a vertex in the graph, and a pair of vertices in the graph has an edge whenever the respective points have inner product t. By this formulation, it is clear that a set on the sphere avoids inner product t if and only if the respective set on the graph is independent.

To properly represent the t-avoiding-set problem for use in optimization problems, an analogue to matrices must be used. The analogue used is *Hilbert-Schmidt kernels*, which we abbreviate to kernels. Kernels are the elements of $L^2(S(\mathbb{R}^n) \times S(\mathbb{R}^n))$. This Hilbert space is the space of square-integrable real-valued functions defined over $S(\mathbb{R}^n) \times S(\mathbb{R}^n)$, with respect to ω, the surface measure on $S(\mathbb{R}^n)$, and with inner product

$$\langle A, B\rangle = \int_{S(\mathbb{R}^n)} \int_{S(\mathbb{R}^n)} A(u, v)B(u, v)\, d\omega(u)\, d\omega(v),$$

for $A, B \in L^2(S(\mathbb{R}^n) \times S(\mathbb{R}^n))$.

The analogue for a characteristic matrix $A_{u,v} = (\chi_U \chi_U^T)_{u,v}$ of $U \subseteq V$ is the *characteristic kernel* $A(u, v) = \chi_U(u)\chi_U(v)$ of $U \subseteq S(\mathbb{R}^n)$, where $A(u, v) = 1$ if $u \in U$ and $v \in U$, $A(u, v) = 0$ elsewhere. The concepts of a positive semidefinite matrix and a matrix invariant also have straightforward analogues for kernels. A matrix $A \in \mathbb{R}^{n\times n}$ is positive semidefinite if for every $x \in \mathbb{R}^n$ $x^tAx = \sum_{u\in V} \sum_{v\in V} x_u A_{u,v} x_v \geq 0$. A kernel $A \in L^2(S(\mathbb{R}^n) \times S(\mathbb{R}^n))$ is *positive definite* if, for every $\rho \in L^2(S(\mathbb{R}^n))$:

$$\int_{S(\mathbb{R}^n)} \int_{S(\mathbb{R}^n)} \rho(u)A(u, v)\rho(v)\, d\omega(u)\, d\omega(v) \geq 0.$$

A *positive kernel* is a kernel that is positive definite. For invariance a similar equivalence can be observed. A matrix is invariant under $\mathrm{Aut}(G)$ iff $A_{u,v} = A_{Tu,Tv}$ for any $u, v \in V$ and $T \in \mathrm{Aut}(G)$. A kernel is invariant under $O(n)$ the orthogonal group iff $A(u, v) = A(Tu, Tv)$ for any $u, v \in S(\mathbb{R}^n)$ and $T \in O(n)$.

A crucial difference between the two problems, is that it does not make sense for the independence number to mean number of vertices in the set, as many measurable subsets of $S(\mathbb{R}^n)$ have an uncountable amount of vertices. De Oliveira Filho expressed the independence number as the surface measure of the t-avoiding set on the sphere. In this report, we instead opted to express it is as the proportion of the sphere that is in the t-avoiding set. This is equivalent to the expression used by de Oliveira Filho when normalizing the surface measure such that the surface measure of the entire sphere is 1.

2.2.2. The Lovász theta number on $S(\mathbb{R}^n)$. Let $\mathcal{F}$ be the family of measurable subsets of $S(\mathbb{R}^n)$. The t-avoiding-set problem is then equivalent to the following independence-number problem:

$$\begin{aligned} \alpha(G(S(\mathbb{R}^n),t)) = \sup\ & \int_{S(\mathbb{R}^n)}\int_{S(\mathbb{R}^n)} A(u,v)\, d\omega(u)\, d\omega(v) \\ & A(u,v) = 0 \quad \forall u,v \in S(\mathbb{R}^n) : \langle u,v\rangle = t, \\ & \int_{S(\mathbb{R}^n)} A(u,u)\, d\omega(u) = 1, \\ & A = \lambda B, \\ & \lambda \geq 0, \\ & B \in \{\chi_U \otimes \chi_U : U \in \mathcal{F}\}. \end{aligned}$$

Recall that all characteristic matrices are positive semidefinite. The formulation for the Lovász theta number on finite graphs was obtained by allowing solutions to be any positive semidefinite matrix that satisfy the other constraints, instead of just scaled characteristic matrices. For $G(S(\mathbb{R}^n),t)$, the formulation for the Lovász theta number is found in a similar fashion. Indeed, as all characteristic kernels are positive definite, we find the Lovász theta number by allowing the solutions to be any positive kernel that satisfy the other constraints:

$$\begin{aligned} \vartheta(G(S(\mathbb{R}^n),t)) = \sup\ & \int_{S(\mathbb{R}^n)}\int_{S(\mathbb{R}^n)} A(u,v)\, d\omega(u)\, d\omega(v) \\ & A(u,v) = 0 \quad \forall u,v \in S(\mathbb{R}^n), \langle u,v\rangle = t, \\ & \int_{S(\mathbb{R}^n)} A(u,u)\, d\omega(u) = 1, \\ & A : S(\mathbb{R}^n)\times S(\mathbb{R}^n) \to \mathbb{R} \text{ is a continuous and positive kernel.} \end{aligned} \tag{2.1}$$

The formulation for the Lovász theta number requires a continuity constraint as the other constraints can be arbitrarily fulfilled without it. While a characteristic kernel is non-continuous, continuous approximations can be used as feasible solutions.

2.2.3. Exploiting symmetry with a theorem of Schoenberg. By a similar process as used on distance-transitive graphs, we can reduce the complexity of a kernel by integration over the orthogonal group $O(n)$, which is the automorphism group of the graph $G(S(\mathbb{R}^n),t)$. The averaging process looks very similar:

$$A'(x,y) = \int_{O(n)} A(Tx,Ty)\, d\mu(T)$$

where μ is the Haar measure for $O(n)$ normalized such that $\mu(O(n)) = 1$. The role of the measure here is to give every transformation in $O(n)$ equal weight much like $1/|\operatorname{Aut}(G)|$ did on the finite graph. Such invariant kernels have the property that $A'(x,y) = A'(Tx,Ty)$ for all $T \in O(n)$. One can verify that, if the kernel A is a feasible solution for optimization problem (2.1) with objective value ϑ', then the kernel obtained by performing invariant integration A' is a feasible solution with the same objective value ϑ'. Consequently, we may restrict the optimization problem to invariant kernels.

Fix $v \in S(\mathbb{R}^n)$, if the function $f : S(\mathbb{R}^n) \to \mathbb{R}$ is such that $f(u)$ is only dependent on $\langle u,v\rangle$, then f is called a *zonal spherical function* with pole $v \in S(\mathbb{R}^n)$. As $\langle u,v\rangle \in [-1,1]$ for every pair of points $u,v \in S(\mathbb{R}^n)$, zonal spherical functions can otherwise be defined over $[-1,1]$. By using the appropriate measure ν for zonal functions over $[-1,1]$, the integral of a zonal function reduces to

$$\int_{S(\mathbb{R}^n)} f(u)\, d\omega(u) = \int_{-1}^{1} f(x) d\nu(x).$$

The group $O(n)$ has the following property: let $u, v, x, y \in S(\mathbb{R}^n)$, there exists $T \in O(n)$ such that $(Tu, Tv) = (x, y)$ if and only if $\langle u, v\rangle = \langle x, y\rangle$. Therefore, the values for an invariant kernel $A'(u, v)$ are described by a function $f : [-1, 1] \to \mathbb{R}$ on the inner product $\langle u, v\rangle$. By fixing u or v, an invariant kernel $A'(u, v)$ is a zonal function with the fixed coordinate as pole.

In order to describe continuous positive invariant kernels, we first introduce the *Jacobi polynomials.* The Jacobi polynomials, parametrized by $\alpha, \beta > -1$, are orthogonal on the interval $[-1, 1]$ with respect to the weight function $(1-x)^\alpha(1+x)^\beta$. That is, whenever $i \neq j$,

$$\int_{-1}^{1} P_i^{(\alpha,\beta)}(x) P_j^{(\alpha,\beta)}(x)(1-x)^\alpha(1+x)^\beta\, dx = 0$$

where $P_k^{(\alpha,\beta)}$ is the Jacobi polynomial of degree k and with parameters α, β. By convention, these polynomials are normalized such that $P_k^{(\alpha,\beta)}(1) = \binom{k+\alpha}{k}$. For use in the Lovász theta number, we instead use the differently normalized Jacobi polynomials $\widetilde{P}_k^{(\alpha,\beta)}$. These polynomials are normalized such that $\widetilde{P}_k^{(\alpha,\beta)}(1) = 1$. For more information on Jacobi polynomials, see [15].

We said that the measure used for integrating $S(\mathbb{R}^n)$-zonal functions over $[-1, 1]$ is such that $d\nu(x) = C \cdot (1-x^2)^{(n-3)/2}\, dx$ for some constant used for normalization C. It follows that the Jacobi polynomials with parameters $\alpha = \beta = (n-3)/2$ are orthogonal with respect to the measure ν. To show the connection between Jacobi polynomials and continuous, positive, invariant kernels, we introduce the following theorem due to Schoenberg [14]:

Theorem 2.1. *A kernel* $A \in L^2(S(\mathbb{R}^n) \times S(\mathbb{R}^n))$ *is continuous, positive, and invariant under* $O(n)$ *if and only if it is of the form*

$$A(u, v) = \sum_{k\in\mathbb{N}} \alpha_k\, \widetilde{P}_k^{((n-3)/2,(n-3)/2)}(\langle u, v\rangle),$$

where $\sum_{k\in\mathbb{N}} \alpha_k < \infty$ *and* $\alpha_k \geq 0$ *for all* $k \in \mathbb{N}$.

As we have seen, we may restrict the Lovász theta number to invariant kernels. By expressing the invariant kernels as in Theorem 2.1, we obtain the new formulation for the Lovász theta number:

$$\begin{aligned} \vartheta(G(S(\mathbb{R}^n), t)) = \sup\ & \alpha_0, \\ \text{s.t.}\ & \textstyle\sum_{k\in\mathbb{N}} \alpha_k = 1, \\ & \textstyle\sum_{k\in\mathbb{N}} \alpha_k \widetilde{P}_k^{((n-3)/2,(n-3)/2)}(t) = 0, \\ & \alpha_k \geq 0 \quad \forall k \in \mathbb{N}. \end{aligned} \tag{2.2}$$

Using the formulation, the problem reduces to a linear program and can consequently be solved using a linear programming solver. To verify that (2.2) is (2.1) restricted to invariant kernels, observe that the objective value of (2.1) for any invariant kernel $A(u, v) = \sum_{k\in\mathbb{N}} \alpha_k \widetilde{P}_k^{((n-3)/2,(n-3)/2)}(\langle u, v\rangle)$ is:

$$\int_{S(\mathbb{R}^n)} \int_{S(\mathbb{R}^n)} A(u, v)\, d\omega(u)\, d\omega(v) = \langle A, \widetilde{P}_0^{((n-3)/2,(n-3)/2)}\rangle = \alpha_0.$$

The constraints follow clearly as $A(u, v) = \sum_{k\in\mathbb{N}} \alpha_k \widetilde{P}_k^{((n-3)/2,(n-3)/2)}(t)$ for all $u, v \in S(\mathbb{R}^n)$ where $\langle u, v\rangle = t$ and $A(u, u) = \sum_{k\in\mathbb{N}} \alpha_k$ for all $u \in S(\mathbb{R}^n)$.

An example is Witsenhausen's problem [16]: what is supremum of the measure of sets on $S(\mathbb{R}^n)$ that avoid orthogonal pairs. Witsenhausen's problem is the t-avoiding-set problem where $t = 0$. The *double-cap conjecture* by Kalai [6] proposes that the measure of a 0-avoiding set can be no larger than the measure of the double-cap set. The double-cap set DC is defined as a $\pi/4$ radius open spherical cap around a pole v and its antipode $-v$. For $n \geq 2$ and the standard uniform probability measure ω, the measure of the double-cap set can be expressed using a closed formula as [8]:

$$\omega(DC) = I_{1/2}\left(\frac{n-1}{2}, \frac{1}{2}\right) = \begin{cases} 1/2 - \dfrac{1}{\pi} \displaystyle\sum_{j=1}^{(n-2)/2} \frac{2^j}{j} \binom{2j}{j}^{-1} & \text{if } n \text{ is even,} \\ 1 - \sqrt{1/2} \displaystyle\sum_{j=0}^{(n-3)/2} 8^{-j} \binom{2j}{j} & \text{if } n \text{ is odd,} \end{cases}$$

where $I_x\big(a, b\big)$ is the regularized incomplete beta function. By solving (2.2) for $t = 0$, we obtain the upper bound $1/n$. This upper bound matches the upper bound found by Witsenhausen using a probabilistic argument. While the formulation does not directly improve the upper bound, such improvements can be found by further constraining the problem. Indeed, the formulation has been extended by Bekker, Kuryatnikova, De Oliveira Filho and Vera [1] to find the upper bounds in Table 1.

n	$\omega(DC)$	Basic upper bound ($1/n$)	Improved upper bound
3	0.292893...	0.333333...	0.297742
4	0.181690...	0.25	0.194297
5	0.116117...	0.2	0.134588
6	0.075587...	0.166666...	0.098095
7	0.049825...	0.142857...	0.075751
8	0.033146...	0.125	0.061178

TABLE 1. Lower and upper bounds for the supremum of measures for 0-avoiding sets on $S(\mathbb{R}^n)$. The lower bound $\omega(DC)$ is the measure of the $\pi/4$ radius double-cap set. The basic upper bound is obtained by the probabilistic argument as shown by Witsenhausen [16] or calculating $\vartheta(G(S(\mathbb{R}^n), 0))$ as in (2.2). The improved upper bound is the lowest upper bound reported in [1].

CHAPTER 3

The t-avoiding-set problem on $S(\mathbb{C}^n)$

The aim of this chapter is to provide a formulation for the Lovász theta number that is an upper bound for the maximum measure of a t-avoiding set on the complex sphere. To accomplish this, we represent the complex sphere as a graph $G(S(\mathbb{C}^n), t)$ where every point on the sphere is a vertex on the graph and a pair of vertices is an edge if and only if the corresponding pair of points has inner product t or $\bar{t}$. In this representation a set on the complex sphere is t-avoiding if and only if the corresponding vertex set is independent. Therefore, an upper bound for the measure of t-avoiding sets can be found by calculating the Lovász theta number, which is a relaxation of the independence-number problem.

We start the chapter by introducing the necessary concepts from functional analysis for working on the complex sphere. The most important concepts are continuous, invariant, positive definite Hilbert-Schmidt kernels and disk polynomials, which provide a basis for such kernels. Next, we outline the process of creating Hilbert-Schmidt kernels from sets on the sphere for use in optimization problems. Afterwards, we formulate the Lovász theta number and create a real-valued disk polynomial to simplify implementation. In the penultimate section, we investigate solutions for the t-avoiding-set problem to gain insight into the Lovász theta number. To conclude the chapter, found values for the Lovász theta number are stated and compared to lower bounds where available.

3.1. Preliminaries for functional analysis on the complex sphere

While working on the complex n-dimensional unit sphere $S(\mathbb{C}^n)$, many concepts used for the real sphere can be used, given some adjustments. On the complex sphere we use the surface measure ω, which is once again normalized such that $\omega(S(\mathbb{C}^n)) = 1$. Generally, square-integrable functions and kernels on $S(\mathbb{C}^n)$ are complex valued. Therefore, the relevant properties outlined by de Oliveira Filho [2] are adjusted to the following:

We denote the Hilbert space of square-integrable complex-valued functions defined over $S(\mathbb{C}^n)$ by $L^2(S(\mathbb{C}^n))$. The inner product for $f, g \in L^2(S(\mathbb{C}^n))$ is defined as:

$$(f, g) = \int_{S(\mathbb{C}^n)} f(u)\overline{g(u)}\, d\omega(u).$$

As on the real sphere, the elements of $L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ are called *Hilbert-Schmidt kernels*, which we will abbreviate to *kernels*. The inner product for the kernels $A, B \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ is defined as:

$$\langle A, B\rangle = \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(u, v)\overline{B(u, v)}\, d\omega(u)\, d\omega(v).$$

Due to conjugate symmetry of inner products, $(f, g) = \overline{(g, f)}$ and $\langle A, B\rangle = \overline{\langle B, A\rangle}$. Therefore, it is important to remain consistent with the order when working with complex -valued functions and kernels.

A kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ is *Hermitian* $A(u, v) = \overline{A(v, u)}$ for all $u, v \in S(\mathbb{C}^n)$. A kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ is positive definite if it is Hermitian and for every $p \in L^2(S(\mathbb{C}^n))$, it holds that:

$$\int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} p(u)A(u,v)\overline{p(v)}\, d\omega(u)\, d\omega(v) \geq 0.$$

As square-integrable functions and kernels are analogues to vectors and matrices respectively, the definition for positive definiteness for complex-valued kernels is likewise similar to the definition for positive semidefiniteness for complex matrices.

To introduce the concept of invariance for kernels, we introduce the automorphism group that preserves the inner product between pairs of points. This group is called the unitary group and is defined as

$$U(n) = \{T \in \mathbb{C}^{n\times n} : T^*T = I\},$$

where I is the identity matrix and T^* the conjugate transpose of T. In general, a function is *invariant* under $U(n)$ if the output of the function does not change after applying any transformation $T \in U(n)$ to the input. The surface measure is *invariant* under $U(n)$. Indeed, for any measurable set $S \in S(\mathbb{C}^n)$ and any transformation $T \in U(n)$

$$\omega(T \cdot S) = \omega(\{Tu : u \in S\}) = \omega(S).$$

As a direct consequence of the surface measure being invariant, we find that integrals over $S(\mathbb{C}^n)$ are invariant over their integration variable. Indeed, for any $T \in U(n)$, $f, g \in L^2(S(\mathbb{C}^n))$ and $A, B \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$

$$\begin{aligned}
(f,g) = \int_{S(\mathbb{C}^n)} f(u)\overline{g(u)}\, d\omega(u) &= \int_{S(\mathbb{C}^n)} f(Tu)\overline{g(Tu)}\, d\omega(u), \\
\int_{S(\mathbb{C}^n)} A(u,v)\overline{B(u,v)}\, d\omega(u) &= \int_{S(\mathbb{C}^n)} A(Tu,v)\overline{B(Tu,v)}\, d\omega(u), \text{ and} \\
\int_{S(\mathbb{C}^n)} A(u,v)\overline{B(u,v)}\, d\omega(v) &= \int_{S(\mathbb{C}^n)} A(u,Tv)\overline{B(u,Tv)}\, d\omega(v).
\end{aligned}$$

By combining the latter two observations, we find that the inner product of two kernels is invariant in both integration variables.

$$\begin{aligned}
\langle A, B\rangle &= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(u,v)\overline{B(u,v)}\, d\omega(u)\, d\omega(v), \\
&= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(T_1u, T_2v)\overline{B(T_1u, T_2v)}\, d\omega(u)\, d\omega(v).
\end{aligned}$$

Integrals over f or A have the same properties as they are special cases for the above equalities. These special cases happen whenever $g(u) = 1$ for all $u \in S(\mathbb{C}^n)$ and $B(u,v) = 1$ for all $u, v \in S(\mathbb{C}^n)$ respectively.

A kernel A is invariant under $U(n)$ whenever $A(Tu, Tv) = A(u,v)$ for any $T \in U(n)$ and any $u, v \in S(\mathbb{C}^n)$. Let μ be the Haar measure on $U(n)$ normalized such that $\mu(U(n)) = 1$. Then, we can make any kernel invariant by integrating it over $U(n)$ with respect to μ. Indeed, given any kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$, the kernel

$$\widetilde{A}(x,y) = \int_{U(n)} A(Tx, Ty)\, d\mu(T)$$

is in $L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ and invariant under $U(n)$. For an invariant kernel B, such as the constant 1 kernel, its inner product with A remains the same after invariant integration. Indeed, by using the Fubini–Tonelli theorem and invariance of B we see

$$
\begin{aligned}
\langle \widetilde{A}, B\rangle &= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} \int_{U(n)} A(Tu, Tv)\, d\mu(T)\, \overline{B(u,v)}\, d\omega(u)\, d\omega(v),\\
&= \int_{U(n)} \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(Tu, Tv)\overline{B(u,v)}\, d\omega(u)\, d\omega(v)\, d\mu(T),\\
&= \int_{U(n)} \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(Tu, Tv)\overline{B(Tu,Tv)}\, d\omega(u)\, d\omega(v)\, d\mu(T),\\
&= \int_{U(n)} \langle A, B\rangle\, d\mu(T) = \langle A, B\rangle.
\end{aligned}
$$

The values for invariant kernels are only dependent on the inner product of the input variables. Indeed, for $u, v, x, y \in S(\mathbb{C}^n)$ with $\langle u, v\rangle = \langle x, y\rangle$ there exists a unitary transformation $T \in U(n)$ such that $Tu = x$ and $Tv = y$, as the unitary group is the automorphism group of $S(\mathbb{C}^n)$ that preserves inner product. Therefore, for the invariant kernel A, we find $A(u, v) = A(x, y)$, whenever $\langle u, v\rangle = \langle x, y\rangle$.

A *zonal spherical function* with pole $v \in S(\mathbb{C}^n)$ is a function $f : S(\mathbb{C}^n) \to \mathbb{C}$ where $f(u)$ is determined only by $\langle u, v\rangle$. As $\langle u, v\rangle \in \overline{\mathbb{D}} = \{re^{i\theta} : r \in [0, 1], \theta \in [0, 2\pi)\}$ for all $u, v \in S(\mathbb{C}^n)$, a zonal function can also be defined over the domain $\overline{\mathbb{D}}$. A $S(\mathbb{C}^n)$-zonal function can therefore be integrated over $\overline{\mathbb{D}}$ using an appropriate measure:

$$
\int_{S(\mathbb{C}^n)} f(u)\, d\omega(u) = \int_{\overline{\mathbb{D}}} f(re^{i\theta})\, d\nu(re^{i\theta}) = \int_0^1 \int_0^{2\pi} f(re^{i\theta})\, d\tau(\theta)\, d\rho(r).
$$

For the Cartesian form of a complex number, the appropriate normalized measure on the unit disk is $d\nu(x+iy) = \frac{1}{\pi}(n-1)(1-x^2-y^2)^{n-2}\, dx\, dy$ [10]. Under the change of variables to polar coordinates this becomes $d\nu(re^{i\theta}) = \frac{1}{\pi}(n-1)r(1-r^2)^{n-2}\, dr\, d\theta$. We separate the measure into normalized measures for the magnitude and the argument as $\nu = \rho \otimes \tau$:

$$
\begin{aligned}
d\tau(\theta) &= \frac{1}{2\pi}\, d\theta,\\
d\rho(r) &= 2(n-1)r(1-r^2)^{n-2}\, dr.
\end{aligned}
$$

Throughout this thesis, we use ρ and τ when integrating zonal functions on $S(\mathbb{C}^n)$. An alternative derivation for the measure has been provided in Appendix A.2. In the derivation, the measure is constructed via the distribution for the first coordinates of uniformly random chosen points on the real sphere.

As the value of an invariant kernel is only dependent on the inner product of the input variables, it follows that all invariant kernels are zonal spherical functions whenever one variable is fixed. Consequently, we simplify the inner product of two invariant kernels $A(u, v), B(u, v) \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$, using their respective zonal functions f, g with pole v:

$$
\begin{aligned}
\langle A, B\rangle &= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(u, v)\overline{B(u, v)}\, d\omega(u)\, d\omega(v),\\
&= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} f(\langle u, v\rangle)\overline{g(\langle u, v\rangle)}\, d\omega(u)\, d\omega(v),\\
&= \int_{S(\mathbb{C}^n)} \int_0^1 \int_0^{2\pi} f(re^{i\theta})\overline{g(re^{i\theta})}\, d\tau(\theta)\, d\rho(r)\, d\omega(v),\\
&= \int_0^1 \int_0^{2\pi} f(re^{i\theta})\overline{g(re^{i\theta})}\, d\tau(\theta)\, d\rho(r).
\end{aligned}
$$

As on the real sphere, we are particularly interested in invariant, positive, continuous kernels. On $S(\mathbb{R}^n)$, the normalized-at-1 Jacobi polynomials $\widetilde{P}_k^{(\alpha,\alpha)}$ with $\alpha = (n-3)/2$ were used to provide an orthogonal basis for invariant, positive, continuous kernels. On $S(\mathbb{C}^n)$, the *disk polynomials* are used for the same function. The disk polynomials, defined as

$$R_{p,q}^{n-2}(z = re^{i\theta}) = r^{|p-q|}\, e^{i(p-q)\theta}\, \widetilde{P}_{\min\{p,q\}}^{(n-2,|p-q|)}(2r^2-1),$$

are polynomials of degree p in z and of degree q in $\overline{z}$. One can verify that the disk polynomials are orthogonal with respect to the measure $\nu(re^{i\theta})$ on $\overline{\mathbb{D}}$. Indeed, $\langle R_{p,q}^{n-2}, R_{a,b}^{n-2}\rangle = 0$ whenever $(p-q) \neq (a-b)$ due to the term $e^{i(p-q)\theta}$. Additionally, $\langle R_{p,q}^{n-2}, R_{a,b}^{n-2}\rangle = 0$ whenever $(p-q) = (a-b)$ and $\min\{p,q\} \neq \min\{a,b\}$, due to orthogonality of the Jacobi polynomials.

Theorem 3.1, as stated and proven by Menegatto and Peron [10], characterizes invariant, positive, continuous kernels.

Theorem 3.1. *A kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ is continuous, positive, and invariant under $U(n)$ if and only if it is of the form*

$$A(u,v) = \sum_{p,q\in\mathbb{N}} a_{p,q}\, R_{p,q}^{n-2}(\langle u,v\rangle),$$

where $\sum_{p,q\in\mathbb{N}} a_{p,q} < \infty$ and $a_{p,q} \geq 0$ for all $p,q \in \mathbb{N}$.

Due to orthogonality of the disk polynomials, the coefficients in Theorem 3.1 for a given continuous, positive, invariant kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ can be found through process of integration:

$$a_{p,q} = \frac{\langle A, R_{p,q}^{n-2}\rangle}{\langle R_{p,q}^{n-2}, R_{p,q}^{n-2}\rangle} = \frac{\int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} A(u,v)\overline{R_{p,q}^{n-2}(\langle u,v\rangle)}\, d\omega(u)\, d\omega(v)}{\int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} R_{p,q}^{n-2}(\langle u,v\rangle)\overline{R_{p,q}^{n-2}(\langle u,v\rangle)}\, d\omega(u)\, d\omega(v)}. \quad (3.1)$$

As a final observation for this section, we find the following relations between the integrals of a continuous, positive, invariant kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ and its coefficients as described in Theorem 3.1:

$$\begin{aligned} \sum_{p,q\in\mathbb{N}} a_{p,q} = \sum_{p,q\in\mathbb{N}} a_{p,q}\, R_{p,q}^{n-2}(1) &= \int_{S(\mathbb{C}^n)} A(u,u)\, d\omega(u), \\ a_{0,0} = \langle A, R_{0,0}^{n-2}\rangle &= \int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} A(u,v)\, d\omega(u)\, d\omega(v). \end{aligned} \quad (3.2)$$

3.2. From sets on $S(\mathbb{C}^n)$ to kernels

In this section we describe set-to-kernel constructions that map any t-avoiding set to a feasible kernel for formulations of the Lovász theta number used in this thesis. This makes the connection between the t-avoiding-set problem and the formulation for the Lovász theta number explicit and shows that the Lovász theta number is an upper bound for the surface measure of t-avoiding sets. To represent a set in an optimization program, we prefer to use continuous, positive, invariant kernels as they can be described by disk polynomials using Theorem 3.1.

Let S be a measurable, not necessarily t-avoiding, set on $S(\mathbb{C}^n)$. A standard way to represent a set is by its characteristic function $\chi_S : S(\mathbb{C}^n) \to \{0,1\}$. The value of the function is 1 for any point in S and 0 elsewhere. It is clear that the surface measure of S can be calculated by the integral of its characteristic function:

$$\omega(S) = \int_{v\in S(\mathbb{C}^n)} \chi_S(u) d\omega(u).$$

For the t-avoiding-set problem, we prefer to use a characteristic kernel over a characteristic function as it explicitly shows whenever a pair of point are in the set together. In particular, this is used to check whether the set is t-avoiding, much like how a characteristic matrix was used to check if a set was independent. The construction of characteristic matrix and its relationship to the measure of S is as follows:

$$\begin{aligned} A(u,v) &= \chi_S(u)\chi_S(v), \\ \omega(S) &= \int_{S(\mathbb{C}^n)} A(u,u)\, d\omega(u), \\ \omega(S)^2 &= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A(u,v)\, d\omega(v)\, d\omega(u). \end{aligned}$$

While the characteristic kernel is straightforward in its concept, it does not yet have the desired properties for use in an optimization program. While the kernel is positive, it is neither continuous nor invariant under $U(n)$. To construct the first kind of continuous, positive, invariant kernel, we perform invariant integration on the characteristic kernel:

$$\widetilde{A}(u,v) = \int_{U(n)} A(Tu, Tv)\, d\mu(T). \tag{3.3}$$

As seen in the preliminaries, $\widetilde{A}$ is invariant under $U(n)$ while maintaining its relation to the measure. Importantly for the t-avoiding-set problem, if S is t-avoiding, then $\widetilde{A}(u,v) = 0$ for every pair of $u, v \in S(\mathbb{C}^n)$ where $\langle u, v\rangle = t$.

To assist in understanding what the values of the kernel mean in terms of the set S, the kernel can be thought of in a probabilistic sense. Let the transformation T be a random element of $U(n)$ chosen according to the Haar probability measure μ. Then the value of the kernel $\widetilde{A}$ for any two points $u, v \in S(\mathbb{C}^n)$ describes the joint probability $\Pr(Tu \in S \text{ and } Tv \in S)$.

The second construction of an invariant kernel differs only in normalization. The kernel A' is constructed as

$$A'(u,v) = \frac{\widetilde{A}(u,v)}{\widetilde{A}(v,v)} = \frac{\int_{U(n)} A(Tv, Tw)\, d\mu(T)}{\int_{U(n)} A(Tv, Tv)\, d\mu(T)}. \tag{3.4}$$

which normalizes the kernel such that $A'(u,u) = 1$ for all $u \in S(\mathbb{C}^n)$. Using the same probabilistic construction as before, these new kernels can be interpreted as a conditional probability function. After the normalization, the relation between the integrals of the kernels and the measure of the sets also changes. Indeed, we see the following properties for the second construction:

$$\begin{aligned} A'(u,v) &= \Pr(u \in TS \mid v \in TS) = \frac{\Pr(u \in TS \text{ and } v \in TS)}{\Pr(v \in TS)}, \\ 1 &= \int_{S(\mathbb{C}^n)} A'(u,u)\, d\omega(u), \\ \omega(S) &= \int_{S(\mathbb{C}^n)} \int_{S(\mathbb{C}^n)} A'(u,v)\, d\omega(v)\, d\omega(u). \end{aligned}$$

As both (3.3) and (3.4) result in a continuous, positive, invariant kernels, they can be described in term of disk polynomials. The coefficients used to describe the corresponding solutions for the Lovász theta number can then be found through process of integration as in (3.1).

3.3. The t-avoiding Lovász-theta number on $S(\mathbb{C}^n)$

We use the formulation for the Lovász theta number described in the previous chapter:

$$\begin{aligned}\vartheta(G(S(\mathbb{C}^n),t)) = \sup\ & \int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} A(x,y)\,d\omega(x)\,d\omega(y)\\ \text{s.t.}\ & \int_{S(\mathbb{C}^n)} A(x,x)\,d\omega(x) = 1,\\ & A(x,y) = 0 \quad \forall x,y \in S(\mathbb{C}^n), \langle x,y\rangle = t,\\ & A \in L^2(S(\mathbb{C}^n)\times S(\mathbb{C}^n)) \text{ is a continuous and positive kernel.}\end{aligned}$$

Next we restrict the problem to invariant kernels and express them in terms of disk polynomials as in Theorem 3.1. We use the same methods to express the objective function and the constraints as we did on $S(\mathbb{R}^n)$. The formulation then becomes as follows:

$$\begin{aligned}\vartheta(G(S(\mathbb{C}^n),t)) = \sup\ & a_{0,0},\\ \text{s.t.}\ & \textstyle\sum_{p,q\in\mathbb{N}} a_{p,q} = 1,\\ & \textstyle\sum_{p,q\in\mathbb{N}} a_{p,q} R^{n-2}_{p,q}(t) = 0,\\ & a_{p,q} \geq 0 \quad \forall p,q \in \mathbb{N}.\end{aligned} \tag{3.5}$$

While the disk polynomials provide a basis for positive invariant kernels on the complex sphere, they introduce unnecessary complexity into the optimization problem. Namely, the polynomials introduce complex values, while characteristic kernels are real valued. To simplify the implementation of the optimization program, new real-valued disk polynomials are created from two disk polynomials which are each other's complex conjugate. By construction $R^{n-2}_{p,q}(z)$ is the conjugate of $R^{n-2}_{q,p}(z)$ for any choice of p and q. We parameterize the real-valued disk polynomial based on the parameters of the complex-valued disk polynomials it is based on: $\gamma = |p-q|$ and $k = \min\{p,q\}$. Using this parameterization, we obtain the following formulation:

$$\begin{aligned}U^{n-2}_{k,\gamma}(z = re^{i\theta}) &= \frac{1}{2}R^{n-2}_{\gamma+k,k},(re^{i\theta}) + \frac{1}{2}R^{n-2}_{k,\gamma+k}(re^{i\theta}),\\ &= r^{\gamma}\frac{e^{i\gamma\theta}+e^{-i\gamma\theta}}{2}\widetilde{P}^{(n-2,\gamma)}_k(2r^2-1),\\ &= r^{\gamma}\cos(\gamma\theta)\widetilde{P}^{(n-2,\gamma)}_k(2r^2-1).\end{aligned}$$

The following new formulation for the Lovász theta number can be created using the real-valued disk polynomials:

$$\begin{aligned}\vartheta(G(S(\mathbb{C}^n),t)) = \sup\ & \alpha_{0,0}\\ & \textstyle\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} = 1,\\ & \textstyle\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t) = 0,\\ & \alpha_{k,\gamma} \geq 0 \quad \forall k,\gamma \in \mathbb{N}.\end{aligned} \tag{3.6}$$

We introduce the following claim about the Lovász theta number to show that the formulation using real-valued disk polynomials is of equivalent strength to the formulation using complex-valued disk polynomials.

Claim 3.2. *There exists a feasible solution for* (3.5) *with objective value* ϑ' *if and only if there exist a feasible solution for* (3.6) *with the same objective value* ϑ'.

Proof. Given a feasible solution for (3.5), with objective value $\vartheta' = a_{0,0}$. Observe that the solution for (3.6) with $\alpha_{k,0} = a_{k,k}$ and $\alpha_{k,\gamma} = a_{\gamma+k,k} + a_{k,\gamma+k}$ for $\gamma \geq 1$ is feasible. As $\alpha_{0,0} = a_{0,0}$, the two solutions have the same objective value.

For the reverse direction, we start with a feasible solution for (3.6), which has an objective value $\vartheta' = \alpha_{0,0}$. Then the solution for (3.5) with $a_{p,p} = \alpha_{p,0}$ and $a_{p,q} = \frac{1}{2}\,\alpha_{\min\{p,q\},\,|p-q|}$ for $p \neq q$ is feasible and has objective value ϑ'. ∎

To further motivate the usage of real-valued disk polynomials in the Lovász theta number, we adapt Theorem 3.1 for real-valued kernels and disk polynomials.

Theorem 3.3. *A kernel $A \in L^2(S(\mathbb{C}^n)\times S(\mathbb{C}^n))$ is continuous, real valued, positive, and invariant under $U(n)$ if and only if it is of the form*

$$A(u,v) = \sum_{\gamma,k\in\mathbb{N}} \alpha_{k,\gamma}\, U^{n-2}_{k,\gamma}(\langle u,v\rangle),$$

in which $\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} < \infty$ and $\alpha_{k,\gamma} \geq 0$ for all $k,\gamma \in \mathbb{N}$.

In the proof for Theorem 3.3, we need the following Lemma. A proof of this Lemma can be found in Appendix A.3.

Lemma 3.4. *Let $K(\langle u,v\rangle)$ be a square-integrable zonal function on $S(\mathbb{C}^n)$ with pole v. Then the following statements hold for all $p,q \in \mathbb{N}$:*

(i) *If $K(z) = K(\overline{z})$ for all $z \in \overline{\mathbb{D}}$, then $\langle K, R^{n-2}_{p,q}\rangle = \langle K, R^{n-2}_{q,p}\rangle$.*
(ii) *If $K(z) \in \mathbb{R}$ for all $z \in \overline{\mathbb{D}}$, then $\langle K, R^{n-2}_{p,q}\rangle = \overline{\langle K, R^{n-2}_{q,p}\rangle}$.*
(iii) *If $\overline{K(z)} = K(\overline{z})$ for all $z \in \overline{\mathbb{D}}$, then $\langle K, R^{n-2}_{p,q}\rangle \in \mathbb{R}$.*

Proof of Theorem 3.3. Theorem 3.1 proves most of Theorem 3.3. What remains to be shown is that a continuous, positive, invariant kernel A is real valued if and only if it is of the form

$$A(u,v) = \sum_{\gamma,k\in\mathbb{N}} \alpha_{k,\gamma}\, U^{n-2}_{k,\gamma}(\langle u,v\rangle) = \sum_{\gamma,k\in\mathbb{N}} \frac{\alpha_{k,\gamma}}{2}\big(R^{n-2}_{k+\gamma,k}(\langle u,v\rangle) + R^{n-2}_{k,k+\gamma}(\langle u,v\rangle)\big).$$

It is trivial to show necessity, as a sum of real-valued functions is itself real valued.

To show sufficiency, we show that if A is real valued, then $a_{p,q} = a_{q,p}$ for all $p,q \in \mathbb{N}$, where $a_{p,q}$ is the coefficient for the $R^{n-2}_{p,q}(\langle u,v\rangle)$. let K be the zonal function where $K(\langle u,v\rangle) = A(u,v)$ for all $u,v \in S(\mathbb{C}^n)$. As A is real valued, in addition to being positive definite and therefore Hermitian, we find

$$K(\langle u,v\rangle) = A(u,v) = \overline{A(u,v)} = A(v,u) = K(\overline{\langle u,v\rangle}).$$

Additionally, one can verify that $\langle R^{n-2}_{p,q}, R^{n-2}_{p,q}\rangle = \langle R^{n-2}_{q,p}, R^{n-2}_{q,p}\rangle$. To complete the proof, we use Lemma 3.4.(i) to show

$$a_{p,q} = \frac{\langle R^{n-2}_{p,q}, K\rangle}{\langle R^{n-2}_{p,q}, R^{n-2}_{p,q}\rangle} = \frac{\langle R^{n-2}_{q,p}, K\rangle}{\langle R^{n-2}_{q,p}, R^{n-2}_{q,p}\rangle} = a_{q,p}. \qquad \blacksquare$$

As invariant characteristic kernels are continuous, real valued and positive, Theorem 3.3 shows those kernels have a real-valued disk polynomial decomposition. Consequently, any such kernel constructed from a t-avoiding set is a feasible solution for (3.6), given the correct normalization is applied.

Remark. *When using the real-valued disk polynomials $U^{n-2}_{k,\gamma}(z)$ instead of complex-valued disk polynomials $R^{n-2}_{p,q}(z)$, the following benefits are observed:*

(i) *As many solvers are only equipped to deal with real numbers, it is no longer necessary to implement a workaround in order to deal with imaginary numbers.*
(ii) *If a real-valued, positive, invariant kernel is described using finitely many complex-valued disk polynomials, then it is described by roughly half as many real-valued disk polynomials.*
(iii) *Using real-valued disk polynomials in the Lovász theta number eliminates the imaginary component beforehand. Therefore, the new problem removes many symmetric solutions that only differ in the ratios between the coefficients of disk polynomials and their conjugates.*
(iv) *The new indices directly encode the relation $U^{n-2}_{k,\gamma}(re^{i\theta}) = \cos(\gamma\theta)U^{n-2}_{k,\gamma}(r)$.*

Remark (*iv*) can be used the perform analysis on the periodicity of a solution of (3.6) by investigating for what γ there are nonzero variables. Likewise, we may restrict the problem to solutions of a certain period by controlling for what γ the variables are allowed to be nonzero.

As an example, assume there exists a value for t such that restricting the t-avoiding-set problem to sets that are closed multiplication by $e^{i\theta}$ does not decrease the optimal value. If a set that are closed under multiplication by $e^{i\theta}$, then the corresponding invariant kernel A' is such that $A'(u, v) = A'(e^{i\theta}u, v)$ for all $u, v \in S(\mathbb{C}^n)$ and for all $\theta \in [0, 2\pi)$. The real-valued disk polynomial decomposition for such invariant kernels only have a nonzero coefficient whenever $\gamma = 0$. Consequently, we may restrict the Lovász theta number to solutions where a variable is nonzero only if $\gamma = 0$. The restricted Lovász theta number still remains an upper bound for the t-avoiding set problem.

3.4. Benchmark bounds for $t = 0$ and $t = e^{i\phi}$

In this section we investigate the t-avoiding-set problem for the cases where $t = 0$ or $t = e^{i\phi}$. For both cases, we prove that we may limit the problem to sets with a specific structure without decreasing the optimal value. To find a lower bound, we show set constructions that are either conjectured or proven to be maximal. In order to find an upper bound, we use the following theorem:

Theorem 3.5. *Let ω the surface measure on $S(\mathbb{C}^n)$ normalized such that $\omega(S(\mathbb{C}^n)) = 1$ and $G(S(\mathbb{C}^n), t)$ be the graph on $S(\mathbb{C}^n)$ where the vertices u, v form an edge if and only if $\langle u, v\rangle = t$. For any finite subgraph $H = (V, E)$, the following inequality holds:*

$$\alpha(G(S(\mathbb{C}^n), t)) \leq \frac{\alpha(H)}{|V|}.$$

Proof. Let I be any measurable independent set on $G(S(\mathbb{C}^n), t)$. As $TI \cap V$ is an independent set on H for all $T \in U(n)$, $|TI \cap V| \leq \alpha(H)$. Let μ be the normalized Haar measure on $U(n)$ and x be any fixed point on $S(\mathbb{C}^n)$, then

$$\omega(I) = \mu(\{T \in U(n) : x \in TI\}) = \int_{U(n)} |TI \cap \{x\}|\, d\mu(T).$$

By taking the average of this measure across each point in V, we find

$$\omega(I) = \frac{1}{|V|} \sum_{x \in V} \int_{U(n)} |TI \cap \{x\}|\, d\mu(T) = \frac{1}{|V|} \int_{U(n)} |TI \cap V|\, d\mu(T) \leq \frac{\alpha(H)}{|V|}.$$

As this holds for every measurable independent set of $G(S(\mathbb{C}^n), t)$, the inequality in Theorem 3.5 follows. ■

3.4.1. Witsenhausen's problem. The maximization problem for 0-avoiding sets is equivalent to the problem posed by Witsenhausen in [16] extended to the complex sphere. The question posed by Witsenhausen was: *"what is the largest set on the unit sphere that avoids orthogonal points?"*. The double-cap conjecture for $S(\mathbb{R}^n)$ by Kalai [6] has been generalized by Montina [12] for $S(\mathbb{C}^n)$. The conjecture proposes that the measure of a 0-avoiding set cannot be larger than the measure of the double-cap set. Let $S(\mathbb{K}^n)$ be the unit sphere, such as $S(\mathbb{R}^n)$ or $S(\mathbb{C}^n)$, then the double-cap set with pole v on $S(\mathbb{K}^n)$ is defined as:

$$DC(v) = \left\{u : u \in S(\mathbb{K}^n), |\langle u, v\rangle| > \sqrt{1/2}\right\}.$$

On $S(\mathbb{R}^n)$, the double-cap set is defined as disjoint union of two open 45 degree caps, one around a pole v and the other around its antipodal $-v$. On $S(\mathbb{C}^n)$, the term "double-cap set" is a misnomer as the set is connected. That is, the set with pole v is a band around the circle $\{e^{i\theta}v : \theta \in [0, 2\pi)\}$. While the term is a misnomer, the naming convention is maintained throughout this work.

In order to calculate the measure of the double-cap set, notice the characteristic function of the set is equal to the zonal function $\chi_{(\sqrt{1/2},1]}(|\langle u, v\rangle|)$. By using the zonal function, we calculate the measure of double-cap set with pole v on $S(\mathbb{C}^n)$ as

$$\begin{aligned}\omega(DC(v)) &= \int_0^1 \int_0^{2\pi} \chi_{(\sqrt{1/2},1]}(r)\, d\tau(\theta)\, d\rho(r),\\ &= \int_{\sqrt{1/2}}^1 2(n-1)r(1-r^2)^{n-2}\, dr = \left(\frac{1}{2}\right)^{n-1}.\end{aligned}$$

The double-cap conjecture has been proven by Witsenhausen for $n = 2$. During the introduction of the problem, he showed that $1/n$ is an upper bound for the measure of 0-avoiding sets through a probabilistic argument. The argument used equates to using Theorem 3.5 with the induced subgraph H with the vertex set $V = \{e_1, e_2, \ldots, e_n\}$. This graph is a complete graph with n vertices and $\alpha(H) = 1$. Using the theorem, we find

$$\alpha(G(S(\mathbb{C}^n), 0)) \leq \frac{\alpha(H)}{|V|} = \frac{1}{n}.$$

As the measure of the double-cap set and the upper bound agree on $n = 2$, the double-cap set is a 0-avoiding set of maximal measure. Both the upper bound $1/n$ and the proof of the double-cap conjecture for $n = 2$ hold for the real and complex spheres.

For $n \geq 3$, the double-cap conjecture has neither been proven nor disproven. Despite this, we are able to formulate statements about the structure of an optimal solution. First of these statements is that there exists an optimal solution that is closed under multiplication by $e^{i\theta}$.

Theorem 3.6. *Let $S \subseteq S(\mathbb{C}^n)$ be a set with no orthogonal points and measure $\omega(S)$. Then $CS = \bigcup_{\theta\in[0,2\pi)} e^{i\theta}S$ has no orthogonal points, is closed under multiplication by $e^{i\theta}$ and has measure $\omega(S) \leq \omega(CS)$.*

Proof of Theorem 3.6. This is a proof by contradiction. Let $S \subseteq S(\mathbb{C}^n)$ be a set with no orthogonal points and construct the set $CS = \bigcup_{\theta\in[0,2\pi]} e^{i\theta}S$. As $S \subseteq CS$, $\omega(S) \leq \omega(CS)$ by monotonicity of the measure. Additionally CS is closed under multiplication by $e^{i\theta}$ by construction. Therefore, we must assume CS has orthogonal points to arrive at a contradiction to the theorem. Let $x, y \in CS$ be the points with inner product $\langle x, y\rangle = 0$. By construction there exist $x', y' \in S$ and $\theta, \psi \in [0, 2\pi)$ such that $x = x'e^{i\theta}$ and $y = y'e^{i\psi}$. Now the assumption implies that $\langle x, y\rangle = \langle x'e^{i\theta}, y'e^{i\psi}\rangle = e^{i(\theta-\psi)}\langle x', y'\rangle = 0$, and consequently $\langle x', y'\rangle = 0$. However, x', y' are points in S and there are no orthogonal points in S. This contradicts the assumption and therefore proves CS has no orthogonal points. ■

Corollary 3.7. *If there is an optimal solution for Witsenhausen's problem, then there is an optimal solution for Witsenhausen's problem on $S(\mathbb{C}^n)$ that is closed under multiplication by $e^{i\theta}$.*

Theorem 3.6 proves that restricting the independence-number problem to only use sets closed under multiplication by $e^{i\theta}$ does not decrease its optimal value. This allows us to restrict the Lovász theta number to only use disk polynomials with $\gamma = 0$, which are the polynomials independent of the argument of the input.

Claim 3.8. *Let $\omega(DC)$ be the surface measure of the double-cap set on $S(\mathbb{C}^n)$. For any set $S \subseteq S(\mathbb{C}^n)$, if S is 0-avoiding and has a characteristic function that is zonal with pole $v \in S(\mathbb{C}^n)$, then $\omega(S) \leq \omega(DC)$.*

PROOF. For $n = 2$, the double-cap conjecture, and therefore the claim, is proven. If $n \geq 3$, a proof by contradiction is used. Let S be a 0-avoiding set with the zonal characteristic function χ_S with pole $v \in S(\mathbb{C}^n)$ and $\omega(S) > \omega(DC)$. As χ_S is zonal, there exists a set $A \subseteq \overline{\mathbb{D}}$ such that $u \in S$ if and only if $\langle u, v\rangle \in A$.

By Theorem 3.6, the set $CS = \bigcup_{\theta \in [0,2\pi)} e^{i\theta} S$ is 0-avoiding with measure $\omega(S) \leq \omega(CS)$. We see that $u \in CS$ if and only if $\langle u, v\rangle \in \bigcup_{\theta\in[0,2\pi)} e^{i\theta}A$. Consequently, there exists a set $D \subseteq [0, 1]$ such that $u \in CS$ if and only if $|\langle u, v\rangle| \in D$. If $D \subseteq (\sqrt{1/2}, 1]$, then clearly $\omega(S) \leq \omega(CS) \leq \omega(DC)$. By assumption $\omega(S) > \omega(DC)$ and therefore $D \cap [0, \sqrt{1/2}] \neq \emptyset$. As $n \geq 3$, there exists two points $w_1, w_2 \in S(\mathbb{C}^n)$ that are orthogonal to each other and to v. Let a be a number in $D \cap [0, \sqrt{1/2}]$, then the points

$$x = av + \sqrt{1-a^2}w_1,$$
$$y = av - \frac{a^2}{1-a^2}\sqrt{1-a^2}w_1 + \sqrt{1-\frac{a^2}{1-a^2}}w_2,$$

are in the set CS. This contradicts the assumption as $\langle x, y\rangle = 0$ and completes the proof. ■

3.4.2. $e^{i\phi}$-avoiding sets. To find an $e^{i\phi}$-avoiding set of maximal measure, we show that we can restrict the problem to a specific type of solutions without decreasing the optimal value. By defining a property of a set called *v-phasic*, we shall prove that restricting solutions to v-phasic sets does not decrease the optimal value.

Fix $v \in S(\mathbb{C}^n)$, this point is used as reference point for the definitions and constructed sets that follow. We define the set of points orthogonal to v as $V^\perp = \{u : u \in S(\mathbb{C}^n), \langle u, v\rangle = 0\}$. Notably, $V^\perp$ is isometric to $S(\mathbb{C}^{n-1})$ and therefore the bijective function $\Phi : S(\mathbb{C}^{n-1}) \to V^\perp$ and its inverse Φ^{-1} exist. As $V^\perp$ is a lower dimensional set than $S(\mathbb{C}^n)$, it has measure 0 on $S(\mathbb{C}^n)$. An important characteristic for the following explanation, is that $V^\perp$ is closed under multiplication by $e^{i\theta}$ ($w \in V^\perp, \theta \in [0, 2\pi) \implies we^{i\theta} \in V^\perp$). As we use v as a reference point, we can decompose a point u in terms of its projection along and perpendicular to v in these three equivalent formulations:

$$u = \langle u, v\rangle v + \sqrt{1 - |\langle u, v\rangle|^2}v_u^\perp, \tag{3.7a}$$
$$u = r_u e^{i\theta_u} v + \sqrt{1 - r_u^2}v_u^\perp, \tag{3.7b}$$
$$u = F(r_u, \theta_u, w_u) = r_u e^{i\theta_u} v + \sqrt{1 - r_u^2}\Phi(w_u). \tag{3.7c}$$

We define the terms r_u, θ_u, $v_u^\perp$ as follows: $r_u = |\langle u, v\rangle|$, $\theta_u = \arg(\langle u, v\rangle)$ and $v_u^\perp = \frac{u - \langle u,v\rangle v}{\sqrt{1-|\langle u,v\rangle|^2}}$. If θ_u or $v_u^\perp$ cannot be determined, which happens when $r_u = 0$ or $r_u = 1$ respectively, the values can be chosen arbitrarily from $[0, 2\pi)$ or $V^\perp$ respectively. After determining $v_u^\perp$, w_u can be found easily by $\Phi^{-1}(v_u^\perp)$.

This notation allows us to parametrize $u \in S(\mathbb{C}^n)$ as $(r_u, \theta_u, w_u) \in [0, 1] \times [0, 2\pi) \times S(\mathbb{C}^{n-1})$ and allows us to integrate any function in $L^2(S(\mathbb{C}^n))$. Indeed, we see that

$$\int_{S(\mathbb{C}^n)} f(u)\, d\omega_n(u) = \int_0^1 \int_0^{2\pi} \int_{S(\mathbb{C}^{n-1})} f(F(r, \theta, w)) d\omega_{n-1}(w)\, d\tau(\theta)\, d\rho(r) \tag{3.8}$$

where ω_m is the normalized surface measure on $S(\mathbb{C}^m)$, and ρ and τ are the normalized measures for the magnitude and argument of on $S(\mathbb{C}^n)$-zonal functions. Additionally, as all the functions we use are square integrable, the order of integration can be freely swapped around.

The subset of set S where all points orthogonal to v are removed is denoted as $\mathring{S} = S \setminus V^\perp = \{u : u \in S, \langle u, v\rangle \neq 0\}$. As the measure of $V^\perp$ is zero, $\mathring{S}$ has the same measure as S.

The theorem to be proven in the following paragraphs is about v-phasic sets.

Definition 3.1 (v-phasic)**.** *A set S is v-phasic, if $\mathring{S}$ can be defined solely on the argument, also called the phase, of the inner product $\langle u, v\rangle$. That is, S is v-phasic, if there exists a set $\Theta \subseteq [0, 2\pi)$ such that, for any point $u \in S(\mathbb{C}^n) \setminus V^\perp$, it holds that $u \in \mathring{S}$ if and only if $\arg(\langle u, v\rangle) \in \Theta$.*

Lemma 3.9. *A set S is v-phasic if for any $u \in \mathring{S}$ with $\arg(\langle u, v\rangle) = \theta_u$, it holds that $w = r_w e^{i\theta_u} v + \sqrt{1 - r_w^2} v_w^\perp \in \mathring{S}$ for all choices of $r_w \in (0, 1]$ and $v_w^\perp \in V^\perp$*

The alternate description found in Lemma 3.9 can be obtained by using the decomposition of a point as in (3.7b). Indeed, the definitions can be shown to be equivalent by taking $\Theta = \{\arg(\langle u, v\rangle) : u \in \mathring{S}\}$ and noticing $S(\mathbb{C}^n) \setminus V^\perp = \{re^{i\theta} v + \sqrt{1 - r^2} v^\perp : r \in (0, 1], \theta \in [0, 2\pi), v^\perp \in V^\perp\}$.

We aim prove that the supremum of the measure for $e^{i\phi}$-avoiding sets does not decrease by restricting the problem to v-phasic sets. To achieve this, it suffices to show that for any $e^{i\phi}$-avoiding set S, there exist a sequence of feasible v-phasic $e^{i\phi}$-avoiding sets that converge in objective value to a value no less than $\omega(S)$. This is a direct consequence of the following theorem:

Theorem 3.10. *Let $S \subseteq S(\mathbb{C}^n)$ be an $e^{i\phi}$-avoiding set. Then there exists a sequence of v-phasic sets $(S_i)_{i\in\mathbb{N}}$, each avoiding $e^{i\phi}$, such that $\omega(S_i) \to M \geq \omega(S)$. In other words, for every such set S, there exists a v-phasic set avoiding $e^{i\phi}$ whose measure is no less than that of S, up to an arbitrarily small error.*

In the proof for Theorem 3.10, sets must be constructed that avoid inner product $e^{i\phi}$. As $|e^{i\phi}| = 1$, the following equivalence relation is defined to assist in the proof:

$$x \sim y \iff |\langle x, y\rangle| = 1.$$

Its equivalence class $[x]$ is $\{e^{i\theta} x : \theta \in [0, 2\pi)\}$. This can be verified by observing the Cauchy-Schwarz inequality $|\langle x, y\rangle| \leq \|x\|\|y\|$ has equality if and only if y is proportional to x. Furthermore, any point $x \in S(\mathbb{C}^n)$ has $\|x\| = 1$. Lastly, the points $x, y \in S(\mathbb{C}^n)$ are proportional to each other if and only if $y = xe^{i\theta}$ for some $\theta \in [0, 2\pi)$.

Lemma 3.11. *Let P be the partition on $S(\mathbb{C}^n) \setminus V^\perp$ induced by $\sim$. Let $R^* = \{rv + \sqrt{1 - r^2} v^\perp : r \in (0, 1), v^\perp \in V^\perp\}$ and $R = R^* \cup \{v\}$, then R forms a complete set of distinct representatives for P.*

Proof of Lemma 3.11. To prove that each point in R represents a distinct equivalence class, it is sufficient to show for two distinct points $u, w \in R$, that $u \sim w$ if and only if $u = w$. By construction, if $u = v$, then $\langle u, w\rangle = r_w$ which only has magnitude 1 if $w = v$. Let both $v, w \in R^*$ and substitute $\langle v_u^\perp, v_w^\perp\rangle$ by $te^{i\phi}$ to arrive at the formulation for the inner product:

$$\begin{aligned}\langle u, w\rangle &= r_u r_w + t\sqrt{1 - r_u^2}\sqrt{1 - r_w^2} e^{i\phi}, \\ &= (r_u r_w + t\sqrt{1 - r_u^2}\sqrt{1 - r_w^2}\cos(\phi)) + i(t\sqrt{1 - r_u^2}\sqrt{1 - r_w^2}\sin(\phi)).\end{aligned} \tag{3.9}$$

Using the found formulation, the squared magnitude shows $|\langle u, w\rangle| \leq 1$:

$$
\begin{aligned}
|\langle u, w\rangle|^2 =&(r_u r_w)^2 + 2(r_u r_w)(t\sqrt{1-r_u^2}\sqrt{1-r_w^2}\cos(\phi)) + (t\sqrt{1-r_u^2}\sqrt{1-r_w^2})^2,\\
\leq&(r_u r_w)^2 + 2(r_u r_w)(t\sqrt{1-r_u^2}\sqrt{1-r_w^2}) + (t\sqrt{1-r_u^2}\sqrt{1-r_w^2})^2,\\
=&(r_u r_w + t\sqrt{1-r_u^2}\sqrt{1-r_w^2})^2,\\
\leq&(r_u r_w + \sqrt{1-r_u^2}\sqrt{1-r_w^2})^2,\\
\leq&(r_u^2 + (1-r_u^2))^2 = 1.
\end{aligned}
\tag{3.10}
$$

To have $u \sim w$, all three inequalities in (3.10) must attain equality. In order, this implies: $\phi = 0$, $t = 1$ and $r_u = r_w$. The desired inner product $\langle v_u^\perp, v_w^\perp\rangle = te^{i\phi} = 1$ is only attained if $v_u^\perp = v_w^\perp$. All together, this implies all three inequalities attain equality if and only if $u = w$.

To prove R forms a complete set of representatives for P, it suffices to show that for every $w \in S(\mathbb{C}^n)/V^\perp$, there is an $u \in R$ such that $w = e^{i\theta}u$. As $w \in S(\mathbb{C}^n)/V^\perp$, $r_w \in (0, 1]$. If $r_w = 1$, then $w \sim v$ and v is an element of R by construction. If $r_w \in (0, 1)$, then u can be found by investigating the (3.7b) decomposition of w:

$$w = r_w e^{i\theta_w} v + \sqrt{1-r_w^2}v_w^\perp = e^{i\theta_w}(r_w v + \sqrt{1-r_w^2}e^{-i\theta_w}v_w^\perp) = e^{i\theta_w}u \tag{3.11}$$

As $V^\perp$ is closed under multiplication by $e^{i\theta}$, $e^{-i\theta_w}v_w^\perp$ is in $V^\perp$ and therefore u is in R. ■

Proof of Theorem 3.10. Let $S \subseteq S(\mathbb{C}^n)$ be an $e^{i\phi}$-avoiding set and let R be defined as in Lemma 3.11. We define the function $\psi : R \to \mathcal{P}([0, 2\pi))$ by:

$$\psi(x) = \{\theta : \theta \in [0, 2\pi),\ e^{i\theta}x \in S\}. \tag{3.12}$$

Each input x in the domain of the function corresponds to its unique equivalence class $[x]$. The output of the function is the set of arguments of the inner products that points in $S \cap [x]$ make with x. By Lemma 3.11, the input of ψ is a complete set of representatives of the partition of $S(\mathbb{C}^n)/V^\perp$ induced by $\sim$. Consequently, ψ can be used to construct $\mathring{S}$:

$$\bigcup_{x\in R}\{e^{i\theta}x : \theta \in \psi(x)\} = \bigcup_{x\in R}(S \cap [x]) = S \cap (S(\mathbb{C}^n) \setminus V^\perp) = \mathring{S}.$$

As S is $e^{i\phi}$-avoiding, for any choice of $x \in R$ there exists no $\theta, \zeta \in \psi(x)$ such that $e^{i(\theta-\zeta)} = e^{i\phi}$. Therefore, for any choice of input x_0, a set can be constructed using $\psi(x_0)$ that is $e^{i\phi}$-avoiding:

$$
\begin{aligned}
S_{\psi(x_0)} &= \{e^{i\theta}x : \theta \in \psi(x_0),\ x \in R\}\\
&= \{e^{i\theta}(rv + \sqrt{1-r^2}v^\perp) : \theta \in \psi(x_0),\ r \in (0, 1], v^\perp \in V^\perp\}
\end{aligned}
$$

Sets constructed in this way are v-phasic, which can be verified using the description found in Lemma 3.9. Indeed, by decomposing a point u in $S_{\psi(x_0)}$ as $u = e^{i\theta_u}(r_u v + \sqrt{1-r_u^2}v_u^\perp)$, we can see that $\arg(\langle u, v\rangle) = \theta_u$. For $S_{\psi(x_0)}$ to be v-phasic, $w = e^{i\theta_u}r_w v + \sqrt{1-r_w^2}v_w^\perp$ must be in $S_{\psi(x_0)}$ for any choice of r_w and $v_w^\perp$. This follows directly from observing that $w = e^{i\theta_u}(r_w v + \sqrt{1-r_w^2}e^{-i\theta_u}v_w^\perp)$ and that $e^{-i\theta_u}v_w^\perp) \in V^\perp$. Additionally, we see that $S_{\psi(x_0)}$ is $e^{i\phi}$-avoiding as any two points $u, w \in S_{\psi(x_0)}$ have:

$$\langle u, w\rangle \begin{cases} \in e^{\psi(x_0)} & \text{if } u \sim w,\\ < 1 & \text{else.}\end{cases}$$

Due to how the set is built, the measure of the constructed set $S_{\psi(x_0)}$ is equal to the normalized Lebesgue measure of $\psi(x_0)$. This can be observed using the characteristic function of $S_{\psi(x_0)}$ using decomposition (3.7c):

$$\chi_{S_{\psi(x_0)}}(u) = \chi_{\psi(x_0)}(\theta_u)\chi_{(0,1]}(r_u)$$

The measure of the set then follows from the integral (3.8):

$$\begin{aligned}
\omega(S_{\psi(x_0)}) &= \int_{u \in S(\mathbb{C}^n)} \chi_{S_{\psi(x_0)}}(u)\, d\omega(u),\\
&= \int_0^{2\pi}\int_0^1\int_{S(\mathbb{C}^{n-1})} \chi_{\psi(x_0)}(\theta)\,\chi_{(0,1]}(r)\, d\omega_{n-1}(w)\, d\rho(r)\, d\tau(\theta),\\
&= \int_0^{2\pi} \chi_{\psi(x_0)}(\theta)\, d\tau(\theta) = \frac{\lambda(\psi(x_0))}{2\pi}.
\end{aligned}$$

Due to the relation between the surface measure of $S_{\psi(x_0)}$ and the Lebesgue measure of $\psi(x_0)$, optimizing the size of the constructed set can be done by finding x_0 that optimizes the Lebesgue measure of $\psi(x_0)$. By constructing characteristic functions and calculating their integral, we can find an upper bound for the measure of $\mathring{S}$:

$$\begin{aligned}
\chi_{\mathring{S}}(u) &= \chi_{\psi(x_u)}(\theta_u)\chi_R(x_u) = \chi_{\psi(r_u v + \sqrt{1-r_u^2}v_u^\perp)}(\theta_u)\chi_{(0,1]}(r_u),\\
\omega(\mathring{S}) &= \int_{S(\mathbb{C}^n)} \chi_{\mathring{S}}(u)\, d\omega_n(u),\\
&= \int_0^1\int_{S(\mathbb{C}^{n-1})}\int_0^{2\pi} \chi_{\psi(rv+\sqrt{1-r^2}\Phi(w))}(\theta)\chi_{(0,1]}(r)\, d\tau(\theta)\, d\omega_{n-1}(w)\, d\rho(r),\\
&= \int_0^1\int_{S(\mathbb{C}^{n-1})} \frac{\lambda\left(\psi(rv+\sqrt{1-r^2}\Phi(w))\right)}{2\pi}\chi_{(0,1]}(r)\, d\omega_{n-1}(w)\, d\rho(r),\\
&\le \sup_{x\in R}\frac{\lambda(\psi(x))}{2\pi}.
\end{aligned}$$

Equality between the measure $\omega(\mathring{S})$ and the bound $\sup_{x\in R}\lambda(\psi(x))/2\pi$ is only found whenever the subset of all points $U \subseteq R$, where $y \in U$ if and only if $\lambda(\psi(y)) \neq \sup_{x\in R}\lambda(\psi(x))$, has measure 0. Clearly

Using the found measure $\omega(S_{\psi(x_0)})$ and the upper bound for $\omega(\mathring{S})$, the theorem can be proven. If a maximum for $\lambda(\psi(x))$ is achieved at x_0, then $\omega(S_{\psi(x_0)}) = \frac{\lambda(\psi(x_0))}{2\pi} \ge \omega(S)$, proving the theorem. As $\lambda(\psi(x))$ is bounded, if it has a supremum that is not achieved, a sequence of $(x_i)_{i\in\mathbb{N}}$ can be found such that $\omega(S_{\psi(x_i)}) = \frac{\lambda(\psi(x_i))}{2\pi} \to \sup_{x\in R}\frac{\lambda(\psi(x))}{2\pi}$. From the upper bound for $\omega(\mathring{S})$, we know $\omega(\mathring{S}) \le \sup_{x\in R}\frac{\lambda(\psi(x))}{2\pi}$ and therefore this sequence of sets $(S_{\psi(x_i)})_{i\in\mathbb{N}}$ proves the theorem. ■

Theorem 3.12. *Let $n \ge 1$. Then $\alpha(G(S(\mathbb{C}^n), e^{i\phi}))$, the supremum for the surface measure of all $e^{i\phi}$-avoiding sets, is as follows:*

(i) *If $\phi = 2\pi\cdot(p/q)$, where $p, q \in \mathbb{N}$, $gcd(p,q) = 1$, then the supremum is attained. If q is even, then $\alpha(G(S(\mathbb{C}^n), e^{i\phi})) = 1/2$. If q is odd, then $\alpha(G(S(\mathbb{C}^n), e^{i\phi})) = 1/2 - 1/(2q)$.*

(ii) *If ϕ is an irrational multiple of 2π, then $\alpha(G(S(\mathbb{C}^n), e^{i\phi})) = 1/2$.*

Proof of Theorem 3.12. In this proof, we bound $\alpha(G(S(\mathbb{C}^n), e^{i\phi}))$ from above and below. That is, we construct $e^{i\phi}$-avoiding sets and use their measure as lower bound while using Theorem 3.5 to find an upper bound. By Theorem 3.10, we know that limiting the $e^{i\phi}$-avoiding-set problem to v-phasic sets conserves the optimal value. As such, we construct the v-phasic set $S_\Theta = \{e^{i\theta}x : \theta \in \Theta,\ x \in R\}$.

The problem then simplifies to optimizing the Lebesgue measure for $\Theta \subseteq [0, 2\pi)$ under the constraint that S_Θ must be $e^{i\phi}$-avoiding. As $e^{i\theta}$ is periodic over 2π, we likewise work periodically over 2π when discussing Θ or whenever we discuss values denoted as $2\pi \cdot \theta$. To further help notation, we define the shift of an argument by ϕ by the group action $\sigma(2\pi \cdot \theta) = 2\pi \cdot \theta + \phi$.

To prove (i), the construction for the argument set Θ is similar for odd and even q. The forbidden argument is represented in its irreducible form $\phi = 2\pi \cdot (p/q)$. We define the half open intervals

$$I_j = \left[2\pi \cdot \frac{jp}{q},\ 2\pi \cdot \frac{jp+1}{q}\right)$$

for every $j \in \{0, 1, 2, \ldots, q-1\}$. As p and q are co-prime, these intervals are disjoint and $\bigcup_{j=0}^{q-1} I_j = [0, 2\pi)$. If θ is an argument in I_j, then $\sigma(\theta) \in I_{j+1}$ if $j < q-1$ and $\sigma(\theta) \in I_0$ if $j = q-1$. Consequently, if

$$\Theta = \bigcup_{j=0}^{\lfloor q/2 \rfloor - 1} I_{2j+1} = \bigcup_{j=0}^{\lfloor q/2 \rfloor - 1} \left[2\pi \cdot \frac{(2j+1)p}{q},\ 2\pi \cdot \frac{(2j+1)p+1}{q}\right), \tag{3.13}$$

then the v-phasic set S_Θ is $e^{i\phi}$-avoiding with $\omega(S_\Theta) = \lambda(\Theta)/(2\pi) = \lfloor q/2 \rfloor / q$. If q is even, then $\omega(S_\Theta) = 1/2$, while if q is odd, then $\omega(S_\Theta) = 1/2 - 1/(2q)$.

We find an upper bound for $\alpha(G(S(\mathbb{C}^n), e^{i\phi}))$ where $\phi = 2\pi \cdot (p/q)$ by using Theorem 3.5. Let H be the induced subgraph of $G(S(\mathbb{C}^n), e^{i\phi})$ with the vertex set $V = \{v, e^{i\phi}v, \ldots, e^{i(q-1)\phi}v\}$. Then H is a cycle graph with q vertices and $\alpha(H) = \lfloor q/2 \rfloor$. We combine the lower bound $\omega(S_\Theta)$ and the upper bound found using the theorem to find

$$\omega(S_\Theta) = \frac{\lfloor q/2 \rfloor}{q} \leq \alpha(G(S(\mathbb{C}^n), e^{i\phi})) \leq \frac{\lfloor q/2 \rfloor}{q} = \frac{\alpha(H)}{|V|}$$

and therefore $\alpha(G(S(\mathbb{C}^n), e^{i\phi})) = \lfloor q/2 \rfloor / q$ whenever $\phi = 2\pi \cdot (p/q)$.

To prove (ii), we start by constructing a sequence of $e^{i\phi}$-avoiding sets that converge in measure to $1/2$. Let φ be the irrational number such that $\phi = 2\pi \cdot \varphi$. We use argument sets as in (3.13) for even q as a basis and shrink each interval slightly away from the right endpoint to account for the error in estimating the irrational number φ. To describe the kth solution, three parameters are used: p_k and q_k to describe the numerator and denominator of the irreducible fraction used to estimate φ, and ε_k used to describe the factor each interval needs to shrink by to avoid $e^{i\phi}$. Define the jth shrunken intervals of the kth solution as

$$I_{j,k} = \left[2\pi \cdot \frac{jp_k}{q_k},\ 2\pi \cdot \frac{jp_k + 1 - \varepsilon_k}{q_k}\right).$$

By assigning the odd intervals to Θ, the measure of the resulting v-phasic set S_Θ becomes $\omega(S_\Theta) = 1/2 - \varepsilon_k/2$. To complete the proof, we must find appropriate expressions for p_k, q_k and ε_k, such that each resulting set is $e^{i\phi}$-avoiding, $\varepsilon_k \to 0$ as k increases and such that p_k, q_k are co-prime with even q_k.

To find the sequence of parameters, we aim to describe φ by $p_k/q_k + \varepsilon_k/q_k$ with increasingly smaller ε_k. To achieve this, first observe that $A = \{x : x \in [0, 2), m, n \in \mathbb{N}, 2m\varphi = x + 2n\}$ is a dense set on $[0, 2)$ as φ is irrational. This means we can choose a sequence $(x_k)_{k \in \mathbb{N}} \subseteq A$ that converges to 1 from above. If m_k, n_k are the integers for which x_k is found, the initial guesses for the kth parameters become $q'_k = 2m_k$, $p'_k = 2n_k + 1$ and $\varepsilon'_k = q'_k\varphi - p'_k$. These initial guesses might not be valid, as the values q'_k and p'_k are not guaranteed to be co-prime. To resolve this, all parameters are divided by a_k, the greatest common denominator of q'_k and p'_k: $q_k = q'_k/a_k$, $p_k = p'_k/a_k$ and $\varepsilon_k = \varepsilon'_k/a_k$. As q'_k and p'_k are even and odd respectively, a_k is odd and therefore q_k is still even and p_k is still odd. Additionally, the sequence of x_k that the new parameters create still converges to 1 from above, and therefore ε_k converges to 0 from above.

As $\varepsilon_k \to 0$ as k increases and p_k, q_k are co-prime with even q_k, what remains to be proven is that each v-phasic set constructed using the parameters avoids $e^{i\phi}$. It is sufficient to show that $\sigma(I_{j,k})$ does not overlap with an interval $I_{l,k}$ where l has the same parity as j. Remember, each set of parameters is chosen such that $\varphi = p_k/q_k + \varepsilon_k/q_k$. By restating the description of $I_{j,k}$ and finding the description of $\sigma(I_{j,k})$, we can show the desired result:

$$\begin{aligned} I_{j,k} &= \left[2\pi \cdot \frac{jp_k}{q_k},\ 2\pi \cdot \frac{jp_k + 1 - \varepsilon_k}{q_k}\right), \\ \sigma(I_{j,k}) &= \left[2\pi \cdot (\frac{jp_k}{q_k} + \varphi),\ 2\pi \cdot (\frac{jp_k + 1 - \varepsilon_k}{q_k} + \varphi)\right), \\ &= \left[2\pi \cdot \frac{(j+1)p_k + \varepsilon_k}{q_k},\ 2\pi \cdot \frac{(j+1)p_k + 1}{q_k}\right). \end{aligned}$$

As seen from the descriptions, $\sigma(I_{j,k}) \cap \bigcup_{l=0}^{q_k-1} I_{l,k} \subset I_{j+1,k}$. As j and $j+1$ have different parity, the claim is proven and therefore S_Θ avoids $e^{i\phi}$ for each constructed set. Therefore, the found parameters describe a sequence of $e^{i\phi}$-avoiding sets that converge to 1/2 in measure. Let H be the induced subgraph of $G(S(\mathbb{C}^n), e^{i\phi})$ with the vertex set $V = \{v, e^{i\phi}v\}$. H is the complete graph with 2 vertices and $\alpha(H) = 1$. By Theorem 3.5, the measure of a $e^{i\phi}$-avoiding set can be no larger than 1/2 which completes the proof. ■

3.5. Resulting Lovász theta numbers

The optimization problem used to calculate the Lovász theta number is (3.6), which uses the real-valued disk polynomials as a basis for solutions. Due to the simplicity of the problem, we may find the optimal value without using an optimization solver. To show the process of finding the optimal value, we start by introducing the following theorem:

Theorem 3.13. *Let $(\alpha_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ be a feasible solution for problem* (3.6) *on $G(S(\mathbb{C}^n), t)$ with $n \geq 2$ and objective value $\alpha_{0,0}$. There exists $k', \gamma' \in \mathbb{N}$ such that $U^{n-2}_{k',\gamma'}(t) \leq \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$. For any such choice, let $\lambda = U^{n-2}_{k',\gamma'}(t)$ and define $(\alpha'_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ by*

$$\alpha'_{k,\gamma} = \begin{cases} \frac{-\lambda}{1-\lambda} & \text{if } (k,\gamma) = (0,0), \\ \frac{1}{1-\lambda} & \text{if } (k,\gamma) = (k',\gamma'), \\ 0 & \text{else.} \end{cases} \tag{3.14}$$

Then $(\alpha'_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ is a feasible solution for problem (3.6) *on $G(S(\mathbb{C}^n), t)$ and objective value $\alpha'_{0,0} \geq \alpha_{0,0}$.*

Proof. First we show that there exists $k', \gamma' \in \mathbb{N}$ such that $U^{n-2}_{k',\gamma'}(t) \leq \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$. Assume there is no such k', γ' and therefore $U^{n-2}_{k,\gamma}(t) > \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$ for all $k, \gamma \in \mathbb{N}$. As $(\alpha_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ is a feasible solution,

$$\sum_{k,\gamma\in\mathbb{N}, 0<k+\gamma} \alpha_{k,\gamma} = \big(\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma}\big) - \alpha_{0,0} = 1 - \alpha_{0,0},$$

$$\sum_{k,\gamma\in\mathbb{N}, 0<k+\gamma} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t) = \big(\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t)\big) - \alpha_{0,0} = -\alpha_{0,0}.$$

As $\alpha_{k,\gamma} \geq 0$, $\sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma}$ converges absolutely to $1-\alpha_{0,0}$ as $M \to \infty$. Additionally, $U^{n-2}_{k,\gamma}(t) \in [-1,1]$ shows that

$$\sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} |\alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t)| \leq \sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma}$$

and consequently $\sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t)$ converges absolutely to $-\alpha_{0,0}$ as $M \to \infty$. By describing $\frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$ in terms of the two series and using the assumption that $U^{n-2}_{k,\gamma}(t) > \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$, we find the following:

$$\begin{aligned}
\frac{-\alpha_{0,0}}{1-\alpha_{0,0}} &= \frac{\lim_{M\to\infty} \sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(t)}{\sum_{k,\gamma\in\mathbb{N},0<k+\gamma} \alpha_{k,\gamma}}, \\
&> \frac{\lim_{M\to\infty} \sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma} \left(\frac{-\alpha_{0,0}}{1-\alpha_{0,0}}\right)}{\sum_{k,\gamma\in\mathbb{N},0<k+\gamma} \alpha_{k,\gamma}}, \\
&= \frac{-\alpha_{0,0}}{1-\alpha_{0,0}} \left(\frac{\lim_{M\to\infty} \sum_{k,\gamma\in\mathbb{N},0<k+\gamma\leq M} \alpha_{k,\gamma}}{\sum_{k,\gamma\in\mathbb{N},0<k+\gamma} \alpha_{k,\gamma}} \right) = \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}.
\end{aligned}$$

This is a contradiction and therefore shows that there exists $k', \gamma' \in \mathbb{N}$ such that $U^{n-2}_{k',\gamma'}(t) \leq \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$.

To complete the proof, let k', γ' be such that $U^{n-2}_{k',\gamma'}(t) \leq \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$. We must show that $(\alpha'_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ is a feasible solution for the problem (3.6) and $\alpha'_{0,0} \geq \alpha_{0,0}$. As $(\alpha_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ is a feasible solution, $\alpha_{0,0} \geq 0$ and consequently $\lambda = U^{n-2}_{k',\gamma'}(t) \leq 0$. It follows that $\alpha'_{k,\gamma} \geq 0$ for all $k, \gamma \in \mathbb{N}$. Next, observe that $\sum_{k,\gamma\in\mathbb{N}} \alpha'_{k,\gamma} = \alpha'_{0,0} + \alpha'_{k',\gamma'} = 1$. To finish showing $(\alpha'_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ is a feasible solution, observe that

$$\sum_{k,\gamma\in\mathbb{N}} \alpha'_{k,\gamma} U^{n-2}_{k,\gamma}(t) = \alpha'_{0,0} + \alpha'_{k',\gamma'}\lambda = \frac{-\lambda}{1-\lambda} + \frac{1}{1-\lambda}\lambda = 0.$$

To show $\alpha'_{0,0} \geq \alpha_{0,0}$, first observe that $\frac{-x}{1-x} \geq \frac{-y}{1-y}$. whenever $x \leq y \leq 0$. Let $x = \lambda$ and $y = \frac{-\alpha_{0,0}}{1-\alpha_{0,0}}$. By construction $x \leq y \leq 0$, which results in the desired inequality:

$$\alpha'_{0,0} = \frac{-x}{1-x} \geq \frac{-y}{1-y} = \alpha_{0,0}. \qquad \blacksquare$$

Corollary 3.14. *Let $n \geq 2$ and $t \in \overline{\mathbb{D}} \setminus \{1\}$. Let $\lambda^* = \inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(t)$ and $\vartheta(G(S(\mathbb{C}^n), t))$ be the optimal value of problem (3.6), then $\vartheta(G(S(\mathbb{C}^n), t)) = \frac{-\lambda^*}{1-\lambda^*}$. Additionally, there exists $k', \gamma' \in \mathbb{N}$ such that $U^{n-2}_{k',\gamma'}(t) = \lambda^*$ if and only if there exist a feasible solution $(\alpha_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ for (3.6) such that $\alpha_{0,0} = \vartheta(G(S(\mathbb{C}^n), t))$.*

Proof. Due to Theorem 3.13, we know that we only need to consider solutions of the form (3.14). The objective function of such a solution is $\frac{-\lambda'}{1-\lambda'}$. Therefore we have the following relation between the optimal value $\vartheta(G(S(\mathbb{C}^n), t))$ and $\lambda^* = \inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(t)$:

$$\vartheta(G(S(\mathbb{C}^n), t)) = \sup_{k,\gamma\in\mathbb{N}} \frac{-U^{n-2}_{k',\gamma'}(t)}{1-U^{n-2}_{k',\gamma'}(t)} = \frac{-\inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k',\gamma'}(t)}{1-\inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k',\gamma'}(t)} = \frac{-\lambda^*}{1-\lambda^*}.$$

The second statement follows clearly. If there exists $k', \gamma' \in \mathbb{N}$ such that $U^{n-2}_{k',\gamma'}(t) = \lambda^*$, then the solution of the form (3.14) for those parameters is feasible with objective value $\frac{-\lambda^*}{1-\lambda^*}$. If there exists a feasible solution $(\alpha_{k,\gamma})_{k,\gamma\in\mathbb{N}}$ for (3.6) such that

$\alpha_{0,0} = \vartheta(G(S(\mathbb{C}^n), t))$, then there exist $k', \gamma' \in \mathbb{N}$ such that

$$\lambda^* = \inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(t) \le U^{n-2}_{k',\gamma'}(t) \le \frac{-\vartheta(G(S(\mathbb{C}^n), t))}{1-\vartheta(G(S(\mathbb{C}^n), t))} = \lambda^*,$$

due to Theorem 3.13. ■

3.5.1. 0-avoiding. For $t = 0$, we were able to express the optimal value and a corresponding solution in closed form. We start by finding $\min_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(0)$. Observe that

$$U^{n-2}_{k,\gamma}(0) = 0^\gamma\, \widetilde{P}^{(n-2,\gamma)}_k(-1) = \begin{cases} (-1)^k \binom{k+n-2}{k}^{-1} & \text{if } \gamma = 0, \\ 0 & \text{else.} \end{cases}$$

Clearly, $U^{n-2}_{k,\gamma}(0) < 0$ if and only if k is odd and $\gamma = 0$. Additionally, the minimum value $-\frac{1}{n-1}$ can be found at $(k,\gamma) = (1,0)$ for all $n \ge 2$. Due to Corollary 3.14, the solution where each coefficient is 0 except for $\alpha_{0,0} = \frac{1}{n}$ and $\alpha_{1,0} = \frac{n-1}{n}$ is optimal with objective value $\frac{1}{n}$.

In comparison to the lower bound $(\frac{1}{2})^{n-1}$ found by the double-cap conjecture, the found bound is tight only for $n = 2$. For $n \ge 3$, the relative gap between the lower bound and upper bound becomes grows with n.

3.5.2. $e^{i\phi}$-avoiding. Whenever $t = e^{i\phi}$, we were able to express the solutions and optimal values for the Lovász theta number like we did for $t = 0$. We again use Corollary 3.14 As $|t| = 1$, all disk polynomials simplify to $U^{n-2}_{k,\gamma}(e^{i\phi}) = \cos(\gamma\phi)$.

If ϕ is not a rational multiple of 2π, then $\inf_{\gamma\in\mathbb{N}} \cos(\gamma\phi) = -1$ yet the infimum is not attained. Consequently the optimal value is $1/2$ but there is no feasible solution that attains that objective value.

For rational multiples of 2π, ϕ can be be described by its irreducible fraction: $2\pi\cdot\frac{p}{q}$. If q is even, the disk polynomial with parameters $(k,\gamma) = (0, q/2)$ is minimal as $U^{n-2}_{0,q/2}(e^{i\phi}) = \inf_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(e^{i\phi}) = -1$ and results in a solution with objective value $\frac{1}{2}$. If q is odd, then there exists $\gamma' \in \mathbb{N}$ such that $\gamma'\frac{p}{q} = \frac{q+1}{2q} + m$ for some $m \in \mathbb{N}$. Using the disk polynomial with parameters $(0, \gamma')$ then results in an optimal solution with objective value:

$$\vartheta(G(S(\mathbb{C}^n), e^{i\phi})) = \frac{-\cos(2\pi\cdot\frac{q+1}{2q})}{1-\cos(2\pi\cdot\frac{q+1}{2q})} = \frac{\cos(\frac{\pi}{q})}{1+\cos(\frac{\pi}{q})}.$$

In comparison to the sets found for Theorem 3.12, the upper bounds found are tight for irrational multiples of 2π and rational multiples of 2π with even denominator. For $\phi = 2\pi\cdot\frac{p}{q}$ and q odd, the bound is tight for $q = 3$. For other odd q, we aim to show:

$$\vartheta(G(S(\mathbb{C}^n), e^{i\phi})) = \frac{\cos(\frac{\pi}{q})}{1+\cos(\frac{\pi}{q})} > \frac{q-1}{2q} = \alpha(G(S(\mathbb{C}^n), e^{i\phi})).$$

Which is only valid if $\cos(\frac{\pi}{q}) > \frac{q-1}{q+1}$. This can be proven by using a bound obtained from Maclaurin series for $\cos(\theta)$: $\cos(\theta) \ge 1 - \frac{\theta^2}{2}$.

$$\begin{aligned} \cos(\frac{\pi}{q}) \ge 1 - \frac{\pi^2}{2q^2} &> \frac{q-1}{q+1}, \\ \iff \frac{2}{q+1} &> \frac{\pi^2}{2q^2}, \\ \iff \frac{4q^2}{q+1} &> \pi^2, \end{aligned}$$

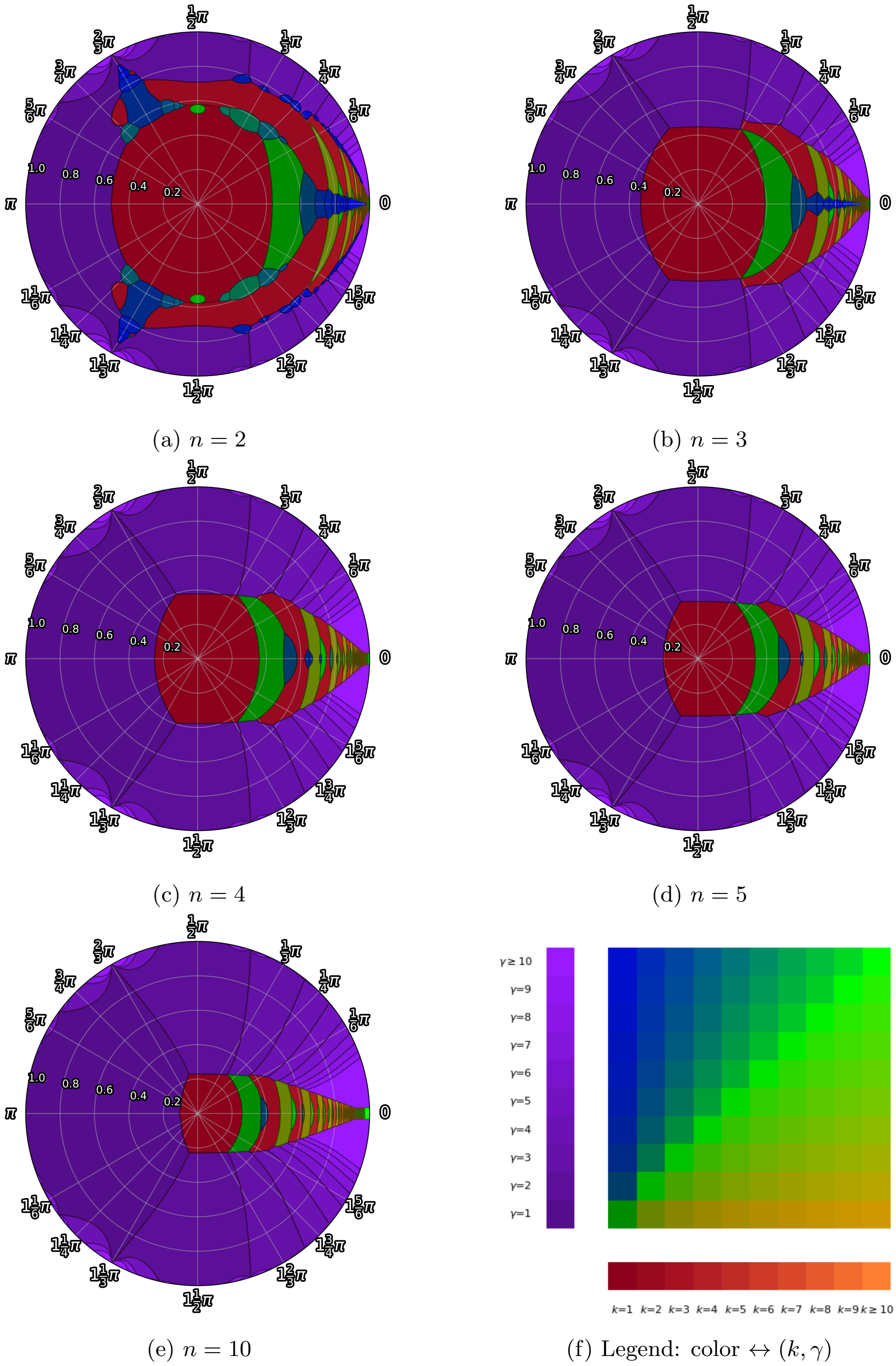
which holds for $q \geq 5$ as desired, so the upper bound does not match the lower bound for those q. The ratio between $\alpha(G(S(\mathbb{C}^n), e^{i\phi}))$ and $\vartheta(G(S(\mathbb{C}^n), e^{i\phi}))$ matches the ratio between the independence number and Lovász theta number for C_q, the cycle graph with q vertices. Indeed, the independence number and Lovász theta number are exactly the independence number and Lovász theta number for C_q after applying the normalization factor $1/q$. This result is a consequence of the graph representation for the $e^{i\phi}$-avoiding-set problem is comprised of uncountable many disconnected graphs, where each graph is a cycle with q vertices.

3.5.3. General t-avoiding. For the remaining values for t, we did not find a closed form expression for the Lovász theta number. Instead, we evaluate $\inf_{k,\gamma} U_{k,\gamma}^{n-2}(t)$ for a dense grid $t_{j,\ell} = r_j e^{i\phi_\ell}$ with r_j uniformly spaced in $(0,1)$ and ϕ_ℓ uniformly spaced in $[0, 2\pi)$. We can only evaluate finitely many disk polynomials. To ensure a found disk polynomial is minimal, we use the following method: As $0 < r_j < 1$, the disk polynomials converge to 0 as $k + \gamma \to \infty$ (see Appendix A.1). Let $\beta_{k,\gamma}$ be an upper bound on $|U_{k,\gamma}^{n-2}(t)|$ like the ones found in Corollary A.3. For any finite $P \subseteq \mathbb{N}^2$ let $P^C = \mathbb{N}^2 \setminus P$ and $\beta_{P^C} = \sup_{(k,\gamma)\in P^C} \beta_{k,\gamma}$. For every $t_{j,\ell}$, we iteratively expand the parameter set P until $\min_{k,\gamma\in P} U_{k,\gamma}^{n-2}(t) < -\beta_{P^C}$. Any parameter set P where the inequality holds ensures that the minimum value for the disk polynomials in P is the minimum value for all disk polynomials.

In the following parts, graphs will be displayed on the unit disk, where the parameters for the minimal disk polynomial are color coded by their type: purely based on k, purely based on γ and a combination of k and γ. The color coding for all those graphs is consistent and can be found in the following legend: The two dimensional case is a special case when it comes to finding the minimal polynomial as observed in Figure 1a. There are areas around $\arg(t) = \pm\frac{2}{3}\pi$, where polynomials with mixed parameters are minimal. These polynomials have a relatively high parameter γ. For $n \geq 3$, the minimal polynomials are for these areas is $U_{0,1}^{n-2}(t)$ with a value around $|t|\cos(\frac{2}{3}\pi) = -|t|/2$. For $n = 2$, the minimal polynomials are instead found whenever γ is an integer multiple of 3, where the Jacobi polynomials cause the disk polynomials to be negative.

For complex dimension $n \geq 3$, a consistent shape starts to emerge when looking at the graphs:

A shape similar to that of a fountain pen tip describes the domain of inner products with nonzero k. Additionally the shape gets less wide as the dimension increases. The shape getting less wide can be attributed to the Jacobi polynomial being the only part of the disk polynomial affected by the dimension.



(a) $n = 2$ (b) $n = 3$

(c) $n = 4$ (d) $n = 5$

(e) $n = 10$ (f) Legend: color $\leftrightarrow (k, \gamma)$

FIGURE 1. For each dimension n, panels (a)–(e) show, for every $t \in \overline{\mathbb{D}}$, parameter pairs $(k, \gamma) \in \mathbb{N}^2$ that achieve the global minimum $\min_{k,\gamma\in\mathbb{N}} U^{n-2}_{k,\gamma}(t)$. Colors encode the selected pair (k, γ) according to the legend in panel (f). When multiple parameter pairs achieve the same minimum, ties are broken by choosing the pair with smallest k, and if still tied, with smallest γ.

CHAPTER 4

The Boolean quadric polytope

To improve the upper bound on the measure of t-avoiding sets, we extend the formulation for the Lovász theta number by introducing additional constraints. To ensure that the extension remains an upper bound for the measure of t-avoiding sets, there must be a construction of feasible solutions from t-avoiding sets that attains equality between objective value and measure. In this chapter, we discuss one such set of constraints: the *Boolean quadric polytope (BQP)* set of constraints introduced by DeCorte, de Oliveira Filho and Vallentin [3].

The Boolean quadric polytope induced by a finite set V is defined as

$$\mathrm{BQP}(V) = \mathrm{conv}\big\{xx^T : x \in \{0,1\}^V\big\}.$$

For a kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ and a finite subset $V \subseteq S(\mathbb{C}^n)$, we use the notation $A(V,V)$ for the matrix constructed as $(A(u,v))_{u,v\in V}$. The BQP constraint set for the t-avoiding Lovász theta number is induced by a finite subset $V \subset S(\mathbb{C}^n)$ and restricts the problem to the kernels $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$ where $A(V,V) \in \mathrm{BQP}(V)$.

In this chapter, we first show that for every set on $S(\mathbb{C}^n)$, an invariant kernel can be constructed that satisfies any BQP constraint. Next, we introduce an alternate formulation for the Lovász theta number, in order to add the BQP set of constraints. To complete the setup of the extended formulation, we describe practical methods for selecting the finite subsets of $S(\mathbb{C}^n)$ that induce the BQP constraints. Finally, we report the optimal objective values obtained from the extended formulation and quantify the improvement in the resulting upper bounds relative to the previous results.

4.1. The BQP constraints for sets on $S(\mathbb{C}^n)$

To gain an understanding on what the Boolean quadric polytope constraint set enforces on kernels, we show the relation between the BQP constraints and kernels constructed from sets on $S(\mathbb{C}^n)$. Let S be any measurable set on $S(\mathbb{C}^n)$, we will use the previously discussed kernel

$$A(u,v) = \int_{U(n)} \chi_S(Tu)\chi_S(Tv)\, d\mu(T)$$

for the remainder of this section. Recall, this construction of a kernel has $A(u,u) = \omega(S)$ for all $u \in S(\mathbb{C}^n)$ and can be thought of as the joint probability $\Pr(Tu \in S \text{ and } Tv \in S)$ for a random $T \in U(n)$ chosen according to the Haar probability measure μ.

To show $A(V,V) \in \mathrm{BQP}(V)$ for any finite $V \subset S(\mathbb{C}^n)$, let $x_W \in \{0,1\}^V$ be the characteristic vector of the subset $W \subseteq V$. Then, the statement $A(V,V) \in \mathrm{BQP}(V)$ is equivalent to

$$A(V,V) = \sum_{W\subseteq V} \lambda_W x_W x_W^T$$

where $\lambda_W \geq 0$ and $\sum_{W\subseteq V} \lambda_W = 1$. One can verify that for any $u, v \in V$, $Tu, Tv \in S$ if and only if there exists $W \subseteq V$ such that $u, v \in W$ and $TV \cap S = TW$. Using this information, we find that the coefficients

$$\lambda_W = \Pr(TV \cap S = TW) = \int_{U(n)} \prod_{u \in V \setminus W} \big(1 - \chi_S(Tu)\big) \cdot \prod_{u \in W} \chi_S(Tu)\, d\mu(T)$$

define $A(V, V)$ as a convex combination of the vertices of $\mathrm{BQP}(V)$. Indeed, we see the coefficients λ_W are nonnegative and sum to 1. Additionally, we verify $A(V, V) = \sum_{W \subseteq V} \lambda_W\, x_W\, x_W^T$ as we find equality for each element of $A(V, V)$ indexed by $u, v \in V$:

$$\begin{aligned} A(u, v) &= \Pr(Tu \in S \text{ and } Tv \in S), \\ &= \sum_{W \subseteq V} \mathbf{1}_{u,v \in W}\ \Pr(TV \cap S = TW) = \big(\sum_{W \subseteq V} \lambda_W\, x_W\, x_W^T\big)_{u,v}. \end{aligned}$$

4.2. The extended t-avoiding Lovász-theta number

In the previous chapter, solutions for the Lovász theta number were kernels that had the property $A(u, u) = 1$. However, as these kernels are generally not in $\mathrm{BQP}(V)$, a new formulation must be constructed using a different normalization. The normalization must be such that the invariant characteristic kernel of the t-avoiding set S with $A(u, u) = \omega(S)$ is a feasible solution. We derive the new formulation using a different formulation for the Lovász theta number on a finite graph $G = (V, E)$. Let $W = \{\xi\} \cup V$ and $\mathcal{S}^W$ be the cone of symmetric matrices in $\mathbb{R}^{W \times W}$. The used formulation for the Lovász theta number on finite graphs is as follows:

$$\max_{Y \in \mathcal{S}^W} \left\{ \sum_{u \in V} Y_{uu} : Y \succeq 0, Y_{\xi\xi} = 1, Y_{\xi u} = Y_{uu} \quad \forall u \in V, Y_{uv} = 0 \quad \forall (u, v) \in E \right\}.$$

The conversion to kernels is done similarly to before. As on the finite case To account for the extension of the kernel with the extra coordinate ξ, we define B, the extension of the invariant positive continuous kernel $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$. Its domain is $\big(\{\xi\} \cup S(\mathbb{C}^n)\big) \times \big(\{\xi\} \cup S(\mathbb{C}^n)\big)$ and the values for B follow the constraints: for $u, v \in S(\mathbb{C}^n)$, $B(\xi, \xi) = 1$, $B(\xi, u) = B(u, \xi) = A(u, u)$ and $B(u, v) = A(u, v)$. As A is a positive invariant continuous kernel, there are the nonnegative weights $\alpha_{k,\gamma}$ such that $A(u, v) = \sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, v \rangle)$. To ensure that B is positive definite, we check using the Schur complement: B is a positive definite-kernel if 1 is invertible and positive semidefinite and the kernel

$$C(u, v) = \sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, v \rangle) - \big(\sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, u \rangle)\big)^2$$

is positive definite. Clearly, 1 is invertible and positive semidefinite. As C is an invariant kernel in $L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$, it is positive definite if and only if the coefficients $\alpha'_{k,\gamma}$ for the disk polynomial decomposition of C are nonnegative. One can verify that $\alpha'_{0,0} = \alpha_{0,0} - (\sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma})^2$ and $\alpha'_{k,\gamma} = \alpha_{k,\gamma}$ elsewhere. For $k, \gamma \in \mathbb{N}$ where $k + \gamma \geq 1$, we see that $\alpha'_{k,\gamma} \geq 0$ as A is positive definite. Then the statement $\alpha'_{0,0} \geq 0$ is equivalent to

$$\begin{pmatrix} 1 & \sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} \\ \sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} & \alpha_{0,0} \end{pmatrix} \succeq 0,$$

which is the constraint that will be used for normalization in the optimization problem. The invariant characteristic kernels induced by sets S used in this section have $\sum_{k,\gamma \in \mathbb{N}} \alpha_{k,\gamma} = \omega(S)$ and $\alpha_{0,0} = \omega(S)^2$ and therefore satisfy the constraints.

To add the set of BQP constraints induced by the set V to the invariant kernel A, we enforce that $A(V, V)$ is a convex sum of vertices of $\mathrm{BQP}(V)$. As seen previously this can be done element-wise, which leads to the formulation for the extended Lovász theta number:

$$\begin{aligned} \sup\ & \textstyle\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} \\ & f(t) = 0, \\ & \begin{pmatrix} 1 & \sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} \\ \sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} & \alpha_{0,0} \end{pmatrix} \succeq 0, \\ & f(\langle u,v\rangle) = \textstyle\sum_{W\subseteq V} \lambda_W \mathbf{1}_{u,v\in W} \quad \forall u,v\in V, \\ & \textstyle\sum_{W\subseteq V} \lambda_W = 1, \\ & f = \textstyle\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}, \\ & \lambda,\alpha \geq 0. \end{aligned} \tag{4.1}$$

Due to the increased complexity of the problem, the process of finding optimal solutions is not as straightforward as finding the values for the original Lovász theta number. We instead use optimization software to find solutions. When implementing the optimization problem into the software, we have to limit the amount of variables included. Due to the increased complexity and the limited amount of variables, we are no longer able to guarantee that the objective value of a solution is optimal or an upper bound for the independence number.

To guarantee that the final objective value remains an upper bound, we first formulate the dual of the problem such that any feasible solution of the problem is an upper bound. Next we further restrict the dual while changing it to a problem with finitely many constraints, instead of infinite. As a result of this process, any feasible solution of the final problem is guaranteed to be an upper bound for the t-avoiding-set problem.

We start by formulating the dual. Let the primal be the problem with the set of BQP constraints induced by the point set V. Then the dual is:

$$\begin{aligned} \inf\ & z_1 + \nu \\ & \begin{pmatrix} z_1 & -z_2/2 \\ -z_2/2 & -z_3 \end{pmatrix} \succeq 0, \\ & z_2 + z_3 + \mu_t + \textstyle\sum_{u,v\in V} \mu_{uv} \geq 1, \\ & z_2 + \mu_t U^{n-2}_{k,\gamma}(t) + \textstyle\sum_{u,v\in V} \mu_{uv} U^{n-2}_{k,\gamma}(\langle u,v\rangle) \geq 1 \quad \forall (k,\gamma)\in\mathbb{N}^2\setminus\{(0,0)\}. \\ & \nu - \textstyle\sum_{u,v\in W} \mu_{uv} \geq 0 \quad \forall W\subseteq V. \end{aligned}$$

Next we restrict the dual by limiting the constraints to those in a finite parameter set P and introducing a constraint that is stronger than the constraints that are not included. Let P^C be the parameters not included in P, that is $P^C = \{(k,\gamma) : (k,\gamma)\in\mathbb{N}^2, (k,\gamma)\notin P\}$. As seen in Appendix A.1, we can calculate upper bounds for $|U^{n-2}_{k,\gamma}(z)|$ for all $(k,\gamma)\in P^C$ where $z = t$ or $z = \langle u,v\rangle$ for $u,v\in V$. Let ε_t and ε_{uv} be the calculated bounds. Then satisfying the inequality

$$z_2 - |\mu_t|\,\varepsilon_t - \sum_{u,v\in V, u\neq v} |\mu_{uv}|\,\varepsilon_{u,v} + \sum_{u\in V} \mu_{uu} \geq 1$$

is sufficient for satisfying each constraint in P^C. By replacing all constraints in P^C with the above inequality, we create the following restriction:

$$\begin{aligned} \inf\ & z_1 + \nu \\ & \begin{pmatrix} z_1 & -z_2/2 \\ -z_2/2 & -z_3 \end{pmatrix} \succeq 0, \\ & z_2 + z_3 + \mu_t + \textstyle\sum_{u,v\in V} \mu_{uv} \geq 1, \\ & z_2 + \mu_t U^{n-2}_{k,\gamma}(t) + \textstyle\sum_{u,v\in V} \mu_{uv} U^{n-2}_{k,\gamma}(\langle u,v\rangle) \geq 1 \quad (k,\gamma)\in P\setminus\{(0,0)\}, \\ & z_2 - |\mu_t|\,\varepsilon_t - \textstyle\sum_{u,v\in V, u\neq v} |\mu_{uv}|\,\varepsilon_{u,v} + \sum_{u\in V} \mu_{uu} \geq 1, \\ & \nu - \textstyle\sum_{u,v\in W} \mu_{uv} \geq 0 \quad \forall W\subseteq V. \end{aligned} \tag{4.2}$$

Any feasible solution for truncated dual is a feasible solution for the original dual. Therefore the objective value of any feasible solution for 4.2 is an upper bound for the measure of t-avoiding sets. As this formulation only has finitely many constraints and variables, this restriction is implementable and is used to calculate the reported upper bounds in the end of this chapter. For a relaxation of the primal that has only finitely many variables, see Appendix A.5.

4.3. Finding point sets for the BQP constraints

To complete the implementation of the BQP constraint set, we outline methods for finding point sets from which to construct the polytope. In this section, we focus on the 3 categories of non-deterministic methods: random vertex choice, vertex choice based on lower bound solution and vertex choice by facet violation.

4.3.1. Random point set. To start, we focus on the simplest approach where the vertices are randomly selected, independent of previous solutions. The methods outlined here use the continuous uniform distribution $U(a, b)$ as a basis for determining the values for coordinates of points. Let $R_1, R_2, \ldots, R_{n-1}$ be realizations of $U(0, 1)$ and $\Theta_1, \Theta_2, \ldots, \Theta_n$ be realizations of $U(0, 2\pi)$. A method constructs a new point v for the set V using an orthonormal basis $\{b_1, b_2, .., b_n\}$ through an iterative process. Let v_k be the resulting vector at kth step in the iteration which is defined as

$$v_k = \sum_{j=1}^{k} \alpha_j e^{i\Theta_k} b_j = \alpha_k e^{i\Theta_k} b_k + v_{k-1},$$

where $v_0 = 0$ and $v_n = v$. To determine α_k for $k < n$, each method introduces a function on R_k and v_{k-1}. For $k = n$, each method fixes $\alpha_n = \sqrt{1 - \|v_{n-1}\|^2}$ to ensure $v \in S(\mathbb{C}^n)$.

The first method is to choose points uniformly random on the sphere according to the surface measure. To do this, we derive the quantile function of the radial measure ρ_m for zonal functions on $S(\mathbb{C}^m)$. As $\rho_m(r) = 2(m-1)r(1-r^2)^{m-2}$, we can integrate ρ_m over the interval $[0, r]$ to find its cumulative density function $F_m(r) = 1-(1-r^2)^{m-1}$. For any $1 <= k < n$, the vector $u_k = \begin{pmatrix} \alpha_k & \alpha_{k+1} & \ldots & \alpha_n \end{pmatrix}^T$ lies on the sphere in $\mathbb{C}^{n-k+1}$ with radius $\sqrt{1 - \|v_{k-1}\|^2}$. As $u_k/\sqrt{1 - \|v_{k-1}\|^2} \in S(\mathbb{C}^m)$, we use the cumulative density function $F(\alpha_k/\sqrt{1 - \|v_{k-1}\|^2})$ for α_k. Then finally the quantile function can be derived to construct the points according to the surface measure:

$$\alpha_j = Q_j(R_j, v_{j-1}) = \sqrt{1 - \|v_{j-1}\|^2}\sqrt{1 - (1 - R_j)^{1/(n-j+1)}}.$$

The second of such methods constructs the vector by applying the realization directly to the remaining radius, that is $\alpha_k = R_k \sqrt{1 - \|v_{k-1}\|^2}$. The bias in this method causes inner products with larger magnitudes to be more likely than when choosing points uniformly random according to the surface measure.

4.3.2. Weighted using lower bound. If there exists a conjectured optimal solution for the t-avoiding-set problem, then the invariant kernel constructed from that solution can be used for the construction of BQP point sets. We form the hypothesis that using larger and better point sets to induce the BQP constraints will cause the optimal solutions for the Lovász theta number to converge to the conjectured maximal t-avoiding set. Based on that hypothesis, we construct a method where we choose point sets such that the inner products are more likely to be where kernels from the Lovász theta number and the t-avoiding-set problem have large differences.

By creating a characteristic kernel for the t-avoiding set S, we can find the coefficients $\alpha^{(S)}_{k,\gamma}$ for the disk polynomial decomposition for the invariant kernel according to Appendix A.4. After solving a relaxed version of the Lovász theta number, we use the solution's coefficients $\alpha^{(\vartheta)}_{k,\gamma}$ to create a difference kernel. The coefficients for the difference kernel are $\alpha^{(\Delta)}_{k,\gamma} = \alpha^{(\vartheta)}_{k,\gamma} - \alpha^{(S)}_{k,\gamma}$. Finally, the kernel is squared to ensure nonnegative values, which results in the invariant kernel described by the zonal function

$$C(\langle u, v\rangle) = \Big(\sum_{k,\gamma\in\mathbb{N}} \alpha^{(\Delta)}_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, v\rangle)\Big)^2 = \sum_{k,\gamma\in\mathbb{N}} \alpha^{(C)}_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, v\rangle).$$

The real disk polynomial $U^{n-2}_{k,\gamma}(z)$ consists of two complex disk polynomials, the first of degree $k+\gamma$ in z and k in $\overline{z}$ and the second the other way around. Therefore, if there exists an $N \in \mathbb{N}$ such that all nonzero coefficients $\alpha^{(\Delta)}_{k,\gamma}$ have $2k + \gamma \le N$, then all nonzero coefficients $\alpha^{(C)}_{k,\gamma}$ have $2k + \gamma \le 2N$.

To create the point set, we use an iterative process similar to the method used when constructing random point sets, independent of previous solutions. Let $B = \{b_1, b_2, \dots, b_n\}$ be the orthonormal basis used. While creating the mth point v_m, the inner products with $v_1, v_2, \dots v_{k-1}$ will be accounted for, where $k = \min\{m, n\}$. During the lth iteration step, we find the complex coefficient $\alpha_{m,l} \in \overline{\mathbb{D}}$. The coefficient is then used to create the vector

$$w_{m,l} = \sum_{j=1}^{l} \alpha_{m,j} b_j = \alpha_{m,l} b_k + w_{m,l-1},$$

where $w_{m,0} = 0$ and after the kth step, we set $w_{m,k} = v_m$.

Let $R_1, R_2, \dots, R_{k-1}$ be realizations of $U(0,1)$ and $\Theta_1, \Theta_2, \dots, \Theta_k$ be realizations of $U(0,1)$. To find the v_ms coefficient for b_l, first observe the function

$$f(r, \theta, m, l) = C\Big(\langle w_{m,l-1}, v_l\rangle + \alpha_{l,l}\, r e^{i\theta}\sqrt{1 - \|w_{m,l-1}\|^2}\Big)$$

with $r \in [0,1]$ and $\theta \in [0, 2\pi)$. This function calculates all possible values for $C(\langle v_m, v_l\rangle)$ given that $\alpha_{m,j}$ is fixed for $j < l$ and undetermined for $j \ge l$. Using $f(r, \theta, m, l)$ and the realization R_l and Θ_l, we use the following equations to find $\alpha_{m,l}$:

$$R_l = \frac{\int_0^x \int_0^{2\pi} f(r, \theta, m, l) \cdot r \, d\theta \, dr}{\int_0^1 \int_0^{2\pi} f(r, \theta, m, l) \cdot r \, d\theta \, dr},$$

$$\Theta_l = \frac{\int_0^\phi f(x, \theta, m, l) \, d\theta}{\int_0^{2\pi} f(x, \theta, m, l) \, d\theta}.$$

By using numerical integration, the first equation is solved to find x and afterwards the second equation is solved to find ϕ. We set v_ms coefficient for the basis vector b_l to $\alpha_{m,l} = x e^{i\phi}\sqrt{1 - \|w_{m,l-1}\|^2}$. For $l = k$, we set $x = 1$ to ensure that $v_m \in S(\mathbb{C}^n)$ and to ensure that $\alpha_{m,l} = 0$ for $m < l \le n$.

4.3.3. Facet-violation optimization. The final BQP set construction method tested is by optimizing the set such that a previous solution for the Lovász theta number is cut as much as possible by adding the BQP constraint set. In other words, we aim to find the BQP set V such that its constraint set is maximally violated by the kernel of the previous solution A. In the formulation for Lovász theta number, inclusion of $A(V, V)$ in the polytope is verified by proving $A(V, V)$ is a convex combination of vertices. However, as optimizing for that constraint set presents implementation issues, we instead optimize for a maximal violation of a facet inequality.

Facet inequalities can be used as an alternative way to verify if $A(V,V)$ is in $BQP(V)$. A facet of $BQP(V)$ is described by the matrix scalar pair (F,β), where every point W in BQP(V) has $\langle F, W\rangle \leq \beta$.

To optimize violation of this facet inequality, we use a non-linear optimizer to solve the following non-linear program with $A \in L^2(S(\mathbb{C}^n) \times S(\mathbb{C}^n))$, the previous solution for the Lovász theta number:

$$\begin{aligned} \max\ & \langle F, A(V,V)\rangle - \beta \\ & u \in S(\mathbb{C}^n) \quad \forall u \in V. \end{aligned}$$

The set V only removes the kernel A from the feasible solutions if the objective value is strictly positive. Additionally, the solver is not guaranteed to find a global maximum for any given facet F, due to non-linearity of the problem. Therefore, to ensure a large violation, we run the program multiple times with different starting guesses for V and for multiple facets. Each of the starting guesses for V can be found using one of the previous methods.

4.4. Results from the extended Lovász-theta problem

The results are separated into 3 categories for forbidden inner product t. Firstly $t = e^{i\phi}$, which has a special BQP set construction such that optimal value equals the maximum measure of an $e^{i\phi}$-avoiding set. Secondly $t = 0$, to thoroughly investigate the Witsenhausen's problem. Lastly, we run the problem for general t to investigate the relation between the value of t and the improvement for the Lovász theta number that can be expected by adding the BQP set of constraints. In general for each test, the primal problem was solved in order to construct BQP sets and the dual problem was used to calculate the reported upper bounds.

4.4.1. $e^{i\phi}$-avoiding. As seen previously, the Lovász theta number matches the maximum measure for most values of ϕ. The only values where equality is not attained are whenever ϕ is a rational multiple of 2π, specifically when $\phi = \frac{p}{q}2\pi$ where q is odd and $q >= 5$. The graph representation for those values consists of infinitely many disconnected q-cycles C_q. Therefore, by selecting V to be one of the cycles, the BQP constraint set implicitly encodes the independence-number problem on C_q into the formulation for the Lovász theta number. Indeed, let $V = \{v, e^{i\phi}v, \ldots, e^{i(q-1)\phi}v\}$ with the edge set E, then the primal is bounded from above by:

$$\begin{aligned} \sup\ & \mathrm{Tr}\big(A(V,V)\big)/|V| \\ & A(u,w) = 0 \qquad \forall (u,w) \in E, \\ & A(V,V) = \textstyle\sum_{W \subseteq V} \lambda_W x_W x_W^T \\ & \textstyle\sum_{W \subseteq V} \lambda_W = 1 \\ & \lambda \geq 0, \\ & A(V,V) \in \mathbb{R}^{V \times V} \quad \text{and is invariant under } \mathrm{Aut}(C_q). \end{aligned}$$

This has an optimal value of $\frac{q-1}{2q}$ which matches the previously found maximal measure of an $e^{i\phi}$-avoiding set.

4.4.2. 0-avoiding. We may use our study of the 0-avoiding-set problem to further strengthen the bound given by the extended Lovász theta number and reduce the size of the optimization problem. Due to Theorem 3.6, we know that we may restrict the 0-avoiding-set problem to sets that are closed under multiplication by $e^{i\theta}$. For any set with this property, the corresponding solution of (4.1) has $\alpha_{k,\gamma} = 0$ whenever $\gamma \neq 0$. Consequently, the formulation for the primal problem

(4.1) may be restricted to the disk polynomials where $\gamma = 0$ while ensuring that the optimal value remains an upper bound for the 0-avoiding-set problem. Similarly, the formulation for the corresponding dual only needs to include the constraints where $\gamma = 0$. The objective value of any feasible solution for this dual remains an upper bound for the 0-avoiding-set problem.

The final benefits obtained through Theorem 3.6 are observed for the truncated dual and the truncated primal. We define the parameter set $P = \{(k, 0) : k \in \mathbb{N}, k \leq N\}$ for some $N \in \mathbb{N}$. The set of excluded parameters is $P^C = \{(k, 0) : k \in \mathbb{N}, k > N\}$. Let $\beta_{k,\gamma}(r)$ be the best bound on $|U^{n-2}_{k,\gamma}(re^{i\theta})|$ obtained by Corollary A.3. As the bounds decrease as k grows, we find

$$\varepsilon_t = \sup_{(k,\gamma)\in P^C} \beta_{k,\gamma}(|t|) = \beta_{N+1,0}(|t|) \quad \text{and}$$
$$\varepsilon_{uv} = \sup_{(k,\gamma)\in P^C} \beta_{k,\gamma}(|\langle u, v\rangle|) = \beta_{N+1,0}(|\langle u, v\rangle|).$$

These bounds are significantly smaller than ones that would be found for a parameter set of the same size if the problem had not been restricted to parameters where $\gamma = 0$.

For every dimension, multiple tests were run for each BQP construction method. Due to the double-cap conjecture, we can use the point set construction based on a lower bound solution. The coefficients used for the construction are those found for the double-cap in Appendix A.4. To find the best upper bound possible, each test was constructed using 4 BQP sets, each containing 18 points. For facet optimization, the size of sets is limited to 6 points per set. To get around that limitation, the sets used to induce the constraints were constructed by generating 3 batches 6 points and taking the union of each batch to construct the BQP set. The results of the test are shown in Table 1 and Table 2.

As seen in Table 2, facet-violation optimization is likely to produce the best results given the same limitations. The closest contender is point generation based on the lower bound, in this case the double cap set. Interestingly, the point set generation based on DC was consistently the best on $n = 8$. That is, all 3 tests run resulted in a lower objective value than the best found through facet-violation optimization.

One of the limitations of the extended Lovász theta number is the size and number of BQP sets able to be used in the solver before running out of memory.

n	$\omega(DC)$ (2^{1-n})	Basic upper bound $(1/n)$	Improved upper bound	Rel. size of new gap
3	0.25	0.333333...	0.290007	48.0%
4	0.125	0.25	0.204317	63.4%
5	0.0625	0.2	0.159185	70.3%
6	0.03125	0.166666...	0.130311	73.2%
7	0.015625	0.142857...	0.110344	74.4%
8	0.0078125	0.125	0.097712	76.7%

TABLE 1. Lower and upper bounds for the supremum of measures for 0-avoiding sets on $S(\mathbb{C}^n)$. The lower bound $\omega(DC)$ is the measure of the double cap set. The basic upper bound is obtained by solving the Lovász theta number for $t = 0$. The improved upper bound is the lowest objective value found using the dual of the extended truncated Lovász theta number. Let x be the basic upper bound and y the improved upper bound, then the relative size of the new objective gap is $(y - \omega(DC))(x - \omega(DC))$.

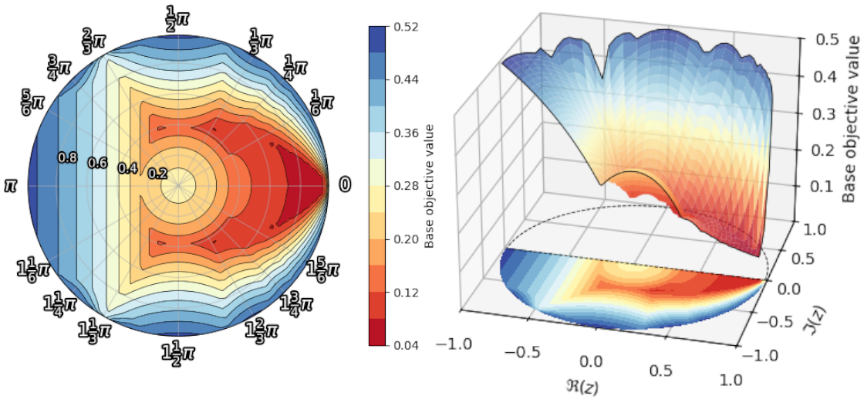
n	Coordinate wise	Uniform w.r.t. ω	weighted by DC	Facet Violation
3	0.293737	0.298155	0.290342	0.290007
4	0.214649	0.221557	0.205532	0.204317
5	0.173107	0.168669	0.160470	0.159185
6	0.141118	0.148623	0.130429	0.130311
7	0.124083	0.127917	0.113130	0.110344
8	0.110000	0.121244	0.097712	0.102607

Table 2. Objective values for different methods of constructing 4 BQP sets of 18 points each. For the facet-violation optimization method, the points were instead generated in batches of 6 to get around the size limitation.

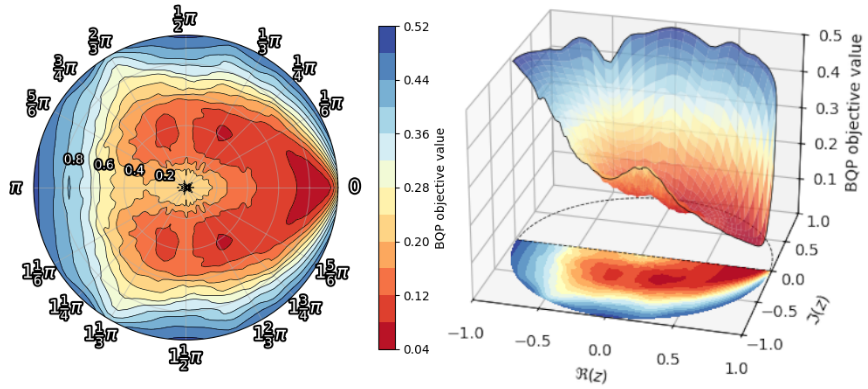
The memory limitation is a consequence of the dual having a constraint for every $W \subseteq V$. Therefore, there are at least $2^{|V|}$ constraints due to the BQP constraint set. The second limitation is the size of sets generated through facet-violation optimization. As the method can only generate point sets of at most 6, the point set generation had to be done in multiple small batches for each BQP set. The drawback of this construction is that the inner products between batches are not accounted for during facet-violation optimization.

4.4.3. General t-avoiding. In addition to the extensive tests run for $t = 0$, we also performed smaller tests for t on a representative subset of the unit disk $\overline{\mathbb{D}}$. The tests were run on $S(\mathbb{C}^4)$ to balance computational efficiency with a diverse set of parameters used in optimal solutions for the original Lovász theta number. Computational efficiency decreases for lower values of n due to slower convergence to 0, while solutions for the original Lovász theta number are primarily constructed using disk polynomials with $k = 0$ for larger values of n. Each test is performed with a single BQP set of size 6 using the biased point set construction where the realizations are applied directly coordinate-wise. The objective values of the t-avoiding Lovász theta number without and with the BQP set added are shown in Figure 1a and Figure 1b respectively.

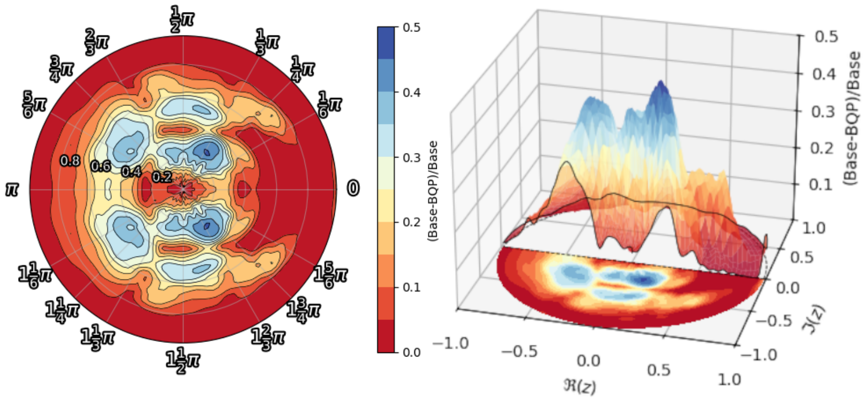
As seen in Figure 1c, the extended formulation significantly lowers the objective value for lower values of $|t|$. These areas have a large overlap with the areas where solutions for the original Lovász theta number are primarily constructed using disk polynomials with $k \leq 1$. It is unclear how much, if any, of the behavior is due to the small size of the BQP sets. For large values of $|t|$, we observed no significant changes, which matches our expectations. Since the $e^{i\phi}$-avoiding set problem and the corresponding Lovász theta number only have a small difference in optimal value, we expect similar behavior for values of t close to $e^{i\phi}$.



(a) $\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); \emptyset)$



(b) $\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); V)$



(c) $\dfrac{\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); \emptyset) - \vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); V)}{\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); \emptyset)}$

FIGURE 1. Effect of adding BQP constraints (induced by vertex sets V with $|V| = 6$) to the truncated dual formulation of the t-avoiding Lovász theta number on $S(\mathbb{C}^4)$. The panels (a) and (b) show the respective optimal values of the truncated dual with no BQP constraints, $\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); \emptyset)$, and with the BQP constraints induced by V, $\vartheta_{\mathrm{tr}}(G(S(\mathbb{C}^4), t); V)$. The panel (c) shows the relative reduction in objective value.

APPENDIX A

Appendix

This chapter is reserved for derivations and proofs obtained in the process of researching the subject, but not directly relevant to understanding the core findings in the thesis. Section A.1 proves that disk polynomials converge to 0 pointwise as the parameters $k + \gamma \to \infty$. This is done by finding converging bounds for the disk polynomials. Section A.2 derives the normalized measure for zonal functions on $S(\mathbb{C}^n)$ using the normalized measure of the first coordinate on $S(\mathbb{R}^n)$. Next, in Section A.3, a version of the Funk-Hecke theorem is found for real-valued disk polynomials. Finally, in Section A.4, the Funk-Hecke theorem is used to find the disk polynomial decomposition for characteristic kernels, with extra attention given to the double-cap set.

A.1. Convergence of the disk polynomials

In this section, we prove that the disk polynomials pointwise converge to 0 as the parameters $k + \gamma \to \infty$. This is done by finding bounds on $U_{k,\gamma}^{n-2}(z)$ and investigating the rate of their convergence. The bounds are of the form $|U_{k,\gamma}^{n-2}(z)| \leq d(z, n-2)/f(k, \gamma, n-2)$. Of the found bounds, the strongest growth of the divisor f is of order $\mathcal{O}\big(k^{n/2-1} + (k+\gamma)^{n/2-3/4}\big)$. The bounds on the disk polynomials are derived from bounds on the Jacobi polynomials and on the function:

$$g_k^{(\alpha,\beta)}(x) = \left(\frac{\Gamma(k+1)\Gamma(k+\alpha+\beta+1)}{\Gamma(k+\alpha+1)\Gamma(k+\beta+1)}\right)^{1/2} \left(\frac{1-x}{2}\right)^{\alpha/2} \left(\frac{1+x}{2}\right)^{\beta/2} P_k^{(\alpha,\beta)}(x)$$

To express the relation between this function and the disk polynomials, let $\alpha = n-2$, $\beta = \gamma$ and $x = 2r^2 - 1$. By accounting for normalization of the Jacobi polynomial, we find the expression:

$$g_k^{(n-2,\gamma)}(2r^2-1) = \left(\frac{\Gamma(k+n-1)\Gamma(k+n+\gamma-1)}{\Gamma(k+1)\Gamma(n-1)^2\Gamma(k+\gamma+1)}\right)^{1/2} (1-r^2)^{n/2-1} U_{k,\gamma}^{n-2}(r)$$

Haagerup and Schlichtkrull [5] found two bounds on $g_k^{(\alpha,\beta)}(x)$. The first bound is stated in the following theorem by Haagerup and Schlichtkrull. The bound is particularly useful to prove convergence of disk polynomials $n = 2$.

Theorem A.1. *There is a constant $C < 12$ such that*

$$|(1-x^2)^{1/4} g_k^{(\alpha,\beta)}(x)| \leq \frac{C}{(2k+\alpha+\beta+1)^{1/4}}$$

for all $x \in [-1, 1]$, $\alpha, \beta \geq 0$ and $k \in \mathbb{N}$.

The second bound is again found in [5] and compiled into the following Lemma by Koornwinder [7]. The bound is useful for practical applications, especially when $|x| \to 1$.

Lemma A.2.

$$|g_k^{(\alpha,\beta)}(x)| \leq \left(\frac{(k+1)(k+\alpha+\beta+1)}{(k+\alpha+1)(k+\beta+1)}\right)^{1/4} \leq 1$$

for all $x \in [-1, 1]$ *and* $\alpha, \beta, k \in \mathbb{N}$.

By using the relation between $g_k^{(\alpha,\beta)}(x)$ and the disk polynomials, we find the following bounds:

Corollary A.3. *There exists a constant* $C < 12$ *such that the disk polynomial* $U_{k,\gamma}^{n-2}(re^{i\theta})$ *is bounded by:*

$$|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq \frac{C \cdot c(k,\gamma,n)}{(1-r^2)^{n/2-1}\left(4\left(2k+\gamma+n-1\right)(r^2-r^4)\right)^{1/4}} \tag{A.1}$$

and

$$|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq \frac{c(k,\gamma,n)}{(1-r^2)^{n/2-1}}\left(\frac{(k+1)(k+\gamma+n-1)}{(k+n-1)(k+\gamma+1)}\right)^{1/4} \leq \frac{c(k,\gamma,n)}{(1-r^2)^{n/2-1}} \tag{A.2}$$

with

$$c(k,\gamma,n) = \left(\binom{k+n-2}{n-2}\binom{k+\gamma+n-2}{n-2}\right)^{-1/2}$$

for all $r \in (0,1)$*,* $\theta \in [0, 2\pi]$*,* $n \in \mathbb{N}$ *where* $n \geq 2$*, and* $k, \gamma \in \mathbb{N}$.

The function $c(k,\gamma,n)$ converges to 0 for $n \geq 3$ where the denominator grows with a rate of order $\mathcal{O}(k^{n/2-1}(k+\gamma)^{n/2-1} + \gamma^{n/2-1})$ and the remaining terms of both inequalities are bounded by a constant. Therefore, $U_{k,\gamma}^{n-2}(z)$ also converges to 0 with a rate of at least order $\mathcal{O}(k^{n/2-1}(k+\gamma)^{n/2-1} + \gamma^{n/2-1})$. For $n = 2$, we use the first inequality to show that $U_{k,\gamma}^{n-2}(z)$ converges to 0 with a rate of order $\mathcal{O}(\sqrt{k+\gamma})$. To show that the bounds are decreasing as the parameters increase, we introduce the following claim

Claim A.4. *Define* $\beta_{k,\gamma}(r)$ *as the best bound on* $|U_{k,\gamma}^{n-2}(re^{i\theta})|$ *obtained by Corollary A.3. Let* $k_0, \gamma_0, k', \gamma' \in \mathbb{N}$*. If* $k' \geq k_0$ *and* $\gamma' \geq \gamma_0$*, then*

$$|U_{k',\gamma'}^{n-2}(re^{i\theta})| \leq \beta_{k',\gamma'}(r) \leq \beta_{k_0,\gamma_0}(r).$$

for all $r \in (0,1)$*,* $\theta \in [0, 2\pi]$*,* $n \in \mathbb{N}$ *where* $n \geq 2$.

PROOF. It suffices to show that $f(k) = \left(\frac{k+1}{k+n-1}\right)^{1/4} / \binom{k+n-2}{n-2}^{1/2}$ is non increasing as k increases, as all the remaining terms in either bound are clearly non increasing as k or γ increases. By investigating the ratio between $f(k+1)$ and $f(k)$, we find

$$\frac{f(k+1)}{f(k)} = \frac{\left(\frac{k+2}{k+n}\right)^{1/4} / \left(\frac{k+1}{k+n-1}\right)^{1/4}}{\binom{k+n-1}{n-2}^{1/2} / \binom{k+n-2}{n-2}^{1/2}} = \left(\frac{(k+2)(k+1)^2}{(k+1)(k+n)(k+n-1)}\right)^{1/4} \leq 1,$$

for all $k \in \mathbb{N}$ which completes the proof. ∎

To complete the set of magnitudes for which we have bounds, we look at $r = 1$ and $r = 0$. Let $n \geq 1$ and $r = 1$, then the bound $|U_{k,\gamma}^{n-2}(e^{i\theta})| \leq 1$ is used for all $k, \gamma \in \mathbb{N}$. Let $n \geq 1$ and $r = 0$, we know that $|U_{k,\gamma}^{n-2}(0)| = 0$ for $\gamma \geq 1$ and $|U_{k,\gamma}^{n-2}(0)| = 1/\binom{k+n-2}{n-2}$ elsewhere. Therefore we use the bound $|U_{k,\gamma}^{n-2}(0)| \leq 0^\gamma / \binom{k+n-2}{n-2}$ which converges to 0 as $k + \gamma \to \infty$ if $n \geq 3$.

The bounds in Corollary A.3 converge slowly as γ grows whenever k and n are small. For such k and n, it is desirable to bounds that converge faster. We find a bound on $|U_{k,\gamma}^{n-2}(z)|$ that holds for fixed k and for all $\gamma \geq N$, where $N \in \mathbb{N}$. All of the following bounds are found by constructing a function $f : \mathbb{R}_+ \times [0,1) \to \mathbb{R}$ where $f(\gamma, r) \geq |\widetilde{P}_k^{(n-2,\gamma)}(2r^2-1)|$ for all $\gamma \in N$. Next, find the smallest $M \geq N$

where $\frac{\partial(r^\gamma f(\gamma,r))}{\partial\gamma} \leq 0$ for all $\gamma \geq M$. Then $|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq r^M f(M,r)$ for all $\gamma \geq N$. A simple example function that holds for all $k \in \mathbb{N}$ and $N \geq n-2$ is

$$f(\gamma, r) = |\widetilde{P}_k^{(n-2,\gamma)}(-1)| = \frac{\Gamma(k+\gamma+1)\Gamma(n-1)}{\Gamma(\gamma+1)\Gamma(k+n-1)}.$$

Here M is the smallest $M \geq N$ where $\sum_{j=1}^{k} \frac{1}{M+j} \leq -\ln(r)$. Then, for all $\gamma \geq N$, $|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq r^M |\widetilde{P}_k^{(n-2,M)}(-1)|$.

As the bounds converge especially slow whenever k is very small, custom bounds are made for $k \leq 2$. For $k = 0$ the best possible bound is $|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq r^N$ for all $\gamma \geq N$. For $k = 1$, the Jacobi polynomial is bounded as $|\widetilde{P}_1^{(n-2,\gamma)}(2r^2-1)| \leq \frac{\gamma+1}{n-1} + (1 - \frac{\gamma+1}{n-1})r^2$. Let $M = \max\{N, -(\ln(r)^{-1} + 1 + \frac{(n-1)r^2}{1-r^2})\}$, then $|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq r^M(\frac{M+1}{n-1} + (1 - \frac{M+1}{n-1})r^2)$ for all $\gamma \geq N$. Finally, for $k = 2$ and $N \geq n-2$, the Jacobi polynomial is bounded as $|\widetilde{P}_2^{(n-2,\gamma)}(2r^2-1)| \leq 1 + (\frac{(\gamma+1)(\gamma+2)}{n(n-1)} - 1)(1-r^2)^2$. Similarly to $k = 1$, let

$$M = \max\{N, \frac{-(3 + \frac{2}{\ln(r)}) + \sqrt{D}}{2} \text{ if } D \geq 0, 0 \text{ else}\},$$
$$D = (2n+1)^2 + \frac{4}{\ln(r)^2} - \frac{4(n^2-n)}{(1-r^2)^2},$$

then $|U_{k,\gamma}^{n-2}(re^{i\theta})| \leq r^M(1 + (\frac{(M+1)(M+2)}{n(n-1)} - 1)(1-r^2)^2)$ for all $\gamma \geq N$.

For different methods, we need to construct a parameter set P such that the bounds are at most $\varepsilon > 0$. To quickly determine a P whenever $n \geq 3$, start by determining the largest radius r_0 for which the bounds need to be calculated. We determine a cut-off value N to construct the parameter set by

$$P = \left\{(k+\gamma) : k, \gamma \in \mathbb{N}, k < N, \gamma < \frac{N^2 - k^2}{\max\{1, k\}}\right\}$$

Using the bounds in Corollary A.3, we can determine a sufficient cut-off value such that $U_{k,\gamma}^{n-2}(z) < \varepsilon$ for all $r \leq r_0$, $(k, \gamma \in \mathbb{N}^2 \setminus P$ by

$$N = \frac{\left((n-2)!/\varepsilon\right)^{1/(n-2)}}{\sqrt{1-r_0^2}}.$$

This method for constructing P works for all $r_0 \in [0,1)$ due to the bounds found earlier for $r = 0$.

A.2. Alternate derivation of measure for zonal spherical functions

In this section we find a normalized measure ν_n on $\overline{\mathbb{D}}$ such that

$$\int_{S(\mathbb{C}^n)} f(\langle u, v\rangle)\, d\omega_n(u) = \int_{\overline{\mathbb{D}}} f(z)\, d\nu_n(z)$$

for every zonal spherical function f with pole v. The derivation uses the normalized measure η_n for the first coordinate x_1 on $S(\mathbb{R}^n)$ as a basis. We use the following formulation for η_n on $S(\mathbb{R}^n)$:

$$d\eta_n(x_1) = \frac{\Gamma(\frac{n}{2})}{2\sqrt{\pi}\Gamma(\frac{n-1}{2})}(1-x_1^2)^{(n-1)/2}\, dx_1. \tag{A.3}$$

To find ν_n, first observe that the measure is invariant under choice of v as the surface measure is invariant under the unitary group $U(n)$. Indeed, for any

$T \in U(n)$ where $Tv = \mathbf{e}_1$:

$$\int_{S(\mathbb{C}^n)} f(\langle u, v\rangle)\, d\omega(u) = \int_{S(\mathbb{C}^n)} f(\langle Tu, Tv\rangle)\, d\omega(u) = \int_{S(\mathbb{C}^n)} f(\langle Tu, \mathbf{e}_1\rangle)\, d\omega(u)$$
$$= \int_{S(\mathbb{C}^n)} f(\langle u, \mathbf{e}_1\rangle)\, d\omega(T^{-1}u) = \int_{S(\mathbb{C}^n)} f(\langle u, \mathbf{e}_1\rangle)\, d\omega(u).$$

Therefore, we assume for the remainder of this section that the pole for the zonal function is $\mathbf{e}_1$ without loss of generality. This means we calculate the measure with respect to the first coordinate of u.

We will show in the following paragraphs is that the measure of u with respect to the first coordinate is equal to:

$$d\nu_n(\langle u, \mathbf{e}_1\rangle = re^{\theta}) = d\tau(\theta) \cdot d\rho_n(r),$$
$$= \big(\frac{1}{2\pi}\, d\theta\big) \cdot \big(2(n-1)r(1-r^2)^{n-2}\, dr\big).$$

As mentioned, we use the normalized measure for the first coordinate η_n on $S(\mathbb{R}^n)$ as a basis. Therefore, we use a parametrization of $u \in S(\mathbb{C}^n)$ on $\hat{u} \in S(\mathbb{R}^{2n})$. Let u be $(u_1 + iu_2, u_3 + iu_4, ..., u_{2n-1} + iu_{2n})$, we define $\hat{u}$ as $(x_1, x_2, ..., x_{2n})$. The measure with respect to the first coordinate of u is then the same as the measure with respect to the first two coordinates of $\hat{u}$. That is

$$d\nu_n(x_1 + ix_2) = d\eta_{2n}(x_1, x_2) = d\eta_{2n}(x_1)\, d\eta_{2n}(x_2|x_1).$$

The measure of the first coordinate $d\eta_{2n}(x_1)$ can be directly obtained from (A.3). To find the conditional measure of the second coordinate with fixed first coordinate $d\eta_{2n}(x_2|x_1)$, observe that $\hat{u}_{2:2n} = (x_2, x_3, ..., x_{2n})$ is on the sphere with radius $\sqrt{1-x_1^2}$ in $\mathbb{R}^{2n-1}$. Consequently, $d\eta_{2n}(x_2|x_1)$ can be found by scaling $\hat{u}_{2:2n}$ by a factor $1/\sqrt{1-x_1^2}$ to find:

$$d\eta_{2n}(x_2|x_1) = \frac{1}{\sqrt{1-x_1^2}}\, d\eta_{2n-1}\left(\frac{x_2}{\sqrt{1-x_1^2}}\right),$$
$$= \frac{\Gamma(n-\frac{1}{2})}{\sqrt{1-x_1^2}\sqrt{\pi}\Gamma(n-1)}\left(1 - \frac{x_2^2}{1-x_1^2}\right)^{n-2} dx_2.$$

Finally the zonal measure $\nu(x_1 + ix_2)$ can be obtained by multiplying the measure of the first coordinate by the measure of the second coordinate with fixed first coordinate.

$$d\nu_n(x_1 + ix_2) = d\eta_{2n}(x_1, x_2) = d\eta_{2n}(x_1) \cdot d\eta_{2n}(x_2|x_1),$$
$$= \left(\frac{\Gamma(n)}{\sqrt{\pi}\Gamma(n-1/2)}(1-x_1^2)^{n-3/2}\, dx_1\right) \cdot d\eta_{2n}(x_2|x_1),$$
$$= \frac{\Gamma(n-\frac{1}{2})\Gamma(n)}{\pi\Gamma(n-1)\Gamma(n-\frac{1}{2})}(1-x_1^2)^{n-2}\left(1 - \frac{x_2^2}{1-x_1^2}\right)^{n-2} dx_1\, dx_2,$$
$$= \frac{1}{2\pi} \cdot 2(n-1)(1-x_1^2-x_2^2)^{n-2}\, dx_1\, dx_2,$$

Lastly we need to change from Cartesian representation of the first complex coordinate $x_1 + ix_2$ to its polar representation $r_1e^{i\theta_1}$ by applying the appropriate change of variables:

$$d\nu_n(r_1e^{i\theta_1}) = r_1\, d\nu_n\big(r_1\cos(\theta_1) + ir_1\sin(\theta_1)\big),$$
$$= \big(\frac{1}{2\pi}\, d\theta_1\big) \cdot \big(2(n-1)r_1(1-r_1^2)^{n-2}\, dr_1\big) = d\tau(\theta_1) \cdot d\rho_n(r_1).$$

The measures τ and ρ_n separate ν_n into parts for θ and r such that $\tau([0, 2\pi)) = 1$ and $\rho_n([0, 1]) = 1$.

A.3. Funk-Hecke for real-valued disk polynomials

Before showing the process of calculating the coefficients for a characteristic kernel, a version of the Funk-Hecke theorem must be formulated for the real-valued disk polynomials. To accomplish this, we first state the Funk-Hecke theorem for complex harmonics and the addition formula for complex-valued disk polynomials. Let $\mathcal{H}_{p,q}(S(\mathbb{C}^n))$ be the space of complex spherical harmonics, as outlined in [13]. The dimension of the space $\mathcal{H}_{p,q}$ is the finite number

$$d(p,q) = (p+q+n-1)\frac{(p+n-2)!(q+n-2)!}{p!q!(n-1)!(n-2)!}.$$

Let ω be the surface measure on $S(\mathbb{C}^n)$ normalized such that $\omega(S(\mathbb{C}^n)) = 1$. The set $\{Y^j_{p,q} : j = 1, 2, \ldots, d(p,q)\}$ will denote an orthonormal basis of $\mathcal{H}_{p,q}$ with respect to the inner product

$$(f,g) = \int_{S(\mathbb{C}^n)} f(u)g(u)\, d\omega(u),$$

for $f, g \in L^2(S(\mathbb{C}^n))$. Finally, let ν be the measure on $\overline{\mathbb{D}}$ for $S(\mathbb{C}^n)$-zonal functions such that

$$d\nu(re^{i\theta}) = \Big(\frac{1}{2\pi}\, d\theta\Big)\Big(2(n-1)r(1-r^2)^{n-2}\, dr\Big).$$

Then the addition formula and Funk-Hecke formula for the complex-valued disk polynomials are as follows:

Lemma A.5 (Addition Formula [13])**.** *Let $n \geq 2$, then*

$$R^{n-2}_{p,q}(\langle u, v\rangle) = \frac{1}{d(p,q)} \sum_{j=1}^{d(p,q)} Y^j_{p,q}(u) Y^j_{p,q}(v)$$

for all $p, q \in \mathbb{N}$.

Theorem A.6 (Funk-Hecke Formula [13])**.** *For $Y(u) \in \mathcal{H}_{p,q}(S(\mathbb{C}^n))$ and complex function with pole v $K(\langle u, v\rangle)$ we have*

$$\int_{S(\mathbb{C}^n)} K(\langle u, v\rangle)\overline{Y(u)}\, d\omega(u) = \lambda_{p,q}\overline{Y(v)},$$

where

$$\lambda_{p,q} = \langle K, R^{n-2}_{p,q}\rangle = \int_{\overline{\mathbb{D}}} K(z)\overline{R^{n-2}_{p,q}(z)}\, d\nu(z).$$

Using the two theorems, we can immediately find the following corollary.

Corollary A.7. *For the disk polynomial $R^{n-2}_{p,q}(\langle u, w\rangle)$ and the complex function with pole v $K(\langle u, v\rangle)$ we have*

$$\int_{S(\mathbb{C}^n)} K(\langle u, v\rangle)\overline{R^{n-2}_{p,q}(\langle u, w\rangle)}\, d\omega(u) = \lambda_{p,q}\overline{R^{n-2}_{p,q}(\langle v, w\rangle)},$$

where

$$\lambda_{p,q} = \langle K, R^{n-2}_{p,q}\rangle = \int_{\overline{\mathbb{D}}} K(z)\overline{R^{n-2}_{p,q}(z)}\, d\nu(z).$$

Proof. This follows directly from observing that for fixed $w \in S(\mathbb{C}^n)$ the disk polynomial $R^{n-2}_{p,q}(\langle u, w\rangle)$ is the complex spherical harmonic $Y(u) \in \mathcal{H}_{p,q}(S(\mathbb{C}^n))$ with the coefficients $a_j = \overline{Y^j_{p,q}(w)}/d(p,q)$. Indeed, by the addition formula:

$$R^{n-2}_{p,q}(\langle u, w\rangle) = \sum_{j=1}^{d(p,q)} \frac{\overline{Y^j_{p,q}(w)}}{d(p,q)} Y^j_{p,q}(u) = \sum_{j=1}^{d(p,q)} a_j Y^j_{p,q}(u) = Y(u). \qquad \blacksquare$$

Theorem A.8. *For the real-valued disk polynomial $U_{k,\gamma}^{n-2}(\langle u,w\rangle)$ and the zonal function with pole v $K(\langle u,v\rangle)$. If $K(z)=K(\overline{z})$ for all $z\in\overline{\mathbb{D}}$, then*

$$\int_{S(\mathbb{C}^n)} K(\langle u,v\rangle)\overline{U_{k,\gamma}^{n-2}(\langle u,w\rangle)}\,d\omega(u)=\Lambda_{k,\gamma}\overline{U_{k,\gamma}^{n-2}(\langle v,w\rangle)},$$

where

$$\Lambda_{k,\gamma}=\langle K,U_{k,\gamma}^{n-2}\rangle=\int_{\overline{\mathbb{D}}}K(z)\overline{U_{k,\gamma}^{n-2}(z)}\,d\nu(z).$$

Additionally, $\Lambda_{k,\gamma}\in\mathbb{R}$ whenever $K(z)\in\mathbb{R}$ for all $z\in\overline{\mathbb{D}}$.

To prove this theorem, we first describe how some properties of the zonal function K affect $\langle K,R_{p,q}^{n-2}\rangle$:

Lemma A.9. *Let $K(\langle u,v\rangle)$ be a square-integrable zonal function on $S(\mathbb{C}^n)$ with pole v. Then the following statements hold for all $p,q\in\mathbb{N}$:*

(i) *If $K(z)=K(\overline{z})$ for all $z\in\overline{\mathbb{D}}$, then $\langle K,R_{p,q}^{n-2}\rangle=\langle K,R_{q,p}^{n-2}\rangle$.*
(ii) *If $K(z)\in\mathbb{R}$ for all $z\in\overline{\mathbb{D}}$, then $\langle K,R_{p,q}^{n-2}\rangle=\overline{\langle K,R_{q,p}^{n-2}\rangle}$.*
(iii) *If $\overline{K(z)}=K(\overline{z})$ for all $z\in\overline{\mathbb{D}}$, then $\langle K,R_{p,q}^{n-2}\rangle\in\mathbb{R}$.*

Proof of Lemma A.9. Observe that $R_{p,q}^{n-2}(\overline{z})=\overline{R_{p,q}^{n-2}(z)}=R_{q,p}^{n-2}(z)$ for all $z\in\overline{\mathbb{D}}$ and for all $p,q\in\mathbb{N}$.
(i) If $K(z)=K(\overline{z})$ for all $z\in\overline{\mathbb{D}}$, then

$$\langle K,R_{p,q}^{n-2}\rangle=\int_{\overline{\mathbb{D}}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)=\int_{\overline{\mathbb{D}}}K(\overline{z})\overline{R_{q,p}^{n-2}(\overline{z})}\,d\nu(z)=\langle K,R_{q,p}^{n-2}\rangle.$$

(ii) If $K\in\mathbb{R}$ for all $z\in\overline{\mathbb{D}}$, then $K(z)=\overline{K(z)}$ and consequently

$$\overline{\langle K,R_{q,p}^{n-2}\rangle}=\overline{\int_{\overline{\mathbb{D}}}K(z)\overline{R_{q,p}^{n-2}(z)}\,d\nu(z)}=\int_{\overline{\mathbb{D}}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)=\langle K,R_{p,q}^{n-2}\rangle.$$

(iii) Let $\overline{\mathbb{D}}^{>}=\{z:z\in\overline{\mathbb{D}},\Im(z)>0\}$ and $\overline{\mathbb{D}}^{<}=\{z:z\in\overline{\mathbb{D}},\Im(z)<0\}$. If $\overline{K(z)}=K(\overline{z})$ for all $z\in\overline{\mathbb{D}}$, then

$$\begin{aligned}\langle K,R_{p,q}^{n-2}\rangle&=\int_{\overline{\mathbb{D}}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z),\\&=\int_{\overline{\mathbb{D}}^{>}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)+\int_{\overline{\mathbb{D}}^{<}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z),\\&=\int_{\overline{\mathbb{D}}^{>}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)+\int_{\overline{\mathbb{D}}^{>}}K(\overline{z})\overline{R_{p,q}^{n-2}(\overline{z})}\,d\nu(z),\\&=\int_{\overline{\mathbb{D}}^{>}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)+\overline{\int_{\overline{\mathbb{D}}^{>}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)},\\&=2\,\Re\left(\int_{\overline{\mathbb{D}}^{>}}K(z)\overline{R_{p,q}^{n-2}(z)}\,d\nu(z)\right)\in\mathbb{R}.\end{aligned}$$

■

Proof of Theorem A.8. Let $K(\langle u,v\rangle)$ be a square-integrable zonal function on $S(\mathbb{C}^n)$ with pole v. Remember, the real disk polynomial $U_{k,\gamma}^{n-2}(z)$ is defined as $U_{k,\gamma}^{n-2}(z)=\big(R_{k+\gamma,k}^{n-2}(z)+R_{k,k+\gamma}^{n-2}(z)\big)/2$. Using Corollary A.7, we find:

$$\int_{S(\mathbb{C}^n)}K(\langle u,v\rangle)\overline{U_{k,\gamma}^{n-2}(\langle u,w\rangle)}\,d\omega(u)=\frac{\lambda_{k+\gamma,k}\overline{R_{k+\gamma,k}^{n-2}(\langle v,w\rangle)}+\lambda_{k,k+\gamma}\overline{R_{k,k+\gamma}^{n-2}(\langle v,w\rangle)}}{2}.$$

If $K(z)=K(\overline{z})$, then $\lambda_{k+\gamma,k}=\lambda_{k,k+\gamma}$ due to Lemma A.9.*(i)*. Consequently,

$$\Lambda_{k,\gamma}=\langle K,U_{k,\gamma}^{n-2}\rangle=\frac{\langle K,R_{k+\gamma,k}^{n-2}\rangle+\langle K,R_{k,k+\gamma}^{n-2}\rangle}{2}=\frac{\lambda_{k+\gamma,k}+\lambda_{k,k+\gamma}}{2}=\lambda_{k+\gamma,k}.$$

Therefore the integral expression simplifies to

$$\int_{S(\mathbb{C}^n)} K(\langle u, v\rangle)\overline{U^{n-2}_{k,\gamma}(\langle u, w\rangle)}\, d\omega(u) = \Lambda_{k,\gamma} U^{n-2}_{k,\gamma}(\langle v, w\rangle).$$

To complete the proof, notice that any combination of two statements in Lemma A.9 is equivalent to the following statement: If $K(z) \in \mathbb{R}$ and $K(z) = K(\overline{z})$ for all $z \in \overline{\mathbb{D}}$, then $\lambda_{k+\gamma,k} = \lambda_{k,k+\gamma}$ and $\lambda_{k+\gamma,k}, \lambda_{k,k+\gamma} \in \mathbb{R}$. Therefore, $\Lambda_{k,\gamma} \in \mathbb{R}$ if those conditions are met. ■

A.4. Disk polynomial decomposition of characteristic kernels

Let $A'(u, v)$ be the invariant characteristic kernel for the set S, then $A'(u, v) = \sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} U^{n-2}_{k,\gamma}(\langle u, v\rangle)$ with $\alpha_{k,\gamma} = \langle A', U^{n-2}_{k,\gamma}\rangle / \langle U^{n-2}_{k,\gamma}, U^{n-2}_{k,\gamma}\rangle$. In order to maintain clarity, we calculate the numerator and denominator separately. We start with the denominator. First we define the function $\varkappa : \mathbb{N} \to \mathbb{R}$ as $\varkappa(\gamma) = 1$ if $\gamma = 0$, $\varkappa(\gamma) = 1/2$ elsewhere. Then the denominator is calculated as:

$$\begin{aligned}
\langle U^{n-2}_{k,\gamma}, U^{n-2}_{k,\gamma}\rangle &= \int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} U^{n-2}_{k,\gamma}(\langle u, v\rangle)\overline{U^{n-2}_{k,\gamma}(\langle u, v\rangle)}\, d\omega(x)\, d\omega(y),\\
&= \int_0^1\int_0^{2\pi} \cos^2(\gamma\theta) r^{2\gamma}\left(\widetilde{P}^{(n-2,\gamma)}_k(2r^2-1)\right)^2 d\tau(\theta)\, d\rho(r),\\
&= \int_0^1 \varkappa(\gamma) r^{2\gamma}\left(\widetilde{P}^{(n-2,\gamma)}_k(2r^2-1)\right)^2 d\rho(r),\\
&= \varkappa(\gamma)\int_0^1 2(n-1) r^{2\gamma+1}(1-r^2)^{n-2}\left(\widetilde{P}^{(n-2,\gamma)}_k(2r^2-1)\right)^2 dr.
\end{aligned}$$

Next we use the substitution $x = 2r^2 - 1$ to complete the calculation:

$$\begin{aligned}
\langle U^{n-2}_{k,\gamma}, U^{n-2}_{k,\gamma}\rangle &= \varkappa(\gamma)\int_{-1}^1 \frac{1}{2}(n-1)\left(\frac{1+x}{2}\right)^\gamma\left(\frac{1-x}{2}\right)^{n-2}\left(\widetilde{P}^{(n-2,\gamma)}_k(x)\right)^2 dx,\\
&= \varkappa(\gamma)\frac{n-1}{2^{(\gamma+n-1)}}\int_{-1}^1 (1+x)^\gamma(1-x)^{n-2}\left(\widetilde{P}^{(n-2,\gamma)}_k(x)\right)^2 dx,\\
&= \varkappa(\gamma)\frac{n-1}{2k+n+\gamma-1}\binom{k+n-2}{k}^{-2}\frac{\Gamma(k+n-1)\Gamma(k+\gamma+1)}{\Gamma(k+n+\gamma-1)\Gamma(k+1)},\\
&= \varkappa(\gamma)\frac{n-1}{2k+n+\gamma-1}\binom{k+n-2}{k}^{-1}\binom{k+n+\gamma-2}{k+\gamma}^{-1}.
\end{aligned}$$

To calculate the numerator, we use the construction for the invariant characteristic kernel where $A'(u, v) = \int_{U(n)} \chi_S(Tu)\chi_S(Tv) d\mu(T)$. If a different normalization is desired, it can easily be applied after calculation of the coefficients. The first observation is that the coefficients for the invariant characteristic kernel $A'(u, v)$ may be calculated by the characteristic kernel $A(u, v) = \chi_S(u)\chi_S(v)$. Indeed, we see that:

$$\begin{aligned}
\langle A', U^{n-2}_{k,\gamma}\rangle &= \int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)}\left(\int_{U(n)} \chi_S(Tu)\chi_S(Tv)\, d\mu(T)\right)\overline{U^{n-2}_{k,\gamma}(\langle u, v\rangle)}\, d\omega(u)\, d\omega(v),\\
&= \int_{U(n)}\int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} \chi_S(Tu)\chi_S(Tv)\overline{U^{n-2}_{k,\gamma}(\langle Tu, Tv\rangle)}\, d\omega(u)\, d\omega(v)\, d\mu(T),\\
&= \int_{S(\mathbb{C}^n)}\int_{S(\mathbb{C}^n)} \chi_S(u)\chi_S(v)\overline{U^{n-2}_{k,\gamma}(\langle u, v\rangle)}\, d\omega(u)\, d\omega(v).
\end{aligned}$$

For special set constructions, the numerator can be simplified further. Namely, if $\chi_S(u)$ is given by a zonal function $f \in L^2(\overline{\mathbb{D}})$ with pole w such that $f(\langle u, w\rangle) =$

$f(\overline{\langle u, w\rangle})$, then the integrals can be calculated piecewise. We can use Theorem A.8 twice by noticing $U_{k,\gamma}^{n-2}(\langle u, v\rangle) = U_{k,\gamma}^{n-2}(\langle v, u\rangle)$:

$$
\begin{aligned}
\langle A', U_{k,\gamma}^{n-2}\rangle &= \int_{S(\mathbb{C}^n)} \left(\int_{S(\mathbb{C}^n)} f(\langle u, w\rangle)\overline{U_{k,\gamma}^{n-2}(\langle u, v\rangle)} d\omega(u) \right) f(\langle v, w\rangle)\, d\omega(v), \\
&= \int_{S(\mathbb{C}^n)} \beta_{k,\gamma} f(\langle v, w\rangle)\overline{U_{k,\gamma}^{n-2}(\langle w, v\rangle)}\, d\omega(v), \\
&= \int_{S(\mathbb{C}^n)} \beta_{k,\gamma} f(\langle v, w\rangle)\overline{U_{k,\gamma}^{n-2}(\langle v, w\rangle)}\, d\omega(v), \\
&= \beta_{k,\gamma}^2 \overline{U_{k,\gamma}^{n-2}(\langle w, w\rangle)} = \beta_{k,\gamma}^2, \\
\beta_{k,\gamma} &= \int_0^1 \int_0^{2\pi} f(re^{i\theta})\overline{U_{k,\gamma}^{n-2}(re^{i\theta})}\, d\tau(\theta)\, d\rho(r).
\end{aligned}
$$

For any set S where there is such a function f with pole w, the set is of the form $S = \{u : u \in S(\mathbb{C}^n), \langle u, w\rangle \in D_S\}$ for some $D_S \subseteq \overline{\mathbb{D}}$. This means $f(re^{i\theta}) = \chi_{D_S}(re^{i\theta})$ and

$$
\beta_{k,\gamma} = \int_{D_S} \overline{U_{k,\gamma}^{n-2}(re^{i\theta})}\, d\nu(re^{\theta}).
$$

If D_S has an especially simple description, which is the case for the double-cap set, then the coefficients can be calculated algebraically. Let D_S be the double-cap set with the pole w defined by $D_S = \{re^{i\theta} : r \in (\sqrt{(}1/2), 1], \theta \in [0, 2\pi)\}$. As the double-cap conjecture is closed under multiplication by $e^{i\theta}$, $\beta_{k,\gamma} = 0$ for $\gamma \geq 1$. Additionally, $\alpha_{0,0} = \beta_{0,0}^2 = \langle A', U_{0,0}^{n0}\rangle = \omega(DC(\mathbb{C}^n))^2 = 2^{-2(n-1)}$. The coefficients that remain to be calculated are for $\gamma = 0$, $k > 0$. In the calculation the following equality is used, see [4, (18.17.1)]:

$$
\begin{aligned}
&2k \int_0^x (1-y)^{\alpha}(1+y)^{\beta} P_k^{(\alpha,\beta)}(y)\, \mathrm{d}y \\
&\qquad = P_{k-1}^{(\alpha+1,\beta+1)}(0) - (1-x)^{\alpha+1}(1+x)^{\beta+1} P_{k-1}^{(\alpha+1,\beta+1)}(x)\,.
\end{aligned}
$$

Using that equality, we calculate $\beta_{k,0}$ and subsequently the coefficient $\alpha_{k,0}$ for the double-cap set.

$$
\begin{aligned}
\beta_{k,0} &= \int_0^{2\pi} \int_0^1 \chi_{(\sqrt{1/2},1]}(r)\overline{U_{k,0}^{n-2}(re^{i\theta})} d\rho(r)\, d\tau(\theta), \\
&= \int_{\sqrt{1/2}}^1 \widetilde{P}_k^{(n-2,0)}(2r^2-1)\, d\rho(r), \\
&= (n-1)\int_0^1 \left(\frac{1-x}{2}\right)^{n-2} \widetilde{P}_k^{(n-2,0)}(x)\, dx, \\
&= 2^{-n}\frac{n-1}{k}\binom{k+n-2}{k}^{-1} P_{k-1}^{(n-1,1)}(0) = 2^{-n}\widetilde{P}_{k-1}^{(n-1,1)}(0), \\
\alpha_{k,0} &= \frac{\beta_{k,0}^2}{\langle U_{k,0}^{n0}, U_{k,0}^{n0}\rangle}, \\
&= 2^{-2n}\frac{(2k+n-1)}{n-1}\binom{k+n-2}{k}^2 \left(\widetilde{P}_{k-1}^{(n-1,1)}(0)\right)^2.
\end{aligned}
$$

A.5. Truncated primal

While the dual for the Lovász theta number is used to obtain the final upper bounds, solutions for the primal are still used to create BQP sets by facet optimization or comparison to a lower bound kernel. During testing, truncating the disk polynomial set in the primal without compensation could cause the primal to be infeasible or have an objective value lower than the lower bound. To resolve this issue, we create a relaxation of the primal that limits the disk polynomials to a parameter set while accounting for the polynomials outside of the parameter set. The relaxation is constructed by creating a slack function ϕ that acts as substitute for the disk polynomials outside of the parameter set. This function has value $\phi(1) = 1$, like all disk polynomials, and may assume any value for $re^{i\theta} \in \overline{\mathbb{D}} \setminus \{1\}$, subject to the bounds ε_r. That is,

$$\phi(re^{i\theta}) = \begin{cases} 1 & \text{if } re^{i\theta} = 1, \\ -\varepsilon_r \leq \phi(re^{i\theta}) \leq \varepsilon_r & \text{else.} \end{cases}$$

Let P be the parameter set and P^C be all parameters not included in P. Let g be any zonal function that is a convex combination of disk polynomials with $k, \gamma \in P^C$. It follows that there exists such a ϕ where $\phi(z) = \sum_{(k,\gamma)\in P^C} \alpha_{k,\gamma} U_{k,\gamma}^{n-2}(z)$ for all $z \in \overline{\mathbb{D}}$. This shows that including ϕ instead of the disk polynomials with $k, \gamma \in P^C$ is a relaxation of the problem. The slack function with coefficient α_ε can be encoded into the primal as follows:

$$\begin{aligned}
\sup\ & \alpha_\varepsilon + \textstyle\sum_{k,\gamma\in\mathbb{N}} \alpha_{k,\gamma} \\
& \textstyle\sum_{(k,\gamma)\in P} \alpha_{k,\gamma} U_{k,\gamma}^{n-2}(t) + \beta_t = 0, \\
& \begin{pmatrix} 1 & \alpha_\varepsilon + \sum_{(k,\gamma)\in P} \alpha_{k,\gamma} \\ \alpha_\varepsilon + \sum_{(k,\gamma)\in P} \alpha_{k,\gamma} & \alpha_{0,0} \end{pmatrix} \succeq 0, \\
& f(\langle u, v\rangle) + \beta_{uv} = \textstyle\sum_{W\subseteq V} \lambda_W \mathbf{1}_{u,v\in W} && \forall u, v \in V, \\
& \textstyle\sum_{W\subseteq V} \lambda_W = 1, \\
& f = \textstyle\sum_{(k,\gamma)\in P} \alpha_{k,\gamma} U_{k,\gamma}^{n-2}, \\
& |\beta_t| \leq \varepsilon_t \alpha_\varepsilon, \\
& |\beta_{uv}| \leq \varepsilon_{uv} \alpha_\varepsilon && \forall u, v \in V, \\
& \beta_{u,u} = \alpha_\varepsilon && \forall u \in V, \\
& \lambda, \alpha \geq 0.
\end{aligned}$$

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