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Universal Gröbner Bases for Designs of Experiments

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Summary. - *Universal Gröbner bases (UGB) are a useful tool to obtain a set of different models identified by an experimental design. Usually, the algorithms to obtain a UGB for the ideal of a design are computationally intensive. Babson et al. (2003) propose a methodology to construct UGB in polynomial time. Their methodology constructs a list of term orders based upon the Hilbert zonotope. We focus on the generation of such a list. We use results on hyperplane arrangements to present a theorem which simplifies the computation of term orders for designs in two dimensions. Our theorem constructs directly the normal fan of the Hilbert zonotope.*

1. Introduction

When analyzing an experiment, it is useful to consider different alternative models; for example in a computer experiment where the cost of every run is high and only a reduced number of runs is possible. In the analysis stage, we may want to have different models at hand, maybe to choose a simulator of our experiment. Then we

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can select a model based on the interpretation as well as the usual statistical criteria. A search through all the potential identifiable models would be impossible and thus we must restrict our class of models. In the present work we consider only the class of hierarchical polynomial models. This class has been studied previously in literature under the names "well-formed", "hierarchical" or "hierarchically well-formulated" models, see Bates *et al.* (2003) and Peixoto (1990). We also restrict the search to full rank models to ensure identifiability.

The search algorithms we are interested in are based on algebraic techniques and return a large subset of the class we are interested in. Depending on the design, sometimes the algebraic techniques return the whole class. However, the algebraic techniques rely on important results from polytopal geometry. For this reason, Sections 2 and 3 introduce both (algebraic and polytopal) notations and explain the link between them. In Section 4 we introduce an important polytope called the Hilbert zonotope, and describe its role in our problem. In Section 5 we give a new theorem which simplifies the current use of the zonotope in two dimensions. Some computational details are in the appendix.

2. Algebra and design of experiments

Pistone and Wynn (1996) pioneered the use of Gröbner bases in experimental design. They demonstrate that computational commutative algebra (CCA) is a useful tool, not only to propose different models, but also to study generalized confounding of models and model terms. We start by defining the experimental design and the class of models we will be considering along this work.

Definition 2.1. *An experimental design is a finite set of n distinct points $\mathcal{D} \subset \mathbb{R}^d$, where d is the number of factors and n is the number of runs.*

The class of hierarchical polynomial models we are interested in is in one-to-one correspondence with the set of staircases defined next.

Definition 2.2. *A staircase is a nonempty subset λ of the set $\mathbb{N}^d$ of non-negative integer vectors such that if $u \in \lambda$ and $v \leq u$ (coordinate-*

wise) then $v \in \lambda$. *Let* $\binom{\mathbb{N}^d}{n}_{stair}$ *denote the finite set of staircases with* n *elements.*

The cardinality of $\binom{\mathbb{N}^d}{n}_{stair}$ for $d = 2, 3$ is computed by MacMahon's classic formulas (see Appendix 7.1), while for $d \geq 4$ it is still an open problem, see Onn and Sturmfels (1999). The log map acts from the terms in $\mathbb{R}[x_1, \ldots, x_d]$ to $\mathbb{Z}^d$ as $\log(x_1^{\alpha_1} \cdots x_d^{\alpha_d}) = (\alpha_1, \ldots, \alpha_d)$. Then, one applies it to the terms in a hierarchical polynomial model and obtains a staircase.

Example 2.3. The hierarchical model $\{1, x_1, x_2, x_1x_2\}$ corresponds to the staircase $\{\binom{0}{0}, \binom{1}{0}, \binom{0}{1}, \binom{1}{1}\} \in \binom{\mathbb{N}^2}{4}_{stair}$.

Definition 2.4. *Let*

$$V_n^d := \bigcup_{\lambda \in \binom{\mathbb{N}^d}{n}_{stair}} \lambda \tag{1}$$

denote the union of all n*-staircases in* $\mathbb{N}^d$.

The computation of V_n^d can be simplified by noting that $V_n^d = \{v \in \mathbb{N}^d : \prod_{i=1}^d (v_i + 1) \leq n\}$. Babson *et al.* (2003) use the asymptotic bound $O(n(\log n)^{d-1})$ for the cardinality of V_n^d.

Example 2.5. For $n = 5$, $d = 2$, we have seven different staircases, and their union is

$$V_5^2 = \{\binom{0}{0}, \binom{1}{0}, \binom{2}{0}, \binom{3}{0}, \binom{4}{0}, \binom{0}{1}, \binom{0}{2}, \binom{0}{3}, \binom{0}{4}, \binom{1}{1}\},$$

see Figure *1* .

Now we give the basic elements for identifying models using CCA. The reader is referred to Cox *et al.* (1996) for a comprehensive resource on algebraic geometry and to Pistone *et al.* (2000) for the use of CCA in statistics.

Definition 2.6. *The design ideal* I *is the set of all polynomials that vanish on the design:* $I = \{f \in \mathbb{R}[x_1, \ldots, x_d] : f(x) = 0 \text{ for all } x \in \mathcal{D}\}$.

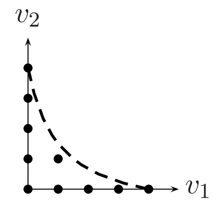

Figure 1: Picture of V_5^2. The dashed curve corresponds to $(v_1 + 1)(v_2 + 1) = 5$

Here $\mathbb{R}[x_1, \ldots, x_d]$ is the ring of polynomials in $x_1, \ldots, x_d$ indeterminates, which for simplicity we write as $\mathbb{R}[x]$. The ideal I is generated by a finite set of polynomials G and we write $I = \langle g : g \in G\rangle = \{\sum_{g\in G} gh, h \in \mathbb{R}[x]\}$. The length of an ideal I is the dimension of the quotient space $\mathbb{R}[x]/I$, where the quotient space $\mathbb{R}[x]/I$ is the class of all polynomials in $\mathbb{R}[x]$ modulo the ideal, e.g. for every f in $\mathbb{R}[x]$ we can construct a representative $[f] = \{g \in \mathbb{R}[x] \text{ such that} f - g \in I\}$. Our search for models identifiable by a design can be expressed precisely as the search for basis for $\mathbb{R}[x]/I$. This important fact enables us to use algebraic techniques to solve our problem.

Definition 2.7. *A term ordering τ is an ordering relation $\succ$ on the terms x^α, $\alpha \in \mathbb{N}^d$ that satisfies i) $x^\alpha \succ 1$ for all x^α and ii) if for $\alpha, \beta, \gamma \in \mathbb{N}^d$ we have $x^\alpha \succ x^\beta$, then $x^\alpha x^\gamma \succ x^\beta x^\gamma$.*

Note that a term ordering corresponds to an ordering relation on $\mathbb{N}^d$. The leading term of a polynomial f is the largest term in f with respect to the term ordering τ. We write $\mathrm{LT}_\tau(f)$.

Definition 2.8. *A Gröbner basis for an ideal I with respect to a term order τ is a finite subset $G_\tau \subset I$ such that $\langle LT_\tau(g) : g \in G_\tau\rangle = \langle LT_\tau(f) : f \in I\rangle$.*

Definition 2.9. *A reduced Gröbner basis (RGB) of I is a Gröb- ner basis $\mathcal{G}_\tau$ such that i) the coefficient of $LT_\tau(g)$ is one for all $g \in \mathcal{G}_\tau$, ii) for all $g \in \mathcal{G}_\tau$, no monomial of g lies in $\langle LT_\tau(f) : f \in \mathcal{G}_\tau \backslash g\rangle$*

A model for the responses at the design is identified by all those terms which cannot be divided by the leading terms of $\mathcal{G}_\tau$. This basis is the hierarchical polynomial model we look for.

Example 2.10. Consider the following non-regular fraction of a factorial 3^2 experiment: $\mathcal{D} = \left\{ \binom{0}{0}, \binom{1}{0}, \binom{0}{1}, \binom{1}{-1}, \binom{-1}{1} \right\}$. For a term ordering in which $x_1 \succ x_2$, we construct the following RGB (leading terms underlined) $\mathcal{G}_\tau = \{\underline{x_1^2} + 2x_1x_2 + x_2^2 - x_1 - x_2, \underline{x_2^3} - x_2, \underline{x_1x_2^2} - x_1x_2 - x_2^2 + x_2\}$ and we identify the model $\{1, x_1, x_2, x_1x_2, x_2^2\}$.

Caboara *et al.* (1997) enlarged upon Pistone and Wynn's ideas, and defined *the fan of an experimental design* as the set of all hierarchical models identifiable by a given design. Caboara *et al.* distinguished between algebraic fan (models obtained with Gröbner basis methods by varying the term ordering), and statistical fan (all hierarchical polynomial models identified by the design). In examples 2.11 and 2.12 we illustrate the algebraic and statistical fan for the design given in example 2.10. Throughout this work, we will use algebra to obtain the algebraic fan of the design.

Next we outline the algebraic approach to computing the fan. The main idea is to construct a *universal Gröbner basis* (UGB) for the design ideal I. The UGB of a (design) ideal is defined as

$$\mathcal{U}(I) := \bigcup_\tau \mathcal{G}_\tau, \tag{2}$$

where $\mathcal{G}_\tau$ is a RGB under the term ordering τ, and τ runs over all term orderings. Once we have $\mathcal{U}(I)$, we can list the algebraic fan of the design. We refer to Weispfenning (1987) for details on properties of UGBs.

Example 2.11. (cont. of Example 2.10) The UGB of I is

$$\begin{aligned}\mathcal{U}(I) = \{&\underline{x_1^2} + 2x_1x_2 + \underbrace{x_2^2} - x_1 - x_2,\ \underbrace{\underline{x_2^3}} - x_2,\ \underbrace{\underline{x_1^3}} - x_1,\\ &\underbrace{\underline{x_1x_2^2}} - x_1x_2 - x_2^2 + x_2,\ \underbrace{\underline{x_1^2x_2}} - x_1^2 - x_1x_2 + x_1\},\end{aligned}$$

where the terms underlined with " $\underline{\ }$ " are the leading terms for the condition $x_1 \succ x_2$; and we underline with " $\underbrace{\quad}$ " the leading terms for $x_1 \prec x_2$. We observe that

1. every polynomial in $\mathcal{U}(I)$ vanishes at every design point, and the set of equations for $\mathcal{U}(I)$ has no other solution than the design points;

2. the set of term orders is partitioned by the conditions $x_1 \succ x_2$ and $x_1 \prec x_2$. Thus $\mathcal{U}(I)$ is indeed a UGB. Moreover, $\mathcal{U}(I)$ is the union of two RGBs and, in this sense, is minimal and unique;

3. the algebraic fan of $\mathcal{D}$ is thus formed by $\{1, x_1, x_2, x_1x_2, x_2^2\}$ and $\{1, x_1, x_2, x_1x_2, x_1^2\}$ which are obtained as those terms not divisible by the leading terms for $x_1 \succ x_2$ and $x_1 \prec x_2$ respectively.

However, in general to compute UGB using Equation (2) directly is not possible, as there is an infinite number of term orderings. Moreover, many different term orderings yield the same $\mathcal{G}_\tau$. A surprising fact proved by Mora and Robbiano (1988) is that for any ideal, the union in Equation (2) is finite. Thus we need an efficient way to generate term orders and to compute UGBs. This will be the topic of the next subsection.

We end this subsection by noting that algebra gives some of the models we seek, but not necessarily all of them. There are staircases that cannot be obtained by algebraic means and still are identifiable.

Example 2.12. (cont. of Example 2.11) The model

$$\{1, x_1, x_2, x_1^2, x_2^2\} \tag{3}$$

is identifiable by the design as the design matrix

1	x_1	x_2	x_1^2	x_2^2
1	0	0	0	0
1	1	0	1	0
1	0	1	0	1
1	1	−1	1	1
1	−1	1	1	1

is full rank. Indeed by exhaustive search one can show that the statistical fan of $\mathcal{D}$ is composed of $\{1, x_1, x_2, x_1x_2, x_2^2\}$, $\{1, x_1, x_2, x_1^2, x_2^2\}$ and $\{1, x_1, x_2, x_1x_2, x_1^2\}$. Now we explain why we cannot obtain Model 3 by algebraic methods. The following is a generating set of polynomials for I: $\{f_1 = x_1^3 - x_1, f_2 = x_2^3 - x_2, f_3 = x_1^2 + 2x_1x_2 + x_2^2 - x_1 - x_2\}$. We have that for any τ, $LT_\tau(f_1) = x_1^3$ and $LT_\tau(f_2) = x_2^3$;

and to obtain Model 3 we need $LT_\tau(f_3) = x_1x_2$ for some τ. The previous statement implies $x_1x_2 \succ x_1^2$ and $x_1x_2 \succ x_2^2$ simultaneously. This in turn means that $x_2 \succ x_1$ and $x_2 \prec x_1$, which is not possible for any term ordering.

3. Polytopes for the algebra

We start this subsection with the basic definitions of polytopal geometry, for which references are Ziegler (1994) and Grümbaum (2003); later we present the use of polytopes in relation to Gröbner bases, for which basic references are Bayer and Morrison (1988), Mora and Robbiano (1988) and Sturmfels (1995).

3.1. Basic definitions

A $d-$dimensional polytope P may be specified as the set of solutions of a system of linear inequalities

$$Ax \leq b,$$

where A is a real matrix of d columns and $b, x \in \mathbb{R}^d$. If the polytope P is not bounded, then we refer to it as a polyhedron. For a bounded polytope, the positions of the vertices may be found using a process called vertex enumeration, see Avis and Fukuda (1991). A particular type of bounded polytopes are zonotopes, which are defined as follows.

DEFINITION 3.1. *The zonotope of a finite set of vectors $V \subset \mathbb{R}^d$ is given by the following Minkowski sum*

$$Z(V) := \sum_{v \in V} [-v, v],$$

where the summand $[-v, v] = [-1, 1] \cdot v$ is the line segment between $-v$ and v in $\mathbb{R}^d$.

EXAMPLE 3.2. Consider $V = \left\{ \binom{1}{0}, \binom{0}{1} \right\} \subset \mathbb{R}^2$. We compute $Z(V)$ by Minkowski-summing the line segments $\left[\binom{-1}{0}, \binom{1}{0}\right]$ and $\left[\binom{0}{-1}, \binom{0}{1}\right]$, e.g. for every vector a in the first line segment, we add every vector b in the second line segment. The result is the square $Z(V) = [-1, 1] \times [-1, 1] = [-1, 1]^2$.

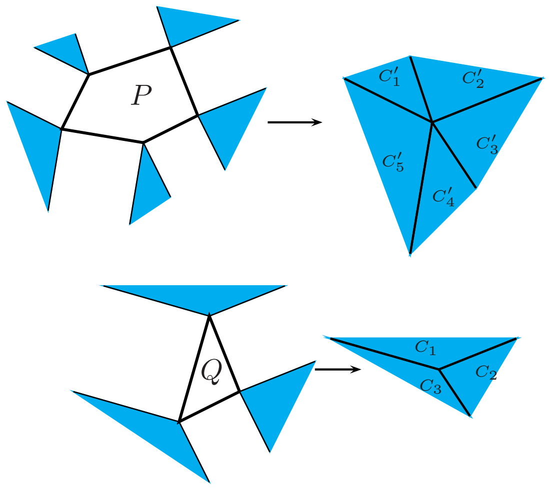

Figure 2: The polytopes P and Q and their normal fans $\mathcal{N}(P)$ and $\mathcal{N}(Q)$. P is a refinement of Q.

A polyhedron of the form $Ax \geq 0$ is called a polyhedral cone. A pointed cone is a cone that contains the origin. Then every polyhedral cone is a pointed cone. Polyhedral cones admit another description, that is as the positive hull of a set of vectors. The positive hull of V is the set $\{\sum v_i \lambda_i : v_i \in V, \lambda_i \geq 0\}$. Now, for a polyhedron $P \subset \mathbb{R}^d$ and $\omega \in \mathbb{R}^d$, we define a face of P as $F = \{u \in P : \omega \cdot u \geq \omega \cdot v \ \forall v \in P\}$.

A *complete fan* is a family of pointed polyhedral cones in $\mathbb{R}^d$ in such a way that its union is all of $\mathbb{R}^d$. The *normal fan* $\mathcal{N}(P)$ of a $d-$polytope $P \subset \mathbb{R}^d$ is the collection C_F of all vectors $a \in \mathbb{R}^d$ such that the linear function $x \to a \cdot x$ on P is maximized by all points on F; where F is a non-empty face of P . The construction of the normal fan is illustrated in Figure *2* for two bidimensional polytopes P and Q. Note that for every vertex h, its normal cone C_h is generated as the positive hull of the normal vectors of adjacent facets.

Theorem 3.3. *(Ziegler, 1994) Let $Z = Z(V) \subseteq \mathbb{R}^d$ be a zonotope. Then the normal fan $\mathcal{N}(Z)$ of Z is the fan $\mathcal{F}_A$ of the hyperplane arrangement*

$$\mathcal{A} = \mathcal{A}_V := \{H_1, \ldots, H_p\}$$

in $\mathbb{R}^d$ *given by*

$$H_i := \{c \in (\mathbb{R}^d)^* : cv_i = 0, v_i \in V\}.$$

Here $(\mathbb{R}^d)^*$ represents the *dual vector space* which is the real vector space of all linear functions $\mathbb{R}^d \to \mathbb{R}$. These are real row vectors of length d.

A polyhedron P is a refinement of a polyhedron Q if the normal fan of P is a refinement of that of Q. The refinement means that the closure of each normal cone of Q is the union of closures of normal cones of P. The closure of a cone is the cone plus its boundary. In Figure *2* we illustrate an example of refinement. The polytope P is a refinement of Q as the cones of $\mathcal{N}(Q)$ can be expressed as unions of the cones in $\mathcal{N}(P)$, namely $C_1 = C'_1 \cup C'_2$, $C_2 = C'_3$ and $C_3 = C'_4 \cup C'_5$.

3.2. Polyhedra to compute UGBs

For the rest of this section, it is necessary to elaborate on design ideals as part of the theory of Hilbert schemes. We refer the reader to Miller and Sturmfels (2004) and just recall that *Hilbert schemes* Hilb_n^d are algebraic varieties that parametrize families of ideals in polynomial rings, where d is the number of indeterminates of factors and n is the dimension of the quotient space, i.e. the number of design points. For example, the Hilbert scheme Hilb_2^2 consists of all ideals $I \subset \mathbb{R}[x_1, x_2]$ for which the quotient space $\mathbb{R}[x_1, x_2]/I$ has dimension 2 as a $\mathbb{R}-$vector space, i.e. in our case, this comprises all the possible polynomial ideals generated by two points in the plane. The starting point for the computation of the UGB for an ideal I is the construction of the state polyhedron $\mathcal{S}(I)$.

A subset $\lambda \subset \mathbb{N}^d$ of n elements is basic for the ideal $I \in \text{Hilb}_n^d$ if the $\mathbb{R}-$vector space $\text{lin}\{x^v : v \in \lambda\} := \{\sum_{v\in\lambda} \alpha_v x^v\}$ satisfies $\text{lin}\{x^v : v \in \lambda\} \cap I = \{0\}$. A hierarchical model obtained with CCA techniques is basic for the design ideal. Now, for a basic set λ, we define its sum as $\sum_{v\in\lambda} v$. The basis polytope of $I \in \text{Hilb}_n^d$ is the convex hull of sums of basic sets of I in V_n^d, that is $\mathcal{B}(I) := \text{conv}\left(\{\sum_{v\in\lambda} v : \lambda \subset V_n^d, \lambda \text{ basic for } I\}\right)$. The state polyhedron of

$I \in \mathrm{Hilb}_n^d$ is given by $\mathcal{S}(I) := \mathcal{B}(I) + \mathbb{R}_+^d$. This last sum is interpreted as a Minkowski sum, and $\mathbb{R}_+^d \subset \mathbb{R}^d$ is the positive orthant.

The vectors $w \in \mathbb{Z}_{>0}^d \subset \mathbb{R}_+^d$ are used to order terms by the product $w \cdot \alpha$, for example we order the terms $x_1^2x_2$, x_2^3, x_1x_2 as $x_1^2x_2 \succ x_1x_2 \succ x_2^3$ with $w = \binom{3}{1}$, but as $x_2^3 \succ x_1^2x_2 \succ x_1x_2$ with $w' = \binom{2}{3}$.

We construct the normal fan of $\mathcal{S}(I)$. Let C_h be the normal cone corresponding to the vertex h of $\mathcal{S}(I)$. We have that $\bigcup_h C_h = \mathbb{R}_+^d$. Now, for every vertex h, Gröbner theory states that the vectors $\{w : w \in \mathbb{Z}_{>0}^d, w \in C_h\}$ will give the same RGB. In this sense, every cone C_h creates an equivalence class of ordering vectors. For this reason, we need only one w for every cone, and let $\mathcal{G}_w$ be the RGB obtained with the ordering vector w. We compute the UGB by

$$\mathcal{U}(I) := \bigcup_w \mathcal{G}_w. \tag{4}$$

Example 3.4. (cont. of Example 2.10) The state polyhedron for the design ideal I is given by $\mathcal{S}(I) = conv\left(\left\{\binom{2}{4}, \binom{4}{2}\right\}\right) + \mathbb{R}_+^2$. We obtain the sum $\binom{2}{4}$ as follows: the log of the model $\{1, x_1, x_2, x_1x_2, x_2^2\}$ gives the staircase $\left\{\binom{0}{0}, \binom{1}{0}, \binom{0}{1}, \binom{1}{1}, \binom{0}{2}\right\}$, then the coordinate-wise sum gives $\binom{2}{4}$. We have that $\binom{4}{2}$ corresponds to $\{1, x_1, x_2, x_1x_2, x_1^2\}$ and we note that the model $\{1, x_1, x_2, x_1^2, x_2^2\}$ corresponds to the sum $\binom{3}{3}$, which is an interior point of $\mathcal{S}(I)$. In Figure *3* we illustrate $\mathcal{S}(I)$ and its normal fan composed of the cones C_1 and C_2. Now, we select an integer vector in the interior of C_1, e.g. $w_1 = \binom{2}{1}$ and obtain $\mathcal{G}_{w_1}$ which is the same RGB as in Example 2.10. We compute the UGB by repeating the computation with a vector w_2 in C_2 and uniting the two RGBs as $\mathcal{U}(I) = \mathcal{G}_{w_1} \cup \mathcal{G}_{w_2}$.

By using the state polyhedron $\mathcal{S}(I)$ we can obtain the adequate ordering vectors w, one for every normal cone, and then compute the UGB using Equation (4). Up to this point, we have solved the initial problem of selecting the right term orders to compute the UGB. However, we need to compute $\mathcal{S}(I)$ for every $\mathcal{D}$. This is a disadvantage because the method has to deal with each specific case in a different way. Another disadvantage of this approach is the inherent complexity of the construction of $\mathcal{S}(I)$.

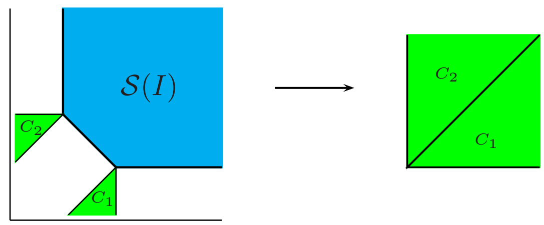

Figure 3: Picture of $\mathcal{S}(I)$ and the cones in $\mathcal{N}(\mathcal{S}(I))$.

For certain types of designs this disadvantage can be partly overcome. Onn and Sturmfels (1999) prove that if a design has a generic configuration (roughly a design whose points are at random), then $\mathcal{S}(I)$ equals the corner cut polyhedron. They also prove that the list of models is enumerable in polytime for a generic design. They give a determinant-based formula to retrieve a model corresponding to a vertex of $\mathcal{S}(I)$ for any vertex. For a random design, Caboara *et al.* (1997) show that all models in $\binom{\mathbb{N}^d}{n}_{stair}$ are identifiable.

In the next section we introduce the Hilbert zonotope, which overcomes the inherent difficulties of the state polyhedron.

4. Hilbert zonotope

We are now arriving at the main point of this paper in which the Hilbert zonotope is the central feature. We follow the definition in Onn and Sturmfels (1999) and Babson *et al.* (2003). We construct the zonotope and then list some of its main features.

Definition 4.1. *The symmetrization of a finite set $A \subset \mathbb{Z}^d$ is*

$$\mathrm{sym(A)} := \{a - b : a \in A, b \in A \backslash a\} \tag{5}$$

The following properties of sym(A) can be easily demonstrated: *i)* sym(A) is centrally symmetric, that is, if $a \in \mathrm{sym(A)}$ then $-a \in \mathrm{sym(A)}$, and *ii)* $0 \notin \mathrm{sym(A)}$.

Definition 4.2. *The primitive elements of a set $A \subset \mathbb{Z}^d \backslash \{0\}$ are all the elements of A that are not non-negative integer multiples of another element of A. We call this set* prim(A)*.*

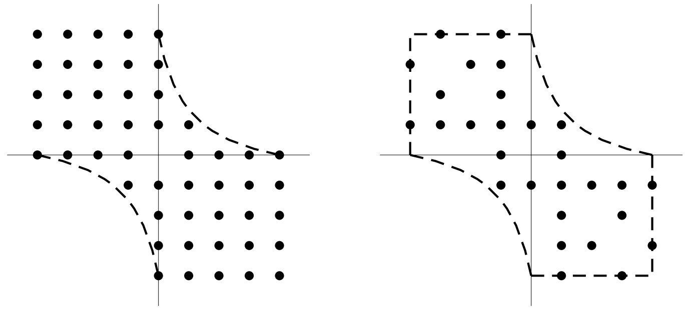

Figure 4: Symmetrization of V_5^2 (left), and D_5^2 (right).

DEFINITION 4.3. *For $n > 1$ let D_n^d be the set of primitive vectors of the symmetrization of V_n^d, that is $D_n^d := \text{prim}(\text{sym}(V_n^d))$. For $n = 1$ let $D_1^d := \pm\{e_1, \ldots, e_d\}$, where e_i is the $i-th$ unit vector.*

EXAMPLE 4.4. Figure *4* gives the symmetrization of V_5^2 and its primitives D_5^2.

When we compute the primitives of $sym(V_n^d)$, it is sufficient to consider only those elements of $sym(V_n^d)$ where the greatest common divisor of its non-zero components is one. The set D_n^d contains vectors pointing in all directions of V_n^d. It has no zero vector and has only one vector for each of the directions from the zero to a point in $\text{sym}(V_n^d)$. This is at the core of the definition of the Hilbert zonotope.

DEFINITION 4.5. *The Hilbert zonotope $\mathcal{H}_n^d$ is the following Min- kowski sum:*

$$\mathcal{H}_n^d := \sum_{v \in D_n^d} [0,1] \cdot v \subset \mathbb{R}^d \tag{6}$$

Clearly, $\mathcal{H}_n^d$ is a zonotope. The Hilbert zonotope is a complicated figure with many facets and vertices, even for small values of d, n (see for example, Table 1 in the Appendix). Next we give two examples and two propositions. Proposition 4.8 gives a recurrence relation between Hilbert zonotopes, and Proposition 4.9 gives a refinement relation between Hilbert zonotopes.

EXAMPLE 4.6. For $n = 1$, $\mathcal{H}_1^d$ is the $d-$cube $[-1,1]^d$.

EXAMPLE 4.7. The vertices of $\mathcal{H}_5^2$ are given by

$$\mathcal{H}_5^2 = \pm\Big\{\tbinom{-27}{23}, \tbinom{-27}{25}, \tbinom{-25}{27}, \tbinom{-23}{27}, \tbinom{-15}{25}, \tbinom{-9}{23}, \tbinom{-5}{21}, \tbinom{1}{17}, \tbinom{9}{11}, \tbinom{11}{9}, \tbinom{17}{1}, \tbinom{21}{-5}, \tbinom{23}{-9}, \tbinom{25}{-15}\Big\}$$

On the left side of Figure *5* we present $\mathcal{H}_5^2$, which is a 28-gon.

PROPOSITION 4.8. *The Hilbert zonotope satisfies the following property:* $\mathcal{H}_n^d \subset \mathcal{H}_{n'}^d$ *for* $n < n'$.

Proof. For a fixed d, if $n < n'$ we have that $V_n^d \subset V_{n'}^d$, and thus $sym(V_n^d) \subset sym(V_{n'}^d)$, and $D_n^d = prim(sym(V_n^d)) \subset prim(sym(V_{n'}^d))$ $= D_{n'}^d$, that is

$$D_{n'}^d = D_n^d \bigcup (D_{n'}^d \backslash D_n^d). \tag{7}$$

Note that $D_{n'}^d \backslash D_n^d$ is a non-empty set. Now we construct the zonotope $\mathcal{H}_{n'}^d$ by Minkowski-summing over $v \in D_{n'}^d$,

$$\mathcal{H}_{n'}^d = \sum_{D_n^d} [0,1] \cdot v + \sum_{D_{n'}^d \backslash D_n^d} [0,1] \cdot v = \mathcal{H}_n^d + \sum_{D_{n'}^d \backslash D_n^d} [0,1] \cdot v \supset \mathcal{H}_n^d,$$

which completes the proof. □

PROPOSITION 4.9. *The Hilbert zonotope* $\mathcal{H}_{n'}^d$ *is a refinement of* $\mathcal{H}_n^d$ *for* $n < n'$.

Proof. We construct the normal fan of $\mathcal{H}_{n'}^d$ using Theorem 3.3 and Equation (7) from Proposition 4.8. The normal fan is then comprised of two groups of hyperplanes. The first group is those hyperplanes corresponding to $\mathcal{N}(\mathcal{H}_n^d)$ (i.e. those hyperplanes orthogonal to $v \in D_n^d$); while the second group comprises the hyperplanes orthogonal to the vectors $v \in D_{n'}^d \backslash D_n^d$. As the set $D_{n'}^d \backslash D_n^d$ is nonempty, the second group of hyperplanes creates the refinement relation. □

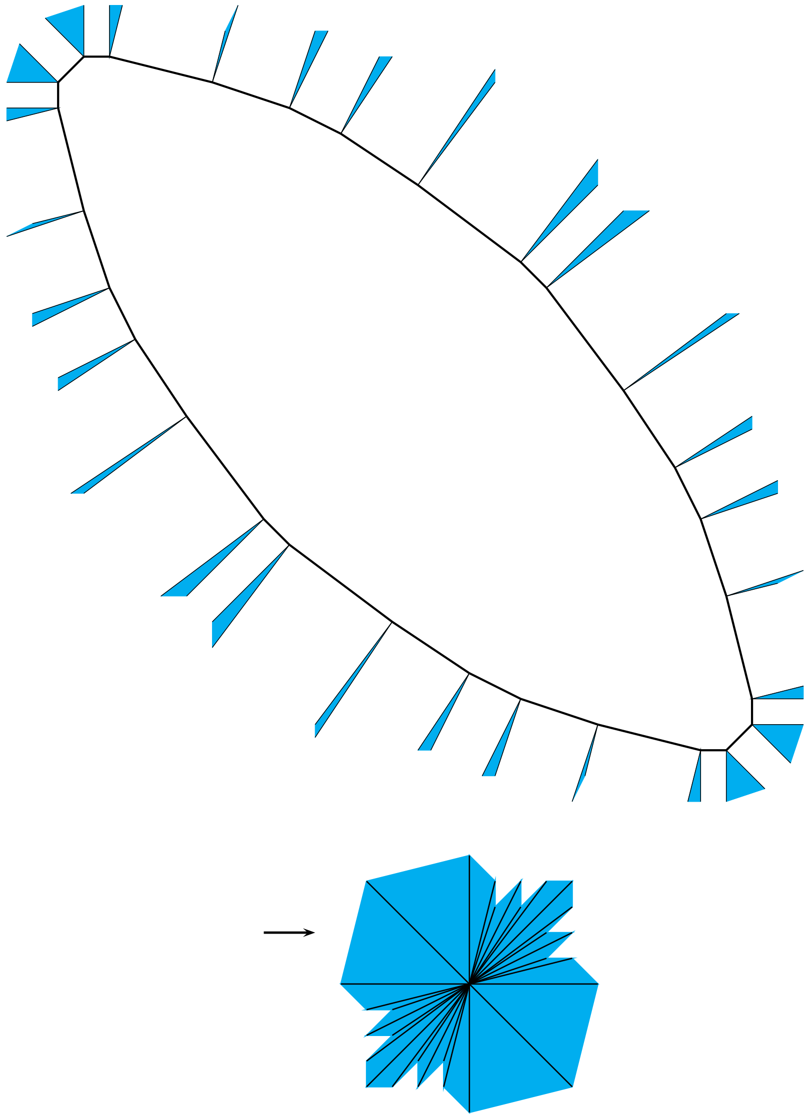

Figure 5: Picture of $\mathcal{H}_5^2$ with its normal cones (above), and the normal fan $\mathcal{N}(\mathcal{H}_5^2)$ (below).

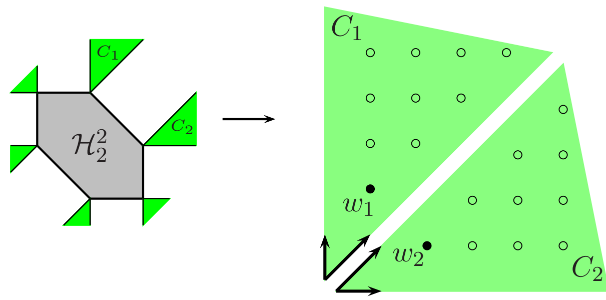

Figure 6: Picture of $\mathcal{H}_2^2$ with its normal fan (left). In the right side of the figure, for every cone C_i we select the ordering vector w_i (pointed in black). We added the vectors that generate C_i.

4.1. The Hilbert zonotope and UGB

In this subsection we illustrate the use of the zonotope to compute universal Gröbner bases. First we recall the important result about the universality of the zonotope.

THEOREM 4.10. *(Babson et al., 2003) The Hilbert zonotope $\mathcal{H}_n^d$ is a refinement of both the basis polytope $\mathcal{B}(I)$ and the state polyhedron $\mathcal{S}(I)$ of every member of the Hilbert scheme* Hilb_n^d.

The previous theorem is used to construct an efficient set of ordering vectors, which is next described. For every vertex h of $\mathcal{H}_n^d$ we construct the corresponding normal cone C_h. Now let $w(h) \in \mathbb{Z}_{\neq 0}^d$ be the vector in the interior of the cone C_h with minimum norm with respect to the standard Euclidean distance. There is a unique $w(h)$ for every vertex h. Let W_n^d be the set of all vectors $w(h)$, that is $W_n^d := \{w(h) : h \text{ vertex of } \mathcal{H}_n^d\}$. We are interested only in those elements of W_n^d which are positive. Let $W_{n+}^d \subset W_n^d$ be the subset of vectors $w(h)$ in the first orthant. This set of positive vectors W_{n+}^d defines a *universal set of term orders* for Hilb_n^d, which can be computed once and for all, and is independent of the configuration of $\mathcal{D}$. The set W_{n+}^d was proposed by Babson *et al.* as part of their polynomial time algorithm to compute UGB and the fan of a design.

EXAMPLE 4.11. Consider $\mathcal{H}_2^2$. Of all the six cones of its normal fan, we only consider the cones which lie in the positive orthant, which are labelled C_1 and C_2 in Figure *6*. The cone C_1 is generated as the positive hull of $\{\binom{0}{1},\binom{1}{1}\}$, while C_2 is generated by $\{\binom{1}{0},\binom{1}{1}\}$. For C_1 we have $w(1)=\binom{0}{1}+\binom{1}{1}=\binom{1}{2}$ and thus $W_{2+}^2=\{\binom{1}{2},\binom{2}{1}\}$.

EXAMPLE 4.12. For the values $n=5, d=2$, we have that W_{5+}^2 is

$$\left\{\begin{pmatrix}1\\5\end{pmatrix},\begin{pmatrix}2\\7\end{pmatrix},\begin{pmatrix}2\\5\end{pmatrix},\begin{pmatrix}3\\5\end{pmatrix},\begin{pmatrix}5\\7\end{pmatrix},\begin{pmatrix}4\\5\end{pmatrix},\begin{pmatrix}5\\4\end{pmatrix},\begin{pmatrix}7\\5\end{pmatrix},\begin{pmatrix}5\\3\end{pmatrix},\begin{pmatrix}5\\2\end{pmatrix},\begin{pmatrix}7\\2\end{pmatrix},\begin{pmatrix}5\\1\end{pmatrix}\right\}.$$

In the right side of Figure *5* we illustrate the complete normal fan $\mathcal{N}(\mathcal{H}_5^2)$. We compare the refinement given by the normal fan of $\mathcal{H}_5^2$ in Figure *5* (with 12 cones in the first orthant) against the normal fan of $\mathcal{S}(I)$ in Figure *3* (with only two cones in the first orthant).

5. Main theorem

Theorem 5.1 gives a fast method to compute the first orthant of $\mathcal{N}(\mathcal{H}_n^2)$. The construction of Theorem 5.1 is intuitively more appealing and easier than the usual construction of $\mathcal{N}(\mathcal{H}_n^d)$. Unfortunately, it cannot be extended to $d\geq 3$ as we shall see in the next section.

THEOREM 5.1. *The cones in the first orthant of* $\mathcal{N}(\mathcal{H}_n^2)$ *are generated by the set* $\operatorname{prim}\left([0,n-1]^2\setminus\{\binom{0}{0}\}\right)$, *where* $[a,b]=\{c\in\mathbb{Z}, a\leq c\leq b\}$.

Proof. Using Definition 4.3, we have $D_n^2=prim(\pm([-n+1,-1]\times[1,n-1]))\bigcup(\pm prim(V_n^d))$. We must keep in mind that D_n^2 is the set of summands in the definition of $\mathcal{H}_n^2$. Next we shall apply Theorem 3.3 to generate all the hyperplanes of the fan. For every vector $\binom{a}{b}\in prim(\pm([-n+1,-1]\times[1,n-1]))$, the corresponding orthogonal hyperplane will be generated by $\binom{-b}{a}\in prim(\pm([1,n-1]^2))$. This last vector is orthogonal to $\binom{a}{b}$. We now have that the horizontal and vertical axes are obtained by $\pm e_i\in\pm prim(V_n^d)$. As we are only concerned with the first orthant, we have that the fan is generated by $prim([1,n-1]^2)\bigcup\{e_i\}=prim\left([0,n-1]^2\setminus\{\binom{0}{0}\}\right)$. The cardinality of $[0,n-1]^2\setminus\{\binom{0}{0}\}$ complies with the bound $O(n^2)$. Now, to obtain the primitives we just need to screen out the non-primitive elements and we can achieve all this with $O(n^2)$ operations. □

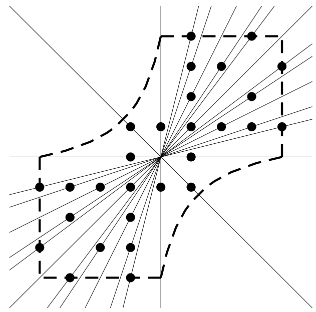

Figure 7: Cones of $\mathcal{N}(\mathcal{H}_5^2)$.

Now we give two examples, the first shows the use of Theorem 5.1 to obtain the ordering vectors, and the second the use of the vectors to obtain the algebraic fan of an experiment.

EXAMPLE 5.2. For $n = 5$, we have that the cones in the first orthant are generated by the set prim $\left([0,4]^2 \setminus \left\{\binom{0}{0}\right\}\right) =$

$$\left\{\binom{0}{1}, \binom{1}{4}, \binom{1}{3}, \binom{1}{2}, \binom{2}{3}, \binom{3}{4}, \binom{1}{1}, \binom{4}{3}, \binom{3}{2}, \binom{2}{1}, \binom{3}{1}, \binom{4}{1}, \binom{1}{0}\right\}.$$

We now explain the generation of the set of ordering vectors W_{5+}^2. We start with the first cone in clockwise direction. For this cone, the generating vectors are $\binom{0}{1}$ and $\binom{1}{4}$, and the corresponding vector in the interior of the cone is $\binom{0}{1} + \binom{1}{4} = \binom{1}{5}$. We proceed similarly with the rest of the cones and we obtain W_{5+}^2 as in Example 4.12.

EXAMPLE 5.3. Consider the experiment $\mathcal{D} = \left\{\binom{-1}{-1}, \binom{-1}{1}, \binom{1}{-1}, \binom{1}{1}, \binom{0}{0}\right\}$, which is a factorial design with a central point. We now use the ordering vectors W_{5+}^2 to compute UGB and obtain the algebraic fan. For this case the algebraic fan has the models $\{1, x_1, x_2, x_1x_2, x_1^2\}$ and $\{1, x_1, x_2, x_1x_2, x_2^2\}$ and coincides with the statistical fan, which can be proved easily.

In the next proposition we identify commonly used term orderings within the structure of $\mathcal{N}(\mathcal{H}_n^2)$. We omit the proof.

Proposition 5.4. *i)For $n > 1$, the set W^2_{n+} includes the vectors $\binom{1}{n}$, $\binom{n}{1}$, $\binom{n-1}{n}$ and $\binom{n}{n-1}$.*

ii) If we order the set V^2_n using the vectors defined in i), we have the following equivalence: $\binom{1}{n}$ corresponds to a `Lex` *ordering in which $x_1 \prec x_2$; $\binom{n}{1}$ to* `Lex` *$x_1 \succ x_2$; $\binom{n-1}{n}$ to* `DegLex` *$x_1 \prec x_2$ and $\binom{n}{n-1}$ to* `DegLex` *$x_1 \succ x_2$.*

6. Discussion

We presented Theorem 5.1, which gives the desired ordering vectors without having to actually compute the Hilbert zonotope and thus saving computational effort. The former methodology of Babson *et al.* (2003) constructs the vectors in $O(n^{2(d-1)}(\log n))^{2(d-1)^2})$ time, which for the case $d = 2$ is $O(n^2(\log n)^2)$, while our proposal in Theorem 5.1 is of order $O(n^2)$.

Our result for the bidimensional Hilbert zonotope can be easily explained in a graphical manner, as follows. The cones of $\mathcal{N}(\mathcal{H}^2_n)$ are generated by rotating D^2_n by 90 degrees. In particular, the first orthant of $\mathcal{N}(\mathcal{H}^2_n)$ is generated by vectors stemming from the origin and pointing towards all possible the directions of the square grid $[0, n-1]^2$. See next example and Figure *10* in Appendix 7.3 for a graphical depiction of this idea.

Example 6.1. Consider the values $d = 2, n = 5$. The set D^2_5 is depicted in Figure *4*. We generate the cones in $\mathcal{N}(\mathcal{H}^2_n)$ by rotating D^2_5, which we illustrate in Figure *7*.

However, there is no immediate generalization for higher dimensions, and Theorem 5.1 and the graphical explanation will be valid only for $d = 2$.

Example 6.2. Consider the case $d = 3$, $n = 3$. A vector that generates a cone in the first orthant is $v = (1, 2, 4)^T$, but we have that $v \notin prim([0, 2]^3 \backslash \{(0, 0, 0)^T\})$.

6.1. Future work

Our problem is one of representation change for polytopes. Polytopes have two representations: first as a set of vertices and secondly as sets of inequalities. Being a zonotope, $\mathcal{H}_n^d$ has a third representation: as a Minkowski sum. While computing the normal fan of $\mathcal{H}_n^d$, we are changing from the third representation to the second. We are interested in the normal fan of $\mathcal{H}_n^d$, and more precisely, in the generating vectors for its normal cones. These generating vectors are precisely the orthogonal vectors to the hyperplanes of the second representation. A difficulty is the complexity of the computation, as the next example shows.

Example 6.3. Consider $D_3^3 = \pm\{(0,0,1)^T, (0,1,0)^T, (1,0,0)^T, (0,1,-1)^T, (1,0,-1)^T, (1,-1,0)^T, (0,1,-2)^T, (1,0,-2)^T, (1,-2,0)^T, (0,2,-1)^T, (2,0,-1)^T, (2,-1,0)^T\}$. Now, to compute the generating vectors of the fan, a rough approach is as follows: i) call the desired set of generators F and initialize it to the empty set, ii) take a set of 3 linearly independent vectors of D_3^3 and construct a 3×3 matrix, iii) by gaussian elimination, we find the set of orthogonal integer vectors which belong to the set of generators of the normal fan of $\mathcal{H}_3^3$, call this set V, iv) update $F = F \bigcup V$ and repeat from i) until all possible linearly independent sets of three vectors have been processed. For the present example, steps i) to iii) would be iterated using all $\binom{24}{3} = 2024$ sets of three vectors to construct the final set F of 50 generating vectors for $\mathcal{N}(\mathcal{H}_3^3)$. This proposal is of order $O(d^2 \cdot \binom{\#D_n^d}{d})$, with the cardinality of D_n^d having the bound $O(\#D_n^d) = O(n^2(\log n)^{2(d-1)})$ (Babson *et al.*, 2003).

7. Appendix

7.1. Cardinality of the set of staircases

The formulas for the cardinality of the set of staircases have a long story, stemming from Euler's work in integer partitions, see Hardy and Wright (1975). The formulas are called after MacMahon, who studied them in early 20th century. MacMahon's formulas are

$$\sum_{n=0}^{\infty} \# \binom{\mathbb{N}^2}{n}_{stair} \cdot z^n = \prod_{k=1}^{\infty} \frac{1}{1-z^k} = 1 + z + 2z^2 + 3z^3 + 5z^4 + 7z^5 + \ldots \tag{8}$$

$$\sum_{n=0}^{\infty} \# \binom{\mathbb{N}^3}{n}_{stair} \cdot z^n = \prod_{k=1}^{\infty} \frac{1}{(1-z^k)^k} = 1 + z + 3z^2 + 6z^3 + 13z^4 + \dots \tag{9}$$

Next we show an example using MacMahon's formulas. The number of staircases with four elements ($n = 4$) in two dimensions ($d = 2$) is 5, which is the coefficient of z^4 in Equation 8. Finally, we see that we can express the number 4 as the following five integer partitions: $4 = 3 + 1 = 2 + 2 = 2 + 1 + 1 = 1 + 1 + 1 + 1$.

7.2. Complexity of the Hilbert zonotope

Table 1 lists the number of vertices, number of facets and number of positive ordering vectors[1] for various values of d and n. The asymptotic order for the first two is discussed in Babson *et al.* (2003). The cardinality of W^2_{n+} is listed on the sequence A049696 (Sloane, 2004); and the following orders of magnitude are reported

$$\#W^2_{n+} = 6n^2/\pi^2 + O(n \log n),$$

and the refinement

$$\#W^2_{n+} = 6n^2/\pi^2 + O(n(\log n)^{2/3}(\log\log n)^{4/3})$$

(Sloane, 2004).

n	1	2	3	4	5	6	7	8	9	10	11	12
# of facets	4	6	10	20	28	48	56	84	100	128	144	192
$\#W^2_{n+}$	1	2	4	8	12	20	24	36	44	56	64	84

Table 1. Values for $\mathcal{H}^2_n$.

n	1	2	3	4	5	6
# of facets	6	14	50	458	1022	4970
# of vertices	8	24	84	720	1500	7320
$\#W^2_{n+}$	1	6	24	192	456	1974

Table 1 (cont.). Values for $\mathcal{H}^3_n$.

[1]See Appendix 7.4 for examples of W^d_{n+}. We have computed tables with the vectors up to the following values (d, n): $(2, 57)$, $(3, 6)$, $(4, 2)$, available from the author by request.

n	1	2
# of facets	8	30
# of vertices	16	120
$\#W^2_{n+}$	1	24

Table 1 (cont.). Values for $\mathcal{H}^4_n$.

7.3. Pictures of zonotopes

We show several zonotopes in Figures *8* and *9*. We give the generating vectors for the cones of $\mathcal{N}(\mathcal{H}^2_n)$ in Figure *10*.

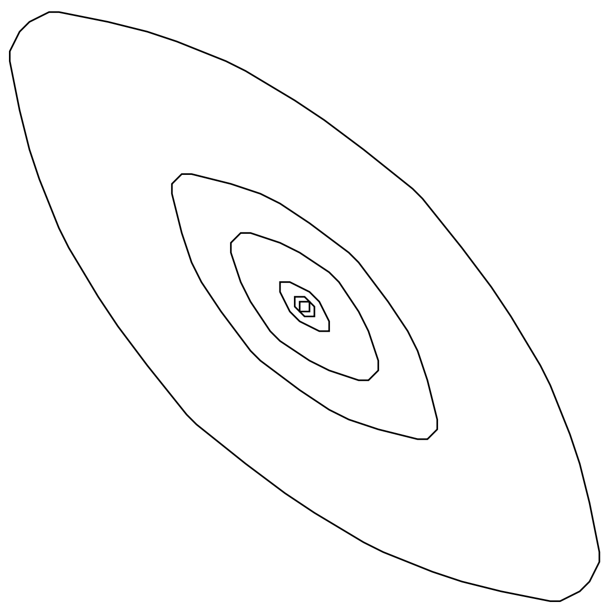

Figure 8: Bidimensional Hilbert zonotopes for $n = 1, \ldots, 6$ (starting from the centre).

7.4. Ordering vectors

We list some examples of ordering vectors. For other values d, n, see Note 1.

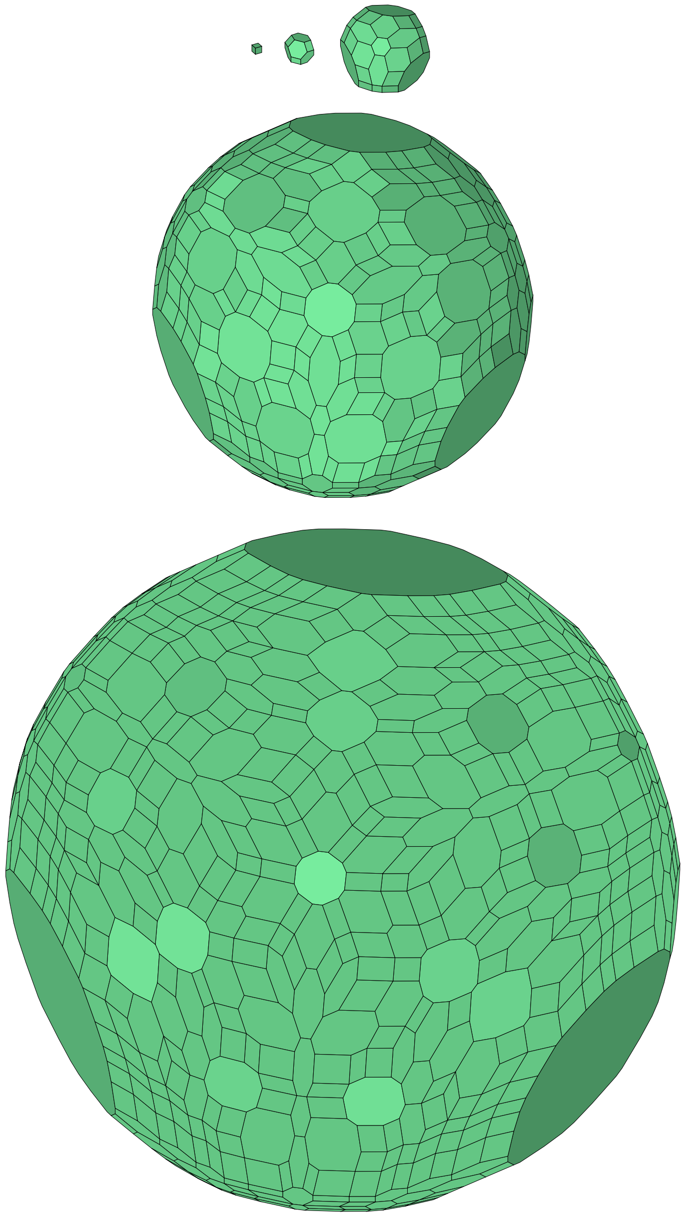

Figure 9: Tridimensional Hilbert zonotope for $n = 1, \dots, 5$ (starting from top left).

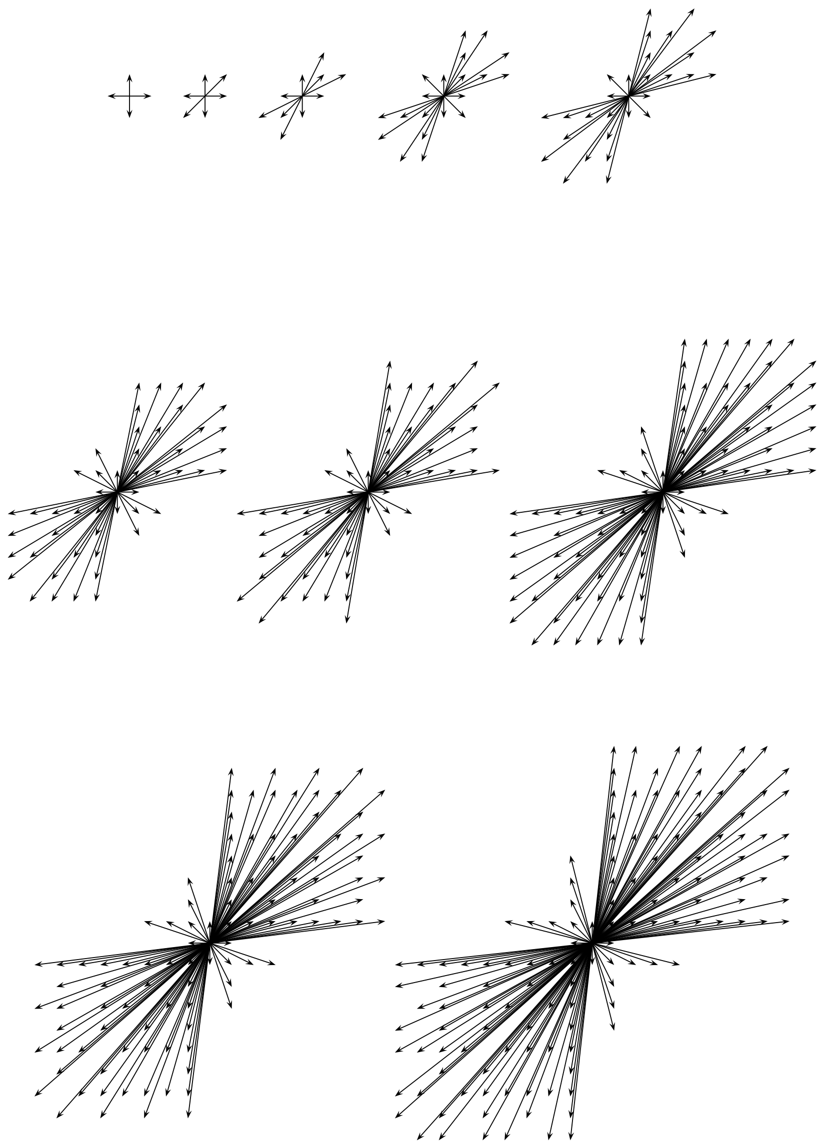

Figure 10: Generating vectors for the cones of $\mathcal{N}(\mathcal{H}_n^2)$ for $n = 1, \ldots, 10$.

7.4.1. Bidimensional case

$W^2_{1+} = \left\{ \binom{1}{1} \right\}$; $W^2_{2+} = \left\{ \binom{2}{1}, \binom{1}{2} \right\}$; $W^2_{3+} = \left\{ \binom{3}{1}, \binom{3}{2}, \binom{2}{3}, \binom{1}{3} \right\}$;
$W^2_{4+} = \left\{ \binom{1}{4}, \binom{2}{5}, \binom{3}{5}, \binom{3}{4}, \binom{4}{3}, \binom{5}{3}, \binom{5}{2}, \binom{4}{1} \right\}$;
$W^2_{5+} = \left\{ \binom{1}{5}, \binom{2}{7}, \binom{2}{5}, \binom{3}{5}, \binom{5}{7}, \binom{4}{5}, \binom{5}{4}, \binom{7}{5}, \binom{5}{3}, \binom{5}{2}, \binom{7}{2}, \binom{5}{1} \right\}$;
$W^2_{6+} = \left\{ \binom{1}{6}, \binom{2}{9}, \binom{2}{7}, \binom{3}{8}, \binom{3}{7}, \binom{4}{7}, \binom{5}{8}, \binom{5}{7}, \binom{7}{9}, \binom{5}{6}, \binom{6}{5}, \binom{9}{7}, \binom{7}{5}, \binom{8}{5}, \right.$
$\left. \binom{7}{4}, \binom{7}{3}, \binom{8}{3}, \binom{7}{2}, \binom{9}{2}, \binom{6}{1} \right\}$;
$W^2_{7+} = \left\{ \binom{1}{7}, \binom{2}{11}, \binom{2}{9}, \binom{2}{7}, \binom{3}{8}, \binom{3}{7}, \binom{4}{7}, \binom{5}{8}, \binom{5}{7}, \binom{7}{9}, \binom{9}{11}, \binom{6}{7}, \binom{7}{6}, \right.$
$\left. \binom{11}{9}, \binom{9}{7}, \binom{7}{5}, \binom{8}{5}, \binom{7}{4}, \binom{7}{3}, \binom{8}{3}, \binom{7}{2}, \binom{9}{2}, \binom{11}{2}, \binom{7}{1} \right\}$.

7.5. Three dimensional case

$W^3_{1+} = \{(1,1,1)^T\}$;
$W^3_{2+} = \{(1,2,3)^T, (1,3,2)^T, (2,3,1)^T, (3,2,1)^T, (3,1,2)^T, (2,1,3)^T\}$.

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