

Good Packings in the Complex Stiefel Manifold using Numerical Methods

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Abstract—For a wireless communication system with multiple transmit and receive antennas, the problem of designing a good performing constellation (namely a constellation with a large diversity) can be converted into a packing problem in a complex Stiefel manifold. In this paper we propose suitable algebraic structures to obtain good packings in a complex Stiefel manifold by numerical methods. The presented design methods work for any dimension and any cardinality of the constellations. The paper summarizes the main results obtained in [7], [8].

Keywords—Space time codes, complex Stiefel manifold.

I. INTRODUCTION

Some 10 years ago it has been recognized that multiple transmit and/or receive antennas can drastically increase the transmission rate on a wireless channel. As a consequence signals have not only to be spread over time but also over space and this explains the term *space time coding*.

After some normalization a codeword consists of a collection of n unitary vectors which are pairwise perpendicular, i.e. a point in a complex Stiefel manifold. Crucial for the design of space time codes are the diversity product and the diversity sum which we will define in a moment. Codes perform well if the diversity sum and diversity product of the code is large.

In this paper we report on progress recently found by the authors on how to derive tight upper bounds

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on the diversity by differential geometric means. The presented upper bound was derived in [8]. We also show how to derive lower bounds on the diversity by numerical methods. The main references for this part of the paper are [5], [6], [7].

Consider a wireless communication system with n transmit antennas and N receive antennas operating in a Rayleigh flat-fading channel. We assume time is discrete and at each time slot, signals are transmitted simultaneously from the n transmit antennas. We can further assume that the wireless channel is static over a time block of length τ . In this context, a codeword can be represented by a $\tau \times n$ unitary matrix, i.e., a point in the complex Stiefel manifold. A unitary space time constellation $\mathcal{V} := \{\Phi_1, \dots, \Phi_m\}$ consists of m complex matrices having size $\tau \times n$ and satisfying $\tau \geq n$ and $\Phi_k^* \Phi_k = I_n$. The scaled matrices $\sqrt{\tau} \Phi_k$, $k = 1, 2, \dots, m$, represent the code words used during the transmission. A fundamental problem for this setting is to design a good performing constellation. There exist two important design criteria for unitary space time constellations: *The diversity product* (DP) and *The diversity sum* (DS).

Definition 1: (See [12]) *The diversity product* of a unitary constellation \mathcal{V} is defined as

$$\prod \mathcal{V} = \min_{l \neq l'} \left(\prod_{i=1}^n (1 - \delta_i(\Phi_l^* \Phi_{l'})^2) \right)^{\frac{1}{2n}},$$

where $\delta_i(\cdot)$ denote the i -th singular value of a matrix.

An important special case occurs when $\tau = 2n$. In this situation it is customary to represent all unitary

matrices Φ_k in the form:

$$\Phi_k = \frac{\sqrt{2}}{2} \begin{pmatrix} I \\ \Psi_k \end{pmatrix}. \quad (1)$$

Since the columns of Φ_k are pairwise perpendicular and have norm 1 it follows that the matrices Ψ_k are $n \times n$ unitary matrices. In terms of unitary matrices the diversity product as defined in Definition 1 has the form:

$$\prod \mathcal{V} = \frac{1}{2} \min_{l \neq l'} |\det(\Psi_l - \Psi_{l'})|^{\frac{1}{n}}. \quad (2)$$

A constellation \mathcal{V} is called fully diverse constellation if $\prod \mathcal{V} > 0$. Many authors tried to construct constellations with a large diversity product. (See e.g. [12], [15], [6], [5], [20], [19], [21]). For the particular situation $\tau = 2n$ with special form (1) the design asks for the construction of a discrete subset $\mathcal{V} = \{\Psi_1, \dots, \Psi_m\}$ of the set of $n \times n$ unitary matrices $U(n)$. One interesting special case happens when this discrete subset has the structure of a discrete subgroup of $U(n)$. The condition that \mathcal{V} is fully diverse is then equivalent to the condition that the identity matrix is the only element of \mathcal{V} having an eigenvalue of 1. In terms of geometry this means that the constellation \mathcal{V} operates fixed point free on the vector space \mathbb{C}^n . Shokrollahi et al. [19], [20] were able to study the complete list of fully diverse finite group constellations inside the unitary group $U(n)$ using a classical classification result of fixed point free unitary representations by Zassenhaus [23]. Some of these constellations have the best known diversity product for given fixed parameters n, N, m . Unfortunately group constellations do not exist for many set of parameters and new methods are needed if one wants to construct constellations with near optimal diversity product.

Definition 2: The *diversity sum* of a unitary constellation \mathcal{V} is defined as

$$\sum \mathcal{V} = \min_{l \neq l'} \sqrt{1 - \frac{\|\Phi_l^* \Phi_{l'}\|_F^2}{n}},$$

where $\|\cdot\|$ denote the Frobenius norm of a matrix.

Again one has the important special case where $\tau = 2n$ and the matrices Φ_k take the special form (1). For the form (1) the diversity sum assumes the following simple form:

$$\sum \mathcal{V} = \min_{l, l'} \frac{1}{2\sqrt{n}} \|\Psi_l - \Psi_{l'}\|_F. \quad (3)$$

Without mentioning the term the concept of diversity sum was used in [11]. Liang and Xia [15, p. 2295] explicitly defined the diversity sum in the situation when $\tau = 2n$ using equation (3). Definition 2 naturally generalizes the definition to arbitrary constellations.

From arguments above, one sees that designing a constellation with a large diversity (DP or DS) is equivalent to finding good packings in a complex Stiefel manifold under a suitable distance measure.

The paper is structured as follows.

In the next section we derive an upper bound for the diversity sum as it has been derived in [8].

In Section III we parameterize constellations which will be efficient for numerical search algorithms. For this purpose we introduce the concept of a *weak group structure* and we classify all weak group structures whose elements are normal and positive. We follow in Section III the ideas as developed by the authors in [7].

Section IV contains the main result of this paper. We investigate an algebraic structure which led to some of the best constellations which we were able to derive. We explain a general method on how one can efficiently design excellent constellations for any set of parameters n, N, τ, m . For this we review the Cayley transform. We conclude this section with an extensive table where we publish a large set of codes having some of the best diversity sums and diversity products in their parameter range.

II. AN UPPER BOUND FOR THE DIVERSITY

In a recent paper Henkel [10] gives upper bounds on the the diversity of a space time constellation (i.e., upper bounds on the minimal “distance” between certain points in a complex Stiefel manifold).

For the special setting when $\tau = 2n$ and the diversity sum and product are given by formulas (3) and (2), we analyzed the geometry of $U(n)$ in [8]. This led to new tight upper bounds. We start with a simple lemma.

Lemma 3: When $\tau = 2n$ then for any unitary space time code \mathcal{V} ,

$$\prod \mathcal{V} \leq \sum \mathcal{V}.$$

Definition 4: Let $\Delta(n, m)$ be the infimum of all numbers such that for every unitary space time code \mathcal{V} of dimension n and size m , one has

$$\sum \mathcal{V} \leq \Delta(n, m).$$

Remark 5: As pointed by Liang and Xia [15] there exists a constellation \mathcal{V} of dimension n and size m

with $\sum \mathcal{V} = \Delta(n, m)$. This is due to the fact that $U(n)^m$ is a compact manifold.

The exact values of $\Delta(n, m)$ are only known in very few special cases. In the case $n = 1$, one checks that $\Delta(1, m) = \sin \frac{\pi}{m}$ for $m \geq 2$. When $n \geq 2$ and $m = 3$, one has $\Delta(n, 3) = \frac{\sqrt{3}}{2}$. When $m = 2$, we have $\Delta(n, 2) = 1$ for $n \geq 2$. For $n = 2$, the following values in I were computed in [15].

The main theorem in [8] provides a general upper bound for $\Delta(n, m)$. For this let

$$D_1 = \{(\theta_1, \theta_2, \dots, \theta_n) \mid -\pi \leq \theta_j < \pi \text{ for } j = 1, 2, \dots, n\},$$

and

$$D_2 = \{(\theta_1, \theta_2, \dots, \theta_n) \mid \sum_{j=1}^n \sin^2 \frac{\theta_j}{2} \leq \frac{r^2}{4}\}.$$

Theorem 6:

$$\Delta(n, m) \leq \sqrt{r^2/n - r^4/(4n^2)},$$

where r is the solution to the following equation:

$$m \iint_{D_1 \cap D_2} \prod_{j < k} |e^{i\theta_j} - e^{i\theta_k}|^2 d\theta_1 d\theta_2 \dots d\theta_n = (2\pi)^n n!. \quad (4)$$

III. CONSTELLATIONS WITH ALGEBRAIC STRUCTURE

In this section we develop geometrical and numerical procedures which allow one to construct unitary constellations with excellent diversity for any set of parameters n, N, τ, m . We follow [7].

Consider a general constellation of square unitary matrices,

$$\mathcal{V} = \{\Psi_1, \Psi_2, \dots, \Psi_m\}.$$

In order to calculate the diversity product, one needs to do $\frac{m(m-1)}{2}$ calculations: $|\det(\Psi_i - \Psi_j)|$ for every different pair i, j . The same statement can be said about the diversity sum.

If one wants to compute the distance of a linear block code then it is enough to compute the Hamming distance between every nonzero vector and the zero vector. Something similar happens when one wants to compute the diversity product of a group constellation. As pointed out in [20] one needs only to calculate $m - 1$ determinants having the form $|\det(I - \Psi_i)|$ in order to compute the diversity product. This is a direct consequence of

$$|\det(\Psi_i - \Psi_j)| = |\det(\Psi_i) \det(I - \Psi_i^* \Psi_j)|$$

$$= |\det(I - \Psi_i^* \Psi_j)|,$$

where $\Psi_i^* \Psi_j$ is still in the group. Group constellations are however very restrictive about what the algebraic structure is concerned, and the constellations found by this approach [20] are really few and far between. In the following we are going to present some constellations which have some small number of generators and whose diversity can be efficiently computed. This will ensure that the total parameter space to be searched is limited as well. We start with an example:

Example 7: Consider the constellation

$$\mathcal{V} = \{A^k B^l \mid A, B \in U(n), k = 0, \dots, p, l = 0, \dots, q\}.$$

(We remark that more specified constellation of this type has been considered in [20].) The parameter space for this constellation is $U(n) \times U(n)$, this is a manifold of dimension $2n^2$ and the number of elements in \mathcal{V} is $(p+1)(q+1)$. If one has to compute $|\det(\Psi_i - \Psi_j)|$ for every distinct pair this would require $\binom{(p+1)(q+1)}{2}$ determinant calculations. We will show in the following that the same result can be obtained by doing $2pq + p + q$ determinant computations.

Let Ψ_i and Ψ_j be two distinct elements having the form $A^{k_1} B^{l_1}$ and $A^{k_2} B^{l_2}$ respectively. We have now several cases. When $k_1 = k_2$, then necessarily $l_1 \neq l_2$ and the distance is computed as

$$|\det(A^{k_1} B^{l_1} - A^{k_2} B^{l_2})| = |\det(I - B^{|l_2 - l_1|})|,$$

where $|l_2 - l_1|$ is an integer between 1 and q . If $l_1 = l_2$, then we have $k_1 \neq k_2$ and the distance is computed as

$$|\det(A^{k_1} B^{l_1} - A^{k_2} B^{l_2})| = |\det(I - A^{|k_2 - k_1|})|,$$

where $|k_2 - k_1|$ is an integer between 1 and p . If $(k_1 < k_2 \text{ and } l_1 < l_2)$ or $(k_1 > k_2 \text{ and } l_1 > l_2)$, we have

$$|\det(A^{k_1} B^{l_1} - A^{k_2} B^{l_2})| = |\det(I - A^{|k_2 - k_1|} B^{|l_2 - l_1|})|,$$

where $1 \leq |k_2 - k_1| \leq p$ and $1 \leq |l_2 - l_1| \leq q$. Similarly if $(k_1 < k_2 \text{ and } l_1 > l_2)$ or $(k_1 > k_2 \text{ and } l_1 < l_2)$ then

$$|\det(A^{k_1} B^{l_1} - A^{k_2} B^{l_2})| = |\det(A^{|k_2 - k_1|} - B^{|l_2 - l_1|})|,$$

with $1 \leq |k_2 - k_1| \leq p$ and $1 \leq |l_2 - l_1| \leq q$. The total number of distances to be computed is in total equal to $2pq + p + q$.

m	2	3	4	5	6	7	8	9	10 through 16
$\Delta(2, m)$	1	$\frac{1}{2}\sqrt{3}$	$\frac{1}{3}\sqrt{6}$	$\frac{1}{4}\sqrt{10}$	$\frac{1}{5}\sqrt{15}$	$\frac{1}{6}\sqrt{21}$	$\frac{1}{7}\sqrt{28}$	$\frac{1}{8}\sqrt{36}$	$\frac{1}{2}\sqrt{2}$

TABLE I
EXACT VALUES OF $\Delta(n, m)$

Following [7] we are going to loosen the constraints imposed by the group structures. As demonstrated in Example 7 it is desirable to have a small dimensional manifold (in Example 7 it was $U(n) \times U(n)$) which parameterizes a set of potentially interesting constellations. Having such a parameterization will help to avoid the problem of “dimension explosion”. The set of constellations parameterized by $U(n) \times U(n)$ in Example 7 are interesting as we are not required to compute all pairwise distances in order to compute the diversity product (sum).

Definition 8: Let X be the set $\{x_1, x_2, \dots, x_n\}$ and F be the free group on the set X . A subset $G \subset U(n)$ is called *freely generated* if there are elements $\{g_1, g_2, \dots, g_n\} \subset G$ such that the homomorphism $\phi : F \rightarrow G$ with $\phi(x_i) = g_i$ is an isomorphism.

An immediate consequence of this definition is that every element in G can be uniquely written as a product of g_i 's and g_i^{-1} 's. The elements g_i are called the generators of G . A freely generated subset G is simply parameterized by the set:

$$\{a_1^{p_1} a_2^{p_2} \dots a_k^{p_k} \mid a_i \text{ is one of } g_i^s, p_i \in \mathbb{Z}\}.$$

Take an element $g \in G$ with its representation $g = \prod_{i=1}^k a_i^{p_i}$, we say that the presentation is *reduced* whenever $a_i \neq a_{i+1}$ for $i = 1, \dots, k-1$. We say that an element $g = \prod_{i=1}^k a_i^{p_i}$ in reduced form is a *normal element* whenever $a_i \neq a_j$ for $i \neq j$. A subset \mathcal{V} of the freely generated set G is said to be a *normal constellation* if every non-identity element in \mathcal{V} is normal. An element g in G with the reduced form $g = \prod_{i=1}^k a_i^{p_i}$ is said to be a *positive element* if $p_i > 0$ for $i = 1, 2, \dots, k$. A subset \mathcal{V} of the freely generated set G is said to be a *positive constellation* if every non-identity element in \mathcal{V} is positive. Positive normal constellations are desirable for space time constellation de

Two unitary matrices $A, B \in G$ are said to be *equivalent* (denote by $A \sim B$) if there is unitary matrix $U \in G$ such that $A = UBU^{-1}$ or $A = UB^{-1}U^{-1}$. $[A]$ will denote all the matrices that are equivalent to A . For a constellation $\mathcal{V} \subset G$, we say $\mathcal{V} = \{\Psi_1, \Psi_2, \dots, \Psi_m\}$ has a *weak group structure*

if for any two distinct elements Ψ_i, Ψ_j the product $\Psi_i^{-1}\Psi_j$ is equivalent to some Ψ_k .

Note also that \mathcal{V} has a group structure as soon as $\Psi_i^{-1}\Psi_j$ is always another element of \mathcal{V} and this explains our wording. The following lemma was proven in [7].

Lemma 9: Let $\mathcal{V} = \{\Psi_0 = I, \Psi_1, \Psi_2, \dots, \Psi_{m-1}\}$ be a constellation with a weak group structure. In order to compute the diversity product (sum) it is enough to do $m - 1$ distance computations.

Based on this lemma we are interested in finite constellations inside G whose elements have a weak group structure and are all normal. The following theorem provides a complete characterization of all these constellations:

Theorem 10: (See [7]) Let $\mathcal{V} \subset G$ be a finite positive normal constellation (including identity element) with $m \geq 3$ elements. If \mathcal{V} has a weak group structure then \mathcal{V} takes one of the following forms:

- $\{I, A, A^2, \dots, A^{m-1}\}$
- $\{I, AB, A^2B^2, \dots, A^{m-1}B^{m-1}\}$

where $A = g_i^{p_i}$, $B = g_j^{p_j}$ for some $i \neq j$.

The proof of Theorem 10 is rather involved and we refer to [7].

IV. UNITARY CONSTELLATIONS WITH LARGE DIVERSITY

As pointed out in [7] for both forms of weak group constellations in Theorem 10, one can always assume that A is diagonal. We can further restrict the search for good 2-dimensional constellations by assuming (see [7]) that B is real orthogonal, i.e., we consider the following 2 dimensional constellation:

$$\mathcal{V} = \{A^k B^k \mid A = \begin{pmatrix} e^{ix} & 0 \\ 0 & e^{iy} \end{pmatrix},$$

$$B = \begin{pmatrix} \cos z & \sin z \\ -\sin z & \cos z \end{pmatrix}, k = 0, 1, \dots, m-1\}. \quad (5)$$

A natural idea is to design the constellation with the help of geometrical intuition. Note that a 2×2 complex matrix can be viewed as a vector in \mathbb{C}^4 . In this context A and B can be viewed as “rotation

transform” (induced by regular matrix multiplication) acting on \mathbb{C}^4 . A constellation of form (5) can be viewed as a set of rotated vectors under the transforms $A^k B^k$, $k = 0, 1, \dots, m - 1$. Using this geometric intuition we were able to find numerically many space time codes with excellent diversity.

The problem of designing 2 dimensional constellations with near optimal diversity was initiated by Liang [15].

2-dimensional constellation design has been studied in [15]. The codes shown in [15] can be achieved by our design as well. In fact, most of Liang’s codes belong to a special form of our parameterization (5). To the best of our knowledge, most of our codes shown on the web site [4] are the best codes ever found or never found before.

The techniques described so far generalize to higher dimensions. The geometric “rotation” idea can be applied to derive other low dimensional constellations. We illustrate it for a 3 dimensional weak group constellation. For this assume that the constellation has the form:

$$\mathcal{V} = \{A^k B^k | A = \begin{pmatrix} \cos x & \sin x & 0 \\ -\sin x & \cos x & 0 \\ 0 & 0 & e^{iy} \end{pmatrix}, \\ B = \begin{pmatrix} e^{iz} & 0 & 0 \\ 0 & \cos w & \sin w \\ 0 & -\sin w & \cos w \end{pmatrix}, k = 0, 1, \dots, m-1\}.$$

where x, y, z, w is assumed to take the multiple of $2\pi/m$. Apparently algebraic design based on geometrical symmetry can be applied to any other structure as well. For instance consider the following specified structures:

$$\mathcal{V} = \left\{ A^k B^l | A = \begin{pmatrix} e^{ix} & 0 \\ 0 & e^{iy} \end{pmatrix}, \right. \\ \left. B = \begin{pmatrix} \cos z & \sin z \\ -\sin z & \cos z \end{pmatrix}, \right. \\ \left. k = 0, 1, \dots, p-1, l = 0, 1, \dots, q-1 \right\}.$$

where we can take x, y to be multiple of $2\pi/p$ and z to be multiple of $2\pi/q$. Some of 2 dimensional geometrically found constellations will be listed together with those numerically found in Table II and Table III. We also refer to [4] for the designed low dimensional constellations from these approaches. However the approach above only works for low dimension due to its computational complexity.

We show next how one can use the theory of complex Stiefel manifolds and the classical Cayley

transform to obtain such a simple parameterization for a unitary constellation.

A. The complex Stiefel manifold

Definition 11: The subset of $\tau \times n$ complex matrices

$$\mathcal{S}_{\tau,n} := \{ \Phi \in \mathbb{C}^{\tau \times n} \mid \Phi^* \Phi = I_n \}$$

is called the *complex Stiefel manifold*.

From an abstract point of view a constellation $\mathcal{V} := \{ \Phi_1, \dots, \Phi_m \}$ having size m , block length τ and operating with n antennas can be viewed as a point in the complex manifold

$$\mathcal{M} := (\mathcal{S}_{\tau,n})^m = \underbrace{\mathcal{S}_{\tau,n} \times \dots \times \mathcal{S}_{\tau,n}}_{m \text{ copies}}.$$

The search for good constellations \mathcal{V} requires hence the search for points in \mathcal{M} whose diversity is excellent.

Stiefel manifolds have been intensely studied in the mathematics literature since their introduction by Eduard Stiefel some 50 years ago. A classical paper on complex Stiefel manifolds is [2], a paper with a point of view toward numerical algorithms is [3]. The major properties are summarized by the following theorem:

Theorem 12: $\mathcal{S}_{\tau,n}$ is a smooth, real and compact sub-manifold of $\mathbb{C}^{n\tau} = \mathbb{R}^{2n\tau}$ of real dimension $2\tau n - n^2$.

Some of the stated properties will follow from our further development. The following two examples give some special cases.

Example 13:

$$\mathcal{S}_{\tau,1} = \left\{ x \in \mathbb{C}^\tau \mid \|x\| = \sqrt{\sum_{i=1}^n x_i \bar{x}_i} = 1 \right\} \subset \mathbb{R}^{2\tau}$$

is isomorphic to the $2\tau - 1$ dimensional unit sphere $S^{2\tau-1}$.

Example 14: When $\tau = n$ then $\mathcal{S}_{\tau,n} = U(n)$, the group of $n \times n$ unitary matrices. It is well known that the Lie algebra of $U(n)$, i.e. the tangent space at the identity element, consists of all $n \times n$ skew-Hermitian matrices. This linear vector space has real dimension n^2 , in particular the dimension of $U(n)$ is n^2 as well.

A direct consequence of Theorem 12 is:

Corollary 15: The manifold \mathcal{M} which parameterizes the set of all constellations \mathcal{V} having size m , block length τ and operating with n antennas forms a real compact manifold of dimension $2m\tau n - mn^2$.

As this corollary makes it clear a full search over the total parameter space is only possible for very moderate sizes of n, m, τ . It is also required to have a good parameterization of the complex Stiefel manifold $\mathcal{S}_{\tau, n}$ and we will go after this task next.

The unitary group is closely related to the complex Stiefel manifold and the problem of parameterization ultimately boils down to the parameterization of unitary matrices. For this assume that Φ is a $\tau \times n$ matrix representing an element of the complex Stiefel manifold $\mathcal{S}_{\tau, n}$. Using Gram-Schmidt one constructs a $\tau \times (\tau - n)$ matrix V such that the $\tau \times \tau$ matrix $[\Phi | V]$ is unitary. Define two $\tau \times \tau$ unitary matrices $[\Phi_1 | V_1]$ and $[\Phi_2 | V_2]$ to be equivalent whenever $\Phi_1 = \Phi_2$. A direct calculation shows that two matrices are equivalent if and only if there is $(\tau - n) \times (\tau - n)$ matrix Q such that:

$$[\Phi_2 | V_2] = [\Phi_1 | V_1] \begin{pmatrix} I & 0 \\ 0 & Q \end{pmatrix}. \quad (6)$$

Identifying the set of matrices Q appearing in (6) with the unitary group $U(\tau - n)$ we get the result:

Lemma 16: The complex Stiefel manifold $\mathcal{S}_{\tau, n}$ is isomorphic to the quotient group

$$U(\tau)/U(\tau - n).$$

This lemma let us verify the dimension formula for $\mathcal{S}_{\tau, n}$ stated in Theorem 12:

$$\begin{aligned} \dim \mathcal{S}_{\tau, n} &= \dim U(\tau) - \dim U(\tau - n) \\ &= \tau^2 - (\tau - n)^2 = 2\tau n - n^2. \end{aligned}$$

The section makes it clear that a good parameterization of the set of constellations \mathcal{V} requires a good parameterization of the manifold \mathcal{M} and this in turn requires a good parameterization of the unitary group $U(n)$.

Once one has a nice parameterization of the unitary group $U(n)$ then Lemma 16 provides a way to parameterize the Stiefel manifold $\mathcal{S}_{\tau, n}$ as well. Parameterizing $U(\tau)$ modulo $U(\tau - n)$ is however an ‘over parameterization’. Edelman, Arias and Smith [3] explained a way on how to describe a local neighborhood of a (real) Stiefel manifold $\mathcal{S}_{\tau, n}$. The method can equally well be applied in the complex case. We do not pursue this parameterization in this paper and leave this for future work.

In the remainder of this paper we will concentrate on constellations having the special form (1). From a numerical point of view we require for this a good parameterization of the unitary group and the next subsection provides an elegant way to do this.

B. Cayley transformation

There are several ways to represent a unitary matrix in a very explicit way. One elegant way makes use of the classical Cayley transformation. In order that the paper is self contained we provide a short summary. More details are given in [18, Section 22] and [9].

Definition 17: For a complex $n \times n$ matrix Y which has no eigenvalues at -1 , the Cayley transform of Y is defined to be

$$Y^c = (I + Y)^{-1}(I - Y),$$

where I is the $n \times n$ identity matrix.

Note that $(I + Y)$ is nonsingular whenever Y has no eigenvalue at -1 . One immediately verifies that $(Y^c)^c = Y$. This is in analogy to the fact that the linear fractional transformation $f(z) = \frac{1-z}{1+z}$ has the property that $f(f(z)) = z$. Note that the set of $n \times n$ skew-Hermitian matrices forms a linear subspace of $\mathbb{C}^{n \times n} \cong \mathbb{R}^{2n^2}$ having real dimension n^2 . The main property of the Cayley transformation is summarized in the following theorem. (See e.g. [9], [18]).

Theorem 18: When A is a skew-Hermitian matrix then $(I + A)$ is nonsingular and the Cayley transform $V := A^c$ is a unitary matrix. Vice versa when V is a unitary matrix which has no eigenvalues at -1 then the Cayley transform V^c is skew-Hermitian.

This theorem allows one to parameterize the open set of $U(n)$ consisting of all unitary matrices whose eigenvalues do not include -1 through the linear vector space of skew-Hermitian matrices. Many optimization algorithm we considered require a parameterization of a neighborhood of one element in $U(n)$. The Cayley transformation can achieve this in a very natural way.

C. Simulated annealing algorithm

The numerical task of searching constellations with large diversity is very involved as there are a large number of target functions and the ambient space has a large dimension. For this reason optimization algorithms such as Newton’s Methods [3], [16] and the Conjugate Gradient Method [3], [16] are difficult to implement. The method which had the most success in our numerical experiments was the *Simulated Annealing (SA) Algorithm*. For more details about this algorithm, we refer to [1], [22], [17].

D. Square constellations design

In Table II and Table III we list the best 2-dimensional constellations we found with the techniques described in Sections IV (For results on the

higher dimensional unitary constellation design, one can check them on the web site [4]). The tabulated constellations have some of the best diversity sums and diversity products published so far. All the constellations searched by simulated annealing (SA) were based on the $A^k B^k$ structure. For the constellations with m elements and parameters x, y, z being multiples of $2\pi/m$, they are found by geometrical methods using the parameterization (5). For the constellations with m elements and parameters x, y, z being decimals, they are found by Brute Force with step size 0.1000 based on the same parameterization (5).

E. Non-square Constellation Design

As first illustrated in [14], one can construct $\tau \times n$ unitary constellations by using the first n columns of $\tau \times \tau$ unitary constellations. With this idea the techniques used above for square unitary constellations can be applied to design general form unitary constellations too. For simplicity we describe the idea with assumption $\tau = 2n$ and consider the following structure:

$$\{A^k B | A \in U(\tau), B = \begin{pmatrix} I_n \\ 0 \end{pmatrix}, k = 0, 1, \dots, m-1\}.$$

One can check at most $2m - 1$ distance calculations are needed to derive the diversity product (sum) with this algebraic structure. We list some of numerically found non-square constellations in Table IV. More results can be found in [4].

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TABLE II
DIVERSITY PRODUCT OF 2 DIMENSIONAL CONSTELLATION BASED ON WEAK GROUP STRUCTURE: [7]

Number of elements	Diversity Product	Codes and Comments
2	1	$x = \pi, y = \pi, z = 0$ (optimal)
3	$\sqrt{3}/2$	$x = 2\pi/3, y = 2\pi/3, z = 0$ (optimal)
4	0.7831	$x = 0.6000, y = 6.0000, z = 4.4000$
5	$\sqrt{5}/8$	$x = 2\pi/5, y = 8\pi/5, z = 4\pi/5$ (optimal)
8	0.7071	$x = 2.3562, y = 3.9270, z = 4.7124$
9	0.6524	SA searched code
10	0.6124	$x = 2\pi/5, y = 8\pi/5, z = \pi/5$
16	$\sqrt[4]{2}/2$	$x = \pi/4, y = 5\pi/4, z = 13\pi/8$
17	0.5255	SA searched code
18	0.5207	SA searched code
19	0.5128	SA searched code
20	0.5011	$x = 1.6500, y = 3.7500, z = 4.0500$
24	0.5000	$x = \pi/12, y = 5\pi/12, z = \pi/2$
37	0.4461	$x = 2\pi/37, y = 6\pi/37, z = 12\pi/37$
39	0.3984	$x = 8\pi/39, y = 34\pi/39, z = 36\pi/39$
40	0.3931	$x = 3\pi/10, y = 11\pi/10, z = 3\pi/4$
55	0.3874	$x = 2\pi/55, y = 68\pi/55, z = 6\pi/11$
57	0.3764	$x = 2\pi/57, y = 40\pi/57, z = 48\pi/57$
75	0.3535	$x = 2\pi/75, y = 98\pi/75, z = 96\pi/75$
85	0.3497	$x = 26\pi/85, y = 94\pi/85, z = 18\pi/17$
91	0.3451	$x = 2\pi/91, y = 128\pi/91, z = 42\pi/91$
96	0.3192	$x = 7\pi/16, y = 29\pi/16, z = \pi/6$
105	0.3116	$x = 2\pi/105, y = 68\pi/105, z = 84\pi/105$
120	0.3090	$x = \pi/30, y = 11\pi/30, z = \pi/4$
135	0.2869	$x = 2\pi/135, y = 28\pi/135, z = 68\pi/135$
145	0.2841	$x = 2\pi/145, y = 64\pi/145, z = 76\pi/145$
165	0.2783	$x = 2\pi/33, y = 20\pi/33, z = 2\pi/5$
203	0.2603	$x = 2\pi/203, y = 290\pi/203, z = 70\pi/203$
225	0.2499	$x = 82\pi/225, y = 118\pi/225, z = 126\pi/225$
217	0.2511	$x = 2\pi/217, y = 250\pi/217, z = 168\pi/217$
225	0.2499	$x = 82\pi/225, y = 118\pi/225, z = 126\pi/225$
240	0.2239	$x = \pi/40, y = 9\pi/40, z = \pi/6$
273	0.2152	$x = 2\pi/273, y = 208\pi/273, z = 142\pi/273$
295	0.2237	$x = 14\pi/295, y = 104\pi/295, z = 22\pi/59$
297	0.1910	$x = 242\pi/297, y = 548\pi/297, z = 54\pi/297$
299	0.1858	$x = 8\pi/299, y = 220\pi/299, z = 18\pi/299$
300	0.1736	$x = \pi/150, y = 51\pi/150, z = 5\pi/6$

TABLE III

DIVERSITY SUM OF 2 DIMENSIONAL CONSTELLATION BASED ON WEAK GROUP STRUCTURE [7]

number of elements	Diversity Sum	Codes and Comments
2	1	$x = \pi, y = \pi, z = 0$ (optimal)
3	$\sqrt{3}/2$	$x = 2\pi/3, y = 2\pi/3, z = 0$ (optimal)
5	$\sqrt{5}/8$	$x = 2\pi/5, y = 8\pi/5, z = 4\pi/5$ (optimal)
9	$3/4$	$x = 10\pi/9, y = 4\pi/3, z = 4\pi/9$ (optimal)
16	$\sqrt{2}/2$	$x = \pi/4, y = 5\pi/4, z = 13\pi/8$ (optimal)
18	0.6614	$x = 4\pi/9, y = 2\pi/3, z = 7\pi/9$
19	0.6391	SA searched code
20	0.6338	SA searched code
21	0.6307	SA searched code
22	0.6154	SA searched code
24	0.6124	$x = \pi/6, y = \pi/4, z = 5\pi/12$
28	0.5996	$x = 3\pi/8, y = \pi/2, z = 2\pi/7$
30	0.5934	$x = 4\pi/15, y = \pi/3, z = 7\pi/15$
31	0.5739	SA searched code
32	0.5734	SA searched code
39	0.5726	$x = 14\pi/39, y = 40\pi/39, z = 18\pi/39$
40	0.5499	$x = 3\pi/20, y = 7\pi/20, z = 3\pi/10$
42	0.5371	$x = 4\pi/7, y = 13\pi/21, z = \pi/3$
45	0.5342	$x = 2\pi/9, y = 4\pi/9, z = 14\pi/15$
52	0.5332	$x = \pi/13, y = 2\pi/13, z = 9\pi/26$
60	0.5000	$x = \pi/15, y = 4\pi/15, z = 3\pi/10$
64	0.4852	$x = 3\pi/16, y = 53\pi/32, z = 55\pi/32$
75	0.4850	$x = 32\pi/75, y = 14\pi/75, z = 2\pi/75$
76	0.4672	$x = 3\pi/19, y = 4\pi/19, z = 11\pi/38$
77	0.4595	$x = 52\pi/77, y = 82\pi/77, z = 60\pi/77$
85	0.4540	$x = 2\pi/17, y = 8\pi/17, z = 14\pi/85$
87	0.4460	$x = 52\pi/87, y = 98\pi/87, z = 82\pi/87$
95	0.4418	$x = 6\pi/19, y = 2\pi/95, z = 36\pi/95$
96	0.4390	$x = 39\pi/48, y = 5\pi/12, z = 11\pi/24$
99	0.4297	$x = 62\pi/99, y = 192\pi/99, z = 142\pi/99$
105	0.4295	$x = 2\pi/105, y = 16\pi/105, z = 28\pi/105$
106	0.4161	$x = 2\pi/53, y = 13\pi/53, z = 12\pi/53$
120	0.4156	$x = \pi/10, y = \pi/6, z = 5\pi/4$
123	0.4077	$x = 188\pi/123, y = 38\pi/123, z = 182\pi/123$
130	0.4071	$x = 26\pi/65, y = 5\pi/13, z = 2\pi/13$
133	0.3971	$x = 2\pi/133, y = 212\pi/133, z = 206\pi/133$
138	0.3963	$x = 16\pi/69, y = 19\pi/69, z = 4\pi/69$
145	0.3949	$x = 138\pi/145, y = 22\pi/145, z = 40\pi/29$
150	0.3758	$x = \pi/15, y = 8\pi/75, z = 19\pi/75$
155	0.3828	$x = 2\pi/5, y = 26\pi/31, z = 58\pi/31$
156	0.3824	$x = 5\pi/39, y = 8\pi/39, z = 15\pi/78$
158	0.3823	$x = 58\pi/79, y = 81\pi/79, z = 64\pi/79$
160	0.3802	$x = 69\pi/80, y = 59\pi/80, z = 37\pi/20$
162	0.3770	$x = 53\pi/21, y = 10\pi/9, z = 19\pi/81$
165	0.3760	$x = 24\pi/165, y = 26\pi/165, z = 34\pi/165$
166	0.3699	$x = 14\pi/83, y = 21\pi/83, z = 10\pi/83$
171	0.3678	$x = 32\pi/171, y = 294\pi/171, z = 6\pi/171$
178	0.3664	$x = 145\pi/89, y = 26\pi/89, z = 10\pi/89$
180	0.3636	$x = \pi/9, y = 97\pi/90, z = 127\pi/90$
193	0.3598	$x = 90\pi/193, y = 98\pi/193, z = 26\pi/193$
204	0.3566	$x = 13\pi/51, y = 4\pi/51, z = 5\pi/34$
208	0.3501	$x = \pi/13, y = 8\pi/13, z = 65\pi/104$
214	0.3476	$x = 98\pi/107, y = 67\pi/107, z = 59\pi/107$
220	0.3459	$x = 19\pi/11, y = 163\pi/110, z = 121\pi/110$
222	0.3438	$x = 19\pi/111, y = 22\pi/111, z = 15\pi/111$
225	0.3420	$x = 2\pi/225, y = 52\pi/225, z = 414\pi/225$
240	0.3371	$x = 71\pi/120, y = 11\pi/10, z = 187\pi/120$
244	0.3335	$x = 39\pi/122, y = 14\pi/61, z = 20\pi/61$
245	0.3305	$x = 16\pi/245, y = 186\pi/245, z = 46\pi/245$
248	0.3291	$x = 103\pi/124, y = 39\pi/31, z = 179\pi/124$
262	0.3274	$x = 142\pi/131, y = 215\pi/131, z = 87\pi/131$
264	0.3247	$x = 79\pi/66, y = 129\pi/66, z = 215\pi/132$
276	0.3237	$x = 23\pi/138, y = 15\pi/69, z = 6\pi/69$
292	0.3164	$x = 65\pi/146, y = 14\pi/73, z = 82\pi/73$
295	0.3147	$x = \pi/5, y = 50\pi/59, z = 22\pi/59$
300	0.3126	$x = \pi/75, y = 17\pi/150, z = 9\pi/25$

TABLE IV
 DIVERSITY PRODUCT AND DIVERSITY SUM FOR NON-SQUARE CONSTELLATIONS ($\tau = 5, n = 2$). [7]

Size	DP	Size	DS
3	0.8527	3	0.8693
4	0.8152	4	0.8589
5	0.7171	5	0.8243
6	0.7668	6	0.7976
7	0.7493	7	0.7960
8	0.7418	8	0.7844
9	0.7183	9	0.7659
10	0.6608	10	0.7737
20	0.6240	20	0.7243
30	0.5985	30	0.6837
40	0.5552	40	0.6576
50	0.5556	50	0.6392
60	0.5088	60	0.6237
90	0.4487	90	0.5775
300	0.3563	300	0.4369
600	0.2821	600	0.3687
900	0.2472	900	0.3358
3000	0.1867	3000	0.2461
6000	0.1545	6000	0.2163
9000	0.1296	9000	0.1874
10000	0.1426	10000	0.1735