Introducing 4D Geometric Shell Shaping

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Abstract—Four dimensional geometric shell shaping (4D-GSS) is introduced and evaluated for reach increase and nonlinearity tolerance in terms of achievable information rates and post-FEC bit-error rate. A format is designed with a spectral efficiency of 8 bit/4D-sym and is compared against polarization-multiplexed 16QAM (PM-16QAM) and probabilistically shaped PM-16QAM (PS-PM-16QAM) in a 400ZR-compatible transmission setup with high amount of nonlinearities. Numerical simulations for a single-span, single-channel show that 4D-GSS achieves increased nonlinear tolerance and reach increase against PM-16QAM and PS-PM-16QAM when optimized for bit-metric decoding (R\textsubscript{BMD}). In terms of R\textsubscript{MBD}, gains are small with a reach increase of 1.6% compared to PM-16QAM. When optimizing for mutual information, a larger reach increase of 3% is achieved compared to PM-16QAM. Moreover, the introduced GSS scheme provides a scalable framework for designing well-structured 4D modulation formats with low complexity.

Index Terms—Constellation shaping, geometric shaping, four-dimensional constellations, probabilistic shaping, nonlinear fiber channel.

I. INTRODUCTION

In recent years, constellation shaping techniques such as probabilistic shaping (PS) [1], [2], [3], [4], [5], [6] and geometric shaping (GS) [7], [8], [9], [10], [11] have been widely investigated to cope with the exponentially increasing capacity demand of optical fiber communication. These techniques can be used to alter the properties of the transmitted constellation to increase the achievable information rates (AIRs) of a communication system. GS imposes a nonuniform probability distribution on the constellation points of a square constellation while GS changes the location of the constellation points and allows for nonequidistant spacing of the points. It has been shown that for the additive white Gaussian noise (AWGN) channel and a given (finite) constellation cardinality, PS outperforms GS [9, Fig. 2], [12, Figs. 2, 3] and also allows for very fine rate-adaptivity [1, Fig. 1]. This comes however at the cost of requiring additional steps in the digital signal processing (DSP) chain. For example, if the probabilistic amplitude shaping (PAS) architecture [1] is used, a shaper and a deshaper are required. GS has the advantage of not requiring extra DSP, but it does require changes to the mapper and demapper. It is well known that demapper complexity increases when increasing demapping dimensionality [13], however, it has been shown that careful design can achieve a good balance between performance and complexity for multidimensional soft demappers (see e.g., [14]).

Designing constellations via GS lifts restrictions previously in place from equally-spaced square quadrature amplitude modulation (QAM). Conventional shaped constellation design is done by targeting the AWGN channel, for which a Gaussian-like constellation shape is optimal [15, Chs. 8, 9]. The resulting increase in performance is called linear shaping gain. PS on square (two-dimensional) QAM achieves this by targeting the same Maxwell-Boltzmann (MB) distribution on every dimension, while GS places constellation points in the 2D I-Q plane allowing nonuniform distance between the constellation points. In the context of optical communication, AWGN-optimized constellations have been applied in nonlinear optical fiber communications [2], [9], [16], [17] by using polarization multiplexing. While this method of designing constellations is relatively simple and provides considerable performance improvements [3], the nonlinear nature of optical fibers results in performance penalties for higher launch powers due to the assumed linearity of the channel [18].

To further improve performance in fiber-optical systems, research has moved towards designing constellations with nonlinear tolerance in mind [18], [19]. It has been shown that multidimensional constellation design is able to provide tolerance against nonlinear fiber effects by reducing nonlinear interference noise (NLIN), in addition to providing linear shaping gains [20], [10]. Therefore, designing constellations in more than two dimensions is necessary for achieving higher AIRs in optical communications limited by NLIN. Currently, 4D constellations optimized under an AWGN channel assumption providing reach increase for optical communications exist up to 10 bits/4D-sym [19, Fig. 2]. Constellations designed under an optical channel assumption also exist up to 10-bits/4D-sym [19, Fig. 3],[21], which employ machine learning to cope with the optimization complexity.

The challenge in designing constellations with more than two dimensions is the exponential increase in degrees of freedom (DOFs) that is generally associated with increasing the number of dimensions while maintaining equal spectral
efficiency (SE) per real dimension. Simple unconstrained optimizations are time consuming, might not lead to a global optimum, and generally provide unstructured results. From a practical point of view, well-structured constellations are always preferred since they allow for more efficient demapping strategies (e.g., by utilizing separability and symmetry of the constellations) [22], [23].

Designing an optimal constellation generally requires some form of iterative optimization for evaluating performance after each iteration. A channel model of the target communication link is thus required. The most straightforward method is using the computationally expensive but very accurate split-step Fourier method (SSFM) method. It is however desirable to reduce complexity of the optimization procedure to a more manageable level by using a simplified model or a simplified optimization objective. For simplified models, closed-form models which approximate the NLIN are available, like the EGN model [24], or its recently introduced extension to dual-polarization [25]. Model-aided optimization is used for example in [18], [26].

Another way of simplifying the design is reducing the DOFs within the optimization problem. This reduction in DOFs is generally achieved by imposing constraints which exploit existing regularities (e.g., symmetries), as used in [27], [11]. However, these works target the AWGN channel for constellation design, which potentially impacts performance negatively when applied to a nonlinear fiber communication system.

In this paper, a novel framework is introduced for geometrically optimizing 4D constellations for symbol-metric decoding (SMD) and bit-metric decoding (BMD) for the nonlinear fiber channel by using shell constraints together with symmetry constraints. This approach, denoted as 4D geometric shell shaping (GSS), provides a well-structured constellation, reduces optimization complexity, and leads to negligible performance degradation, all while providing increased nonlinear tolerance. 4D-GSS is studied for a SE of 8 bits/4D-sym such that the constellation cardinality.1 Throughout this paper, \( \mathbf{x}_i \triangleq (x_{1i}, x_{2i}, x_{3i}, x_{4i}) \in \mathbb{R}^4 \) is a vector denoting the \( i \)-th constellation point of \( \mathbf{X} \) with \( x_{1i} \neq x_j \) for \( i \neq j \). The 2D coordinates of the \( x \)- and \( y \)-polarization are represented by \( x_{1i}, x_{2i} \) and \( x_{3i}, x_{4i} \), respectively, and the rows of \( \mathbf{X} \) are labeled using a fixed binary labeling. In other words, the \( i \)-th symbol \( x_i \) is associated with a unique binary label \( b_i = (b_{1i}, b_{2i}, \ldots, b_{mi}) \).

B. Achievable Information Rates

A number of metrics exist for evaluating the performance of a fiber optical system. For systems based on SMD, the mutual information (MI) is often used. Using Monte-Carlo simulations, the MI can be approximated as

\[
\text{MI} = \frac{1}{D} \sum_{i=1}^{D} \log_2 \frac{q_{Y|X}(y_i|x_i)}{\sum_{j=1}^{M} P_X(x_j)q_{Y|X}(y_i|x_j)},
\]

where \( P_X(x_j) \) is the probability of the symbol \( x_j \), \( D \) is the number of transmitted symbols and \( q_{Y|X} \) is the auxiliary channel, which is an approximation of the actual channel law \( f_{Y|X} \) from which the samples \( y_1, y_2, \ldots, y_D \) are taken from. We use mismatched decoding [29] in this paper for which \( q_{Y|X} \) in (1) is considered to be the AWGN channel, i.e.,

\[
q_{Y|X}(y|x) = \frac{1}{(\pi \sigma^2/2)^2} \exp \left(-\frac{||y-x||^2}{\sigma^2/2}\right),
\]

where \( \sigma^2 \) is the total noise variance of the 4D AWGN channel. The expression in (1) is a modified version of [30, Eq. (30)] that takes probabilities into account (for PS).

For bit-interleaved coded modulation (BICM) systems with BMD and uniform signaling, a popular performance metric is the generalized mutual information (GMI) [30]. When PS is included in such a system, the BMD rate [3] is calculated instead, which extends GMI to take nonuniform probabilities into account and is equivalent to GMI for uniform probabilities. We approximate the BMD rate via Monte-Carlo simulations as [3, Eq. (8)]

\[
R_{\text{BMD}} = \sum_{k=1}^{m} \left( I(C_k; Y) - m \right) H(C_k) + H(C)
\]

\[
\approx - \sum_{j=1}^{M} P_X(x_j) \log_2 P_X(x_j) - \frac{1}{D} \sum_{k=1}^{m} \sum_{i=1}^{D} \log_2 \left( 1 + e^{(-1)^{k+1} L_k,i} \right),
\]

\[1\text{Notation convention:} \ \text{Calligraphic letters} \ X \ \text{represent sets. Blackboard bold letters} \ \mathcal{X} \ \text{denote matrices in which} \ x_i \ \text{are row vectors denoting the} \ \mathbf{x}^\text{th} \ \text{row. Conditional probability density functions (PDFs)} \ \text{are denoted by} \ f_{Y|X}(y|x), \ \text{where} \ Y \ \text{and} \ X \ \text{denote random (4D) vectors and} \ x \ \text{and} \ \mathbf{x} \ \text{denote their realizations. Probability mass functions (PMFs)} \ \text{are denoted by} \ P_X(x), \ \text{expectations are denoted by} \ E[\cdot] \ \text{and} \ \mathbb{E}\mathbb{E}\mathbb{E} \ \text{denotes binary negation. The squared Euclidean norm of a matrix is denoted by} \ ||X||^2 = ||x_1||^2 + \ldots + ||x_M||^2, \ \text{where} \ ||x_i||^2 = x_{1i}^2 + \ldots + x_{4i}^2. \ \text{The indicator function is denoted by} \ I[\cdot], \ \text{which is 1 when its argument is true and 0 otherwise, and} \ \mathbb{R} \ \text{and} \ \mathbb{N} \ \text{denote the set of all real and natural numbers, respectively, with} \ \mathbb{R}_{\geq 0} \ \text{denoting the set of all positive real numbers.} \]
where \( C_k \) is the random variable representing the transmitted bit at bit position \( k \), \( I(C_k; Y) \) is the bit-wise MI between \( C_k \) and output \( Y \). \( c_{k,i} \) are the transmitted coded bits and \( L_{k,i} \) are the log-likelihood ratios (LLRs) defined as

\[
L_{k,i} = \log \frac{\sum_{j \in j^i_k} q_{j}^Y | X(y_j | x_j) P_X(x_j)}{\sum_{j \in j^i_k} q_{j}^Y | X(y_j | x_j) P_X(x_j)}, \tag{5}
\]

where \( j^i_k \) is the set of constellation point indices with \( b \in \{0, 1\} \) at bit position \( k \).

In this work we consider GS to have uniform symbol probabilities with independent bit levels. This implies \( -\sum_{j=1}^{M} P_X(x_j) \log_2 P_X(x_j) = m - \sum_{k=1}^{m} H(C_k) + H(C) = 0 \) in (4) and \( P_X(x_j) \) in (5) is not needed, resulting in

\[
R_{\text{BMD}} = \sum_{k=1}^{m} I(C_k; Y) \tag{6}
\]

\[
\approx m - \frac{1}{D} \sum_{k=1}^{m} \sum_{i=1}^{D} \log_2 \left( 1 + e^{(-1)^{t_k,i} L_{k,i}} \right), \tag{7}
\]

where

\[
L_{k,i} = \log \frac{\sum_{j \in j^i_k} q_{j}^Y | X(y_j | x_j)}{\sum_{j \in j^i_k} q_{j}^Y | X(y_j | x_j)}. \tag{8}
\]

To evaluate the performance predictions made by the above-mentioned AIRs, post-forward error correction (FEC) bit error rates (BERs) will also be calculated. The system model is shown in Fig. 1 indicating the performance metrics which are considered in this paper.

### C. Optimizing Geometric Shaping in 4D

The constellation \( \mathcal{X} \) is typically designed to maximize a certain performance metric \[9\]. In this paper, \( R_{\text{BMD}} \) is the chosen metric and the optimal constellation is denoted by \( \mathcal{X}^* \).

The resulting optimization problem is defined as

\[
\mathcal{X}^* = \arg \max_{\mathcal{X} \in \mathcal{X}} R_{\text{BMD}}(\mathcal{X}), \tag{9}
\]

where \( R_{\text{BMD}} \) is given by (6) and (8), and \( \mathcal{X} \) is the set containing all \( 4 \times M \) real-valued matrices satisfying a variance (power) constraint, i.e.,

\[
\mathcal{X} \triangleq \{ \mathbf{x} : \mathbf{x}_i \in \mathbb{R}^4, i = 1, 2, \ldots, M, E[||\mathbf{x}||^2] \leq P \}. \tag{10}
\]

The optimization problem in (9) has four DOFs per constellation point, one for each dimension, resulting in \( 4M \) DOFs.

We call this the \textit{unconstrained optimization} and denote it by \textbf{4D-GS}. The DOFs are directly related to the dimensionality 4 and the constellation cardinality \( M = 2^m \). From this we see that for increasing constellation sizes, the DOFs grow exponentially and the optimization becomes challenging.

In this paper, instead of solving the unconstrained optimization in (9), we define a set of constraints which reduce the DOFs, while minimizing the potential loss in performance.

The optimization under these constraints is defined as

\[
\mathcal{X}^* = \arg \max_{\mathcal{X} \in \mathcal{X}_{\text{GSS}}} R_{\text{BMD}}(\mathcal{X}), \tag{11}
\]

where the optimization space is constrained to \( \mathcal{X}_{\text{GSS}} \subset \mathcal{X} \).

As we will show below, the imposed constraints make the optimization problem in (11) to only have 28 DOFs instead of 1024 DOFs for the chosen system (\( m = 8 \)).

In this paper we propose to impose three constraints on the constellation, which we call (i) “uniform t-shell division”, (ii) “X-Y symmetry”, and (iii) “orthant symmetry”. We call the optimization under these constraints \textbf{4D-GSS}. In what follows, we explain these three constraints and how they lead to 28 DOFs for \( m = 8 \). As we will show in Sec. IV-A, the loss in performance by introducing these three constraints is minimal.

### D. GSS Constraints

Each of the three constraints mentioned in Sec. II-C is associated with a part of the binary labeling, which is considered to be fixed. Fig. 2 provides an example of how the bit allocation is predefined under the considered constraints in a 4D constellation with \( m = 8 \) bits and \( t = 4 \) shells. The left side of Fig. 2 shows 16 constellation points belonging to a single orthant\(^2\) with their corresponding binary labels. The binary labels are grouped into sets of bits referred to by (a) through (d). The four bits in (a) define an orthant. In Fig. 2 only the first orthant is shown and thus, all \( x_i \) have the same binary label (all zeros) for (a). The two bits in (b) determine the shell, with each shell having the same amount of points (2 in this case). The bits in (c) select between two points on a shell, and (d) selects between two X-Y symmetric points.

The three GSS constraints described above reduce the number of 4D constellation points to be optimized from \( 2^8 = 256 \) to only \( 2^{m-5} = 8 \) (filled circles in Fig. 2) with a reduction in DOFs from 1024 to 28. In what follows, we formally describe the set \( \mathcal{X}_{\text{GSS}} \) together with two symmetry operations that make up these three GSS constraints.

\(^2\)An orthant is a generalization in \( N \)-dimensional Euclidean space of what a quadrant is in the 2D plane.
Definition 1 (Uniformly divided t-shell constraint):

\[
\mathcal{X}_{\text{GSS}} \triangleq \{ \mathbf{x} : \mathbf{x}_1 \in \mathbb{R}^4_{>0}, \| \mathbf{x}_1 \| \in \mathcal{R}_t, \\sum_{i=1}^t \| \mathbf{x}_i \| = r_j \} = \frac{2^{m-5}}{t}, \tag{12a}
\]

\[
i = 1, 2, \ldots, 2^{m-5}, j = 1, 2, \ldots, t, \tag{12b}
\]

and \(r_j\) is the radius of the \(j\)-th 4D shell out of a total of \(t\) 4D shells.

The \(2^{m-5}\) shell constraint forces constellation points to be equally divided on the \(t\) concentric 4D shells in the all positive \(\mathbb{R}^4_{>0}\) space (first orthant). This uniformly divided part of this constraint is provided by (12b). The upper limit for \(t\) is given by \(2^{m-5}\) (see (13)), which is equivalent to having a dedicated shell for each constellation point. In the case of \(t = 1\), this constraint turns into a constant modulus constraint, effectively creating a generalization of the format proposed in [10]. By forcing each point to be on top of a certain shell, we take away one additional DOF per constellation point, such that 3 DOFs per constellation point remain. However, \(t\) extra DOFs are added due to the number of the shells. This results in \(3 \cdot 2^{m-5} + t\) DOFs. The advantage of having an integer power of two \((t = 2^p)\) shells is that \(p\) out of \(m - 5\) bits can be used to select the shell. In Fig. 2, \(p = 2\). This offers the possibility of achieving rate-adaptivity by adding PS on top of GSS using the PAS architecture [1], which is called hybrid shaping. In this case, only the bits which select the shell are shaped. The remaining \(m - p - 5\) uniform bits select the specific constellation points on a shell.

In the remainder of this section we will assume an identical setup to the one in the example in Fig. 2. As a result \(|\mathcal{X}_{\text{GSS}}| = 8\) and the 8 constellation points are labeled by \(\mathbf{l}_i = [b_{5i}, b_{6i}, b_{7i}] \in \{0, 1\}^3\).

Operation 1 (X-Y symmetry): An X-Y symmetry operation applied to 8 points \(\mathbf{x}_i\) with \(i = 1, 2, \ldots, 8\) results in 16 points and binary labels

\[
\mathbf{x}_{i+8} = [x_{3i}, x_{4i}, x_{xi}, x_{2i}], \quad \mathbf{l}_{i+8} = [l_i, b_{5i}], \quad \mathbf{l}_{i+8} = [l_i, b_{6i}], \tag{14}
\]

X-Y symmetry mirrors the points in the \(\mathcal{X}_{\text{GSS}}\) set over its two polarizations. A single bit added to the labeling end is used to distinguish between the two X-Y symmetric points. The X-Y symmetry also ensures identical average transmit power over the two polarizations. In Fig. 2, this mirroring causes for example \(\mathbf{x}_0\) to become \(\mathbf{x}_{15}\) and the extra bit added to the binary labels is \(d\) and \(\overline{d}\), resp. After applying the X-Y symmetry operation to \(\mathcal{X}_{\text{GSS}}\), we must apply the orthant symmetry operation, defined as follows.

Operation 2 (Orthant symmetry): The orthant symmetry operation applied to 16 points \(\mathbf{x}_{i}\) with \(i = 1, 2, \ldots, 16\) gives

\[
\mathbf{x}_{i+16(j-1)} = [x_{2i}, x_{3i}, x_{4i}, x_{xi}], \quad \mathbf{l}_{i+16(j-1)} = [l_1, l_2, l_3, l_4, \mathbf{l}], \tag{15}
\]

for \(j = 1, 2, \ldots, 16\), and where \(\mathbb{H}_j\) is the mirroring matrix of the \(j\)-th orthant

\[
\mathbb{H}_j = \begin{bmatrix}
(-1)^{\tilde{j}_1} & 0 & 0 & 0 \\
0 & (-1)^{\tilde{j}_2} & 0 & 0 \\
0 & 0 & (-1)^{\tilde{j}_3} & 0 \\
0 & 0 & 0 & (-1)^{\tilde{j}_4}
\end{bmatrix}, \tag{16}
\]

where \([l_1, l_2, l_3, l_4]\) is the binary representation of \(j\), i.e., \(j - 1 = \sum_{k=1}^4 l_k 2^{k-1}\) with \(l_k \in \{0, 1\}\).

The mirroring matrices transform each of the 16 points in \(\mathbf{x}_i\) to all \(2^8 = 16\) orthants with corresponding binary labels \(\mathbf{b}_i\), resulting in a total of 256 constellation points and label combinations, given by

\[
\begin{align*}
\mathbf{x}_i &= [x_{1i}, x_{2i}, x_{3i}, x_{4i}, \mathbf{b}_i] = [0, 0, 0, 0, \mathbf{l}], \\
\mathbf{x}_{i+16} &= [-x_{1i}, x_{2i}, x_{3i}, x_{4i}, \mathbf{b}_{i+16}] = [1, 0, 0, 0, \mathbf{l}], \\
\mathbf{x}_{i+32} &= [x_{1i}, -x_{2i}, x_{3i}, x_{4i}, \mathbf{b}_{i+32}] = [0, 1, 0, 0, \mathbf{l}], \\
\vdots \\
\mathbf{x}_{i+240} &= [-x_{1i}, -x_{2i}, -x_{3i}, -x_{4i}, \mathbf{b}_{i+240}] = [1, 1, 1, 1, \mathbf{l}].
\end{align*}
\]

The first orthant \(\mathbb{R}^4_{>0}\) in Definition 1 only considers 4D symbols with all their components to be positive. Orthant symmetry is achieved by mirroring the \(2^{m-4}\) constellation points (after applying the X-Y symmetry operation) with respect to the origin along the axes of the 4 dimensions and by changing the bits \(b_1, b_2, b_3, b_4\) (see (15)), where each of these bits is associated with the sign of one real dimension.

An advantage of assigning bits in this manner is that it ensures the orthants themselves are Gray-labeled (adjacent orthants differ only in one bit), which provides higher AIRs compared to other labeling strategies when used in BICM systems [31]. In the context of optical communications, the mirroring procedure was first used in [11, Sec. II-B].
Example 1 (Application to 400ZR): The described constraints are applied to 4D constellations targeting the same SE as uniform PM-16QAM, therefore \( m = 8 \). The number of shells is chosen to be \( t = 4 \). First, the uniformly divided \( t \)-shell constraint is applied to the \( 2^m - 5 = 8 \) constellation points within the first orthant. This results in the set \( X_{\text{GSS}} \) with \( 3 \cdot 2^m - 5 + t = 28 \) DOFs. Since \( t = 4 \), two bits are used to index the shell. Applying the X-Y symmetry operation to \( X_{\text{GSS}} \) increases the number of constellation points in the first orthant by a factor 2 to \( 2^m - 4 = 16 \). When applying the orthant symmetry operation, four bits are assigned to select the orthant with groups of two bits assigned to the quadrants in the X and Y polarization respectively, which together define the orthant. This increases the number of constellation points by a factor 2, which results in the desired total amount of \( 2^8 = 256 \) 4D constellation points.

By using the three constraints described above, the DOFs are reduced from an unconstrained 1024 \((4 \cdot 2^8)\) to 28 \((3 \cdot 2^8 - 4)\). Fig. 3 compares the DOFs when using 4D-GSS compared to the unconstrained case of 4D-GS for increasing constellation sizes. Table I shows the DOFs and the number of 4D shells for a number of different constellation types at a fixed SE of \( m = 8 \).

III. SYSTEM SETUP AND OPTIMIZATION

A. Link specification

For designing constellations with high nonlinear tolerance in mind, a suitable transmission scenario needs to be chosen which is expected to have high NLIN. For this reason an unamplified 400ZR link is chosen [28], for which the transmitted constellation is PM-16QAM which matches the desired cardinality of the considered 4D-GSS constellation.

The considered system transmits a dual-polarized, single channel waveform over a single span of standard single-mode fiber (SSMF). This setup is simulated via the split-step Fourier method (SSFM) with 1000 steps per span and fiber parameters \( \alpha = 0.2 \) dB/km, \( \beta_2 = -21.68 \) ps\(^2\)/km and \( \gamma = 1.20 \) (W-km\(^{-1}\)). The symbol rate is matched to the 400ZR specification will be used as a guideline.

B. Transceiver impairments

At the transmitter side, the 400ZR specification requires the in-band optical signal-to-noise ratio (OSNR) to have a minimum value of 34 dB/0.1nm. At the receiver side, the concatenated FEC scheme in the 400ZR standard is specified to operate error-free (post-FEC BER = \( 10^{-15} \)) when a pre-FEC BER of \( 1.25 \cdot 10^{-2} \) or lower is achieved. The receiver sensitivity requires least \(-20\) dBm of power to be present at the input of the receiver. These previous two conditions combined with the minimum of 34 dB OSNR at the transmitter guarantee error-free operation.

In simulations, the transmitter is emulated by adding AWGN to the transmitted waveform such that the OSNR value is equal to the in-band OSNR limit. For the receiver it is possible to calculate the necessary AWGN addition using [32, Eq. (18)]

\[
P_e \approx \frac{4}{m} \left(1 - \frac{1}{\sqrt{M}}\right)^{\frac{M}{2}} \sum_{i=1}^{M} Q\left(\frac{(2i - 1) \sqrt{E_b}}{N_0 (M - 1)}\right)\]

where \( P_e \) is the targeted BER, \( Q(\cdot) \) is the Q-function and \( E_b/N_0 \) is the accompanying SNR per bit under a Gray-coded \( M \)-QAM assumption in an AWGN channel. For 16QAM and a BER of \( 1.25 \cdot 10^{-2} \), (18) provides an \( E_b/N_0 \) of 7.53 dB, which translates to a signal-to-noise ratio (SNR) of 13.5 dB. Assuming that an input power of \(-20\) dBm is present at the receiver in a back-to-back scenario, the amount of noise power added in the receiver is equal to \(-33.5\) dBm. This is added as AWGN after simulating the optical fiber.

C. Forward Error Correction

400ZR uses a concatenated FEC scheme as defined in [28, Sec. 10] consisting of an outer staircase code (SCC) with hard-decision (HD) decoding of rate 0.937, and an inner Hamming code with soft-decision (SD) decoding of rate 0.930, resulting in a total overhead of 14.8%. The SCC in 400ZR is defined to be taken from [33, Annex A], which describes a \((255, 239)\) SCC with blocks of size 512 \times 510 and a \((1022, 990)\) Bose-Chaudhuri-Hocquenghem (BCH) code as the component code. The FEC code is a double-extended \((128, 119)\) Hamming code using a parity-check matrix as described in [28, Sec. 10.5].

Instead of implementing the full concatenated FEC as described above, in this paper we only implemented the Hamming code and a SD decoder based on a Chase-I decoder [34]. A post-FEC BER after the Hamming decoder of \( 4.5 \cdot 10^{-3} \) is targeted, which is the required pre-FEC BER for the \((255, 239)\)
SCC to achieve a BER of $10^{-15}$ at the output. The scrambling and interleaving steps are approximated by using a bit-wise fixed random permutation after FEC encoding and the inverse operation before FEC decoding. The full system diagram is shown in Fig. 4.

D. Optimization

In (20), the optimization problem for determining $X^*$ was defined. If the constraints from Sec. II are applied, the optimization only needs to be performed for the 28 resulting DOFs. To enforce the shell constraints, each point out of the 8 points in $X^*$ is now represented in spherical coordinates $(r_i, \theta_j, \phi_j, \omega_j)$, where $i = 1, 2, 3, 4$ and $j = 1, 2, \ldots, 8$. The optimization problem can now be defined as

$$\{r^*, \theta^*, \phi^*, \omega^*\} = \arg\max \text{R}_{BMD}(r, \theta, \phi, \omega) \quad (19)$$

where the parameters $(r, \theta, \phi, \omega)$ are constrained such that the corresponding points are in $X^*$.

Since there are no existing constellations which strictly adhere to the chosen constraints, selecting an initialization for the optimization procedure is not straightforward. It was determined on a trial-and-error basis that there were no clear differences in resulting performance after optimization between randomly initialized constellations and constellations which were initialized with a distinct structure. For that reason it was chosen to initialize all parameters at the halfway point between the upper and lower bounds, which are shown in (19).

Optimization over the system in Fig. 4 is performed using a patternsearch optimizer [35], which is a derivative-free multidimensional optimization algorithm. Patternsearch automatically finds the optimal way to spread out the constellation. To enhance stability during the optimization procedure, fixed random seeds are used for the sequence generation and AWGN noise additions.

IV. RESULTS

A. $R_{BMD}$ optimized constellations

Conventional PM-16QAM, as used in the 400ZR standard, is considered as a baseline. Next to that, PS is applied on top of PM-16QAM by shaping each real dimension with an ideal amplitude shaper, where amplitudes are randomly drawn from a predefined distribution. The distribution is optimized for each pair of launch power and transmission distance, and is not constrained to be a MB distribution. The proposed 4D-GSS-4 constellations are also optimized and evaluated for each pair of launch power and distance. Lastly, a 4D sphere packed constellation is also considered, specifically the 256 point Welti constellation (w4-256) [36]. Sphere packed constellations are optimal for the AWGN channel for a given SE and will provide insight into the maximum expected performance in the linear region later in this paper. For $R_{BMD}$ evaluation, w4-256 uses the optimized binary labeling from [37].

Fig. 5(a) shows $R_{BMD}$ results for a distance sweep between 120 and 180 km in which 4D-GSS-4 achieves 1.3% gain in $R_{BMD}$ and 1.6% gain in distance compared to PM-16QAM around 160 km. Since in this specific scenario, the 400ZR link is loss-limited, results are shown at optimal launch power until the distance is too large to satisfy the received power requirement of at least $-20$ dBm. The point after which this occurs is indicated by solid markers. Beyond these markers, the constellations are pushed to launch powers above the optimal value to satisfy the received power requirement. In Fig. 5(a), it is shown that the distance for which 4D-GSS-4 can operate at optimal launch power is approximately 5 km larger than the other considered constellations. This increase in maximum optimal launch power is also reflected in Fig. 5(b) where 4D-GSS-4 has 0.5 dB higher optimal launch power ($P^*$) compared to the baselines and hence, the highest nonlinear tolerance among the considered schemes. The region where NL tolerance is observed is indicated in yellow. In the linear domain, 4D-GSS-4 has similar performance to PM-16QAM and loses in performance compared to PM-16QAM-PS. Even though an optimized binary labeling is used for the w4-256 constellation, since it is not designed to maximize $R_{BMD}$, it performs poorly.

To evaluate the performance losses induced by the GSS constraints, optimized 4D constellations which have either only orthant symmetry as the constraint (denoted with 4D-OS), or a combination of orthant symmetry and X-Y symmetry (denoted as 4D-OS+X-Y), are evaluated around the optimal launch power. It is shown in Fig. 5(b) that removing the shell constraints from 4D-GSS-4 increases the performance by 0.012 bit/4D-sym, which is less than 0.2%. Additionally, removing the X-Y constraint, and thus only leaving the orthant symmetry constraint, has almost zero impact. Furthermore, it has been shown in [11, Fig. 6] that lifting the orthant symmetry constraint has a marginal impact on performance. All this indicates that the proposed symmetry constraints as used in 4D-GSS-4 have very little impact on total performance, but do reduce the optimization complexity significantly. Fig. 5(b) also includes MI results for 4D-GSS-4 (denoted by 4D-GSS-4 MI). This indicates the theoretical upper limit for the $R_{BMD}$ where it is clear that quite a large gap still exists between the
Fig. 5. $R_{\text{BMD}}$ vs transmission distance at optimal launch power (left) and launch power for a distance of 160 km (right). Solid markers show the transition to pushing above optimal launch power. Constellation inset shows received symbols at optimal launch power for a distance of 120 km.

One possible explanation of the increased nonlinear tolerance of 4D-GSS-4 can be observed from Fig. 6, which shows the peak-to-average power rating (PAPR) of the considered constellations. The accompanying table shows that PM-16QAM has a PAPR of 1.8, while 4D-GSS-4 constellations have a PAPR of 1.25 on average over the considered distances, which is a reduction of 40% compared to PM-16QAM. Note that PAPR is only a rough indicator for evaluating nonlinear tolerance, and other factors also play a role [11, Sec. 2-D].

Fig. 7 shows the post-FEC BER of 4D-GSS-4 compared to PM-16QAM when the inner Hamming code is SD-decoded as described in Sec. III-C, together with HD decoding of the same code. The outer SCC has a FEC limit of $4.5 \times 10^{-3}$, which is used as the minimum required BER after the Hamming code for error-free operation. A gain of 2% in transmission distance between 4D-GSS-4 and PM-16QAM is achieved at the SCC-FEC limit, which is very close to the observed 1.6% gain in $R_{\text{BMD}}$. The HD-decoded Hamming code shows similar gains between the two constellation types but cannot satisfy the SCC-FEC limit over similar distances. When only the Hamming codes are considered without the outer SCC, gains increase to in-between 2.5% and 3.3% depending on the specific distance and code, as indicated by the $10^{-3}$ BER line.

B. MI optimized constellations

It was observed in Fig. 5(b) that the $R_{\text{BMD}}$ for the optimized 4D-GSS-4 constellations was consistently lower than the MI by about 0.08 bits/4D-sym. This could indicate an issue with the binary labeling since PM-16QAM-PS (PM-16QAM-PS) did not show such a gap. To find the potential upper performance limit of 4D-GSS-4, the optimization procedure was repeated using the MI as the performance metric, using (1) for evaluating the MI. This results in the following optimization problem

$$X^* = \arg\max_{X \in \mathcal{X}} \text{MI}(X).$$

Fig. 8(a) shows MI results for a distance sweep between 120 and 180 km. In this case 4D-GSS-4 shows gains of 3% in distance and 2.5% in MI vs. PM-16QAM and is slightly outperformed by w4-256. Again, Fig. 8(b) shows that 4D-GSS-4 has the largest optimal launch power. Moreover, due to the rapidly-vanishing MI of w4-256, 4D-GSS-4 outperforms w4-256 at very high powers ($P > 14$). However, for lower
transmission distances and optimal launch power (left) and average PAPR over the shown distances (right).

PAPR results in Fig. 9 show similar results to Fig. 6, with the main difference being that the MI optimized 4D-GSS-4 constellations have even lower average PAPR, increasing the difference against PM-16QAM from to 49%. Against w4-256, 4D-GSS-4 shows a reduction in PAPR of 10%, which could contribute to 4D-GSS-4 gaining performance in terms of MI over w4-256 for launch powers larger than 14 dBm.

C. Bitwise MI

To investigate possible causes of the binary labeling penalty for 4D-GSS-4, we look at the bit-wise MI as given by (6). Table II compares the bit-wise MI of 4D-GSS-4, PM-16QAM and w4-256 at the optimal launch powers. The individual bits are denoted by \( b_i \) for \( i = 1, \ldots, m \) and \( \text{R}_{\text{BMD}} \) is added in (6) as a reference. For PM-16QAM, the bits are reordered such that the bits which determine the signs are the first four bits (same as 4D-GSS-4). This does not effect the performance since PM-16QAM is a Cartesian product of 4 independent pulse amplitude modulation (PAM)-4 constellations. As a result, this also implies symmetry across all four dimensions and thus, PM-16QAM also has orthant symmetry.

| Constellation | Average PAPR |
|---------------|--------------|
| 4D-GSS-4      | 1.21         |
| PM-16QAM      | 1.80         |
| PM-16QAM-PS   | 1.89         |
| w4-256        | 1.33         |

\( \text{R}_{\text{BMD}} = 13.5 \text{ dBm} \) and \( \text{MI} = 7.45 \) bit/4D-sym for PM-16QAM, whereas bit \( b_5 \) through \( b_8 \) determine the amplitude of each of the PAM-4 signals for PM-16QAM. For 4D-GSS-4, the bits \( b_5 \) and \( b_6 \) select the shell, bit \( b_7 \) selects between 2 points on a shell, and bit \( b_8 \) selects between X-Y symmetric points.

In terms of bit-wise MI, \( b_1 \) through \( b_4 \) perform identically for both PM-16QAM and 4D-GSS-4, which is expected due to both constellations employing orthant symmetry. Bits \( b_5, b_6 \) and \( b_8 \) have larger bit-wise MI for 4D-GSS-4 compared to PM-16QAM, whereas bit \( b_7 \) incurs a penalty. This suggests that the proposed structure combined with the chosen constellation cardinality does not allow for a good labeling of \( b_7 \). It is furthermore observed that the gap between \( \text{R}_{\text{BMD}} \) and MI of 0.08 bits/4D-sym is equal to the difference between the bit-wise MI of \( b_7 \) and \( b_8 \) in Table II. Lastly, as expected, w4-256 has much worse performance in general compared to the other two constellations since the structure of this constellation is not optimized for allowing a good binary labeling at all.

V. CONCLUSIONS

A novel framework is proposed for generating families of well-structured 4D geometrically-shaped constellations which are more nonlinearity-tolerant than conventional PM-16QAM. Numerical simulations show that the newly proposed 4D-GSS-4 constellations outperform both PM-16QAM and PS-PM-16QAM in a 400ZR-compatible transmission setup when optimized for \( \text{R}_{\text{BMD}} \). It was shown that the imposed constraints...
lead to negligible performance degradation while considerably reducing the optimization space and resulting in well-structured constellations. It was also found that the chosen constraints combined with the chosen SE do not allow for structured constellations. It was also found that the chosen abl...able reducing the optimization space and resulting in well-

Investigating better combinations of constellation cardinality (≥ 10 bits/4D-sym) and GSS (e.g., modifying shell constraints) is left for further investigation. Another area of possible research is to increase the dimensionality across channel time slots or number of wavelength channels (e.g., 8D-GSS).

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