# Classification of Six-Point Metrics

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#### Abstract

There are 339 combinatorial types of generic metrics on six points. They correspond to the 339 regular triangulations of the second hypersimplex  $\Delta(6,2)$ , which also has 14 non-regular triangulations.

### 1 The Metric Fan

We consider the cone of all metrics on the finite set  $\{1, 2, ..., n\}$ :

$$C_n = \{ d \in \mathbb{R}^{\binom{n}{2}} : d_{ij} \ge 0 \text{ and } d_{ij} + d_{jk} \ge d_{ik} \text{ for all } 1 \le i, j, k \le n \}.$$

This is a closed convex pointed polyhedral cone. Its extreme rays have been studied in combinatorial optimization [4, 5]. Among the extreme rays are the *splits*. The splits are the metrics  $\sum_{i \in A} \sum_{j \notin A} e_{ij} \in \mathbb{R}^{\binom{n}{2}}$  as A ranges over nonempty subsets of  $\{1, 2, \ldots, n\}$ . There is an extensive body of knowledge (see [5, 9]) also on the facets of the subcone of  $C_n$  generated by the splits.

Our object of study is a canonical subdivision of the metric cone  $C_n$ . It is called the *metric fan* and denoted  $MF_n$ . A quick way to define the metric fan  $MF_n$  is to say that it is the secondary fan of the second hypersimplex

$$\Delta(n,2) = \operatorname{conv}\{e_i + e_j : 1 \le i < j \le n\} \subset \mathbb{R}^n$$

Every metric d defines a regular polyhedral subdivision  $\Delta_d$  of  $\Delta(n, 2)$  as follows. The vertices of  $\Delta(n, 2)$  are identified with the edges of the complete graph  $K_n$ , and subpolytopes of  $\Delta(n, 2)$  correspond to arbitrary subgraphs of  $K_n$ . A subgraph G is a cell of  $\Delta_d$  if there exists an  $x \in \mathbb{R}^n$  satisfying

$$x_i + x_j = d_{ij}$$
 if  $\{i, j\} \in G$  and  $x_i + x_j > d_{ij}$  if  $\{i, j\} \notin G$ .

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Two metrics d and d' lie in the same cone of the metric fan  $MF_n$  if they induce the same subdivision  $\Delta_d = \Delta_{d'}$  of the second hypersimplex  $\Delta(n, 2)$ . We say that the metric d is generic if d lies in an open cone of  $MF_n$ . This is equivalent to saying that  $\Delta_d$  is a regular triangulation of  $\Delta(n, 2)$ .

These triangulation of  $\Delta(n, 2)$  and the resulting metric fan  $MF_n$  were studied by De Loera, Sturmfels and Thomas [3], who had been unaware of an earlier appearance of the same objects in phylogenetic combinatorics [1, 6]. In [6], Dress considered the polyhedron dual to the triangulation  $\Delta_d$ ,

$$P_d = \{ x \in \mathbb{R}^n_{>0} : x_i + x_j \ge d_{ij} \text{ for } 1 \le i < j \le n \},\$$

and he showed that its complex of bounded faces, denoted  $T_d$ , is a natural object which generalizes the phylogenetic trees derived from the metric d. Both [3] and [6] contain the description of the metric fans  $MF_n$  for  $n \leq 5$ :

- The octahedron  $\Delta(4, 2)$  has three regular triangulations  $\Delta_d$ . They are equivalent up to symmetry. The corresponding *tight span*  $T_d$  is a quadrangle with an edge attached to each of its four vertices. The three walls of the fan  $MF_4$  correspond to the trees on  $\{1, 2, 3, 4\}$ .
- The fan  $MF_5$  has 102 maximal cones which come in three symmetry classes. The tight spans  $T_d$  of these three metrics are depicted in [6, Figure A3], and the corresponding triangulations  $\Delta_d$  appear (in reverse order) in [3, page 414]. For instance, the *thrackle triangulation* of [3, §2] corresponds to the planar diagram in [6]. All three tight spans  $T_d$  have five two-cells. (The type  $T_{X,D_3}$  is slightly misdrawn in [6]: the two lower left quadrangles should form a flat pentagon).

The aim of this article is to present the analogous classification for n = 6. The following result was obtained with the help of Rambau's software TOPCOM [13] for enumerating triangulations of arbitrary convex polytopes.

**Theorem 1** There are 194, 160 generic metrics on six points. These correspond to the maximal cones in  $MF_6$  and to the regular triangulations of  $\Delta(6,2)$ . They come in 339 symmetry classes. The hypersimplex  $\Delta(6,2)$  has also 3,840 non-regular triangulations which come in 14 symmetry classes.

This paper is organized as follows. In Section 2 we describe all 12 generic metrics whose tight span  $T_d$  is two-dimensional, and in Section 3 we describe all 327 generic metrics whose tight span has a three-dimensional cell. Similarly, in Section 4, we describe the 14 non-regular triangulations of  $\Delta(6, 2)$ . In each case a suitable system of combinatorial invariants will be introduced. In Section 5 we study the geometry of the metric fan  $MF_6$ . The rays of  $MF_6$  are precisely the *prime metrics* in [12]. We determine the maximal cones incident to each prime metric, and we discuss the corresponding minimal subdivisions of  $\Delta(6, 2)$ . In Section 6 we present a software tool for visualizing the tight span  $T_d$  of any finite metric d. This tool was written written in POLYMAKE [10] with the help of Michael Joswig and Julian Pfeifle. We also explain how its output differs from the output of SPLITSTREE [8].

A complete list of all six-point metrics has been made available at

### bio.math.berkeley.edu/SixPointMetrics

For each of the 339+14 types in Theorem 1, the regular triangulation, Stanley-Reisner ideal, and numerical invariants are listed. The notation is consistent with that used in the paper. In addition, the webpage contains interactive pictures in JAVAVIEW [11] of the tight span of each metric.

# 2 The 12 Two-Dimensional Generic Metrics

We identify each generic metric d with its tight span  $T_d$ , where the exterior segments have been contracted<sup>1</sup> so that every maximal cell has dimension  $\geq 2$ . With this convention, generic four-point metrics are quadrangles and five-point metrics are glued from five polygons (cf. [6, Figure A3]). The generic six-point metrics, on the other hand, fall naturally into two groups.

**Lemma 2** Each generic metric on six points is either a three-dimensional cell complex with 26 vertices, 42 edges, 18 polygons and one 3-cell, or it is a two-dimensional cell complex with 25 vertices, 39 edges and 15 polygons. There are 327 three-dimensional metrics and 12 two-dimensional metrics.

We first list the twelve types of two-dimensional metrics. In each case the tight span consists of 15 polygons which are either triangles, quadrangles or pentagons. Our first invariant is the vector  $B = (b_3, b_4, b_5)$  where  $b_i$  is the number of polygons with *i* sides. The next two invariants are the order of the symmetry group and the number of cubic generators in the Stanley-Reisner ideal of the triangulation  $\Delta_d$ . The last item is a representative metric  $d = (d_{12}, d_{13}, d_{14}, d_{15}, d_{16}, d_{23}, d_{24}, d_{25}, d_{26}, d_{34}, d_{35}, d_{36}, d_{45}, d_{46}, d_{56})$ :

Type 1: (1, 10, 4), 1, 2, (9, 9, 10, 13, 18, 18, 17, 6, 11, 17, 14, 9, 11, 8, 17)Type 2: (1, 10, 4), 1, 3, (8, 8, 8, 14, 15, 16, 14, 6, 9, 12, 12, 7, 8, 7, 13)Type 3: (1, 10, 4), 1, 5, (5, 6, 7, 8, 12, 11, 10, 5, 7, 11, 6, 6, 7, 5, 10)Type 4: (1, 10, 4), 2, 3, (7, 5, 7, 12, 12, 12, 12, 5, 7, 10, 9, 7, 7, 5, 10)Type 5: (1, 10, 4), 2, 4, (6, 7, 8, 10, 14, 13, 12, 6, 8, 13, 9, 7, 6, 6, 10)Type 6: (1, 10, 4), 2, 5, (7, 7, 7, 11, 14, 12, 12, 6, 7, 14, 10, 7, 6, 7, 11)Type 7: (1, 10, 4), 8, 6, (5, 5, 5, 8, 10, 10, 8, 5, 5, 8, 5, 5, 5, 5, 8)Type 8: (2, 8, 5), 1, 3, (5, 5, 7, 10, 11, 10, 10, 5, 8, 10, 7, 6, 5, 4, 7)Type 10: (2, 8, 5), 2, 4, (7, 7, 8, 10, 14, 14, 13, 5, 9, 13, 9, 7, 10, 6, 14)

<sup>&</sup>lt;sup>1</sup>Note that the exterior segments do appear in Figures 1–5 of this paper and in the diagrams on our webpage. They are drawn in green for extra clarity.

Type 11: (2, 8, 5), 2, 4, (4, 5, 5, 8, 9, 9, 7, 4, 7, 8, 5, 4, 5, 4, 7)

Type 12: (3, 6, 6), 12, 3, (3, 3, 5, 6, 6, 6, 6, 3, 5, 6, 5, 3, 3, 3, 6)

The three metrics of types 9, 10 and 11 cannot be distinguished by the given invariants. In Section 5 we explain how to distinguish these three types.

The metric with the largest symmetry group is Type 12. Its symmetry group has order 12. This combinatorial type of this metric is given by the Stanley-Reisner ideal of the corresponding regular triangulation of  $\Delta(6, 2)$ :

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 \langle x_{36}x_{14}, x_{25}x_{34}, x_{35}x_{46}, x_{16}x_{45}, x_{35}x_{12}, x_{26}x_{35}, x_{36}x_{45}, x_{15}x_{36}, x_{26}x_{45}, x_{12}x_{46}, \\ x_{12}x_{56}, x_{25}x_{36}, x_{45}x_{23}, x_{24}x_{13}, x_{45}x_{12}, x_{34}x_{12}, x_{25}x_{46}, x_{23}x_{46}, x_{16}x_{25}, x_{13}x_{46}, \\ x_{24}x_{36}, x_{35}x_{14}, x_{13}x_{56}, x_{26}x_{14}, x_{26}x_{13}, x_{15}x_{46}, x_{36}x_{12}, x_{45}x_{13}, x_{25}x_{14}, x_{25}x_{13}, \\ x_{15}x_{26}x_{34}, x_{23}x_{56}x_{14}, x_{16}x_{24}x_{35} \rangle.
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The number of quadratic generators is 30, and this number is independent of the choice of generic metric. The number of cubic generators of this particular ideal is three (the last three generators), which is the third invariant listed under "Type 12". These cubic generators correspond to "empty triangles" in the triangulation  $\Delta_d$ . For instance, the cubic  $x_{15}x_{26}x_{34}$  means that conv $\{e_1 + e_5, e_2 + e_6, e_3 + e_4\}$  is not a triangle in  $\Delta_d$  but each of its three edges is an edge in  $\Delta_d$ . In the tight span  $T_d$  this can be seen as follows:

> {geodesics between 1 and 5}  $\cap$  {geodesics between 2 and 6}  $\cap$  {geodesics between 3 and 4} =  $\emptyset$ ,

but any two of these sets of geodesics have a common intersection. This can be seen in the picture of the tight span of the type 12 metric in Figure 1.

The twelve generic metrics listed above demonstrate the subtle nature of the notion of *combinatorial dimension* introduced in [6]. Namely, the combinatorial dimension of a generic metric d can be less than that of a generic split-decomposable metric [1]. This implies that the space of all *n*-point metrics of combinatorial dimension  $\leq 2$  is a polyhedral fan whose dimension exceeds the expected number 4n - 10 (cf. [7, Theorem 1.1 (d)]).

For six-point metrics, this discrepancy can be understood by looking at the centroid  $(\frac{1}{3}, \frac{1}{3}, \frac{1}{$ 

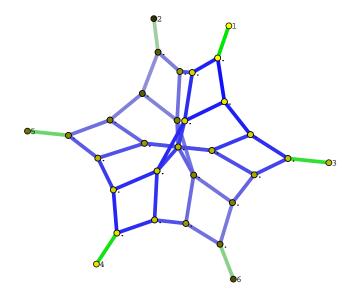


Figure 1: The tight span of the metric # 12

# 3 The 327 Three-Dimensional Generic Metrics

We next classify the 327 three-dimensional metrics. It turns out that in each case, the unique 3-dimensional cell is a simple polytope, so its numbers v of vertices and e of edges are determined by its number f of faces:

$$v = 2f - 4$$
 and  $e = v + f - 2$ .

We consider the two vectors  $R = (r_3, r_4, r_5, r_6)$  and  $B = (b_3, b_4, b_5, b_6)$  where  $r_i$  is the number of polygons with *i* edges on the 3-cell and  $b_i$  is the number of polygons with *i* edges not on the 3-cell. It turns out that no type has a polygon with 7 or more sides. Hence the number of facets of the 3-cell is  $f = r_3 + r_4 + r_5 + r_6$ . Our third invariant is the pair  $S = (s_2, s_3)$  where  $s_2$  (resp.  $s_3$ ) is the number of 2/4-splits (resp. 3/3-splits) lying on the cone of the metric fan containing *d*. The fourth invariant is the pair  $C = (c_5, c_6)$  where  $c_i$  is the number of cubic generators of the Stanley-Reisner ideal which involve *i* of the points. And finally we list (g, t) where *g* is the order of the symmetry group and *t* is the number of types which share these invariants. These invariants divides the 327 three-dimensional metrics into 251 equivalence classes. We order the classes lexicographically according to the vector (f, R, B, S, C, (g, t)). The 251 invariants are given in the following long list of strings R B S C gt:

40000a22600241	40000941501111	40000941502121	40001751401011
40001751402011	40001832501111	40001832502111	40002642402011
40002642402021	40002642403021	40002642404021	40002723502121
40003533404011	40004424406081	23000a21512121	23000850401011
23000850502111	23000931402011	23000931501111	$\underline{23000940510122}$

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0000 00 40 51 11 10	0000 00 40 51 01 00	0000 00 40 61 01 01	00001000100011
2300 0940 51 11 13	2300 0940 51 21 22	2300 0940 61 01 21	2300 1660 40 20 11
2300 1660 40 40 21	2300 1741 40 20 12	2300 1741 40 30 11	2300 1741 50 21 11
2300 1750 51 11 13	2300 1750 51 21 12	2300 1822 40 40 21	2300 1831 51 21 11
23002551404012	23002560512122	2300 2632 40 40 11	23002641512121
23003442406021	06000a11411011	06000a20420022	06000a20520012
06000a20620041	$\underline{06000c006300c1}$	06000840410011	06000840410021
06000840411011	06000840412021	06000840420022	06000840510021
06000921410021	06000930410011	06000930411011	06000930510012
06000930511011	06001650403021	06001650404021	06001650411011
06001650412012	06001650422011	06001731412011	06001740411011
06001740412011	06001740511011	06001821411011	06001821413011
06001830422011	06001830522011	06002460404011	06002460412021
06002460424041	06002541414021	06002631413011	06002640424041
06003270406041	22200840402011	22200840502121	22200921402021
22200930511113	22200930512113	22201650403021	22201650404011
22201650404021	22201731404011	22201740512113	22202460404011
22202541406021	22203270406041	05200a01310021	05200a10420012
05200a10520011	05200b00530021	05200830410011	05200830411011
05200920310011	05200920410011	05200920410021	05200920411011
$\underline{05200920420014}$	05200920510021	05200920520021	05201640411011
05201640412012	05201640422011	05201730312011	05201730411011
05201730412011	05201730413011	05201730422012	05201811312011
05201820422012	05201820522011	05202450414011	05202450424021
05202540413011	05202621314021	05202630424021	13300830411011
13300830412011	13300920410111	13300920411012	13300920411111
13300920511011	13301640404011	13301640412013	13301640422011
13301730411111	13301730412011	13301730413012	13301820422011
13301820522011	13302450406021	13302450414011	13302450424021
13302540413011	13302630424021	22210920512122	23020920512121
30311640404011	30312450406021	04400a00420021	04400a00430021
04400910320012	04400910410011	04400910420011	04401720311012
04401720312014	04401720321014	04401720322011	04401720411012
04401720422011	04401810321014	04401810421012	04401810421022
04401810422011	04401900431011	04402530312012	04402530314011
04402530323012	04402620323012	06020a00420021	06020a00430041
06020820420041	06021720422011	06022440424041	06022620424041
1331 0820 41 10 11	1331 0910 41 10 11	1331 1720 31 20 12	13311720413011
13311720422012	1331 1810 42 20 11	1331 2440 41 40 11	13312440424021
13312530314011	13312620424021	1412 0910 41 11 11	20602440424041
2141 0820 41 20 21	2141 2620 42 40 41	2222 1720 41 30 11	2222 2440 40 60 41
2222 2440 41 40 21	4004 2440 40 60 81	0360 0900 32 00 21	0360 0900 33 00 61
$\begin{array}{c} 2222 \\ 2440 \\ 4140 \\ 211 \\ 0360 \\ 1710 \\ 3110 \\ 11 \end{array}$	03601710322011	0360 2610 22 20 13	0360 2610 32 20 13
0360 2700 33 20 11	0360 2700 33 20 21	0360 3420 22 40 23	$0300\ 2010\ 32\ 2010\ 10\ 20\ 10\ 20\ 10\ 20\ 10\ 20\ 10\ 20\ 10\ 20\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 1$
03002700332011 $04411710311011$	03002700332021 $04411710321011$	0300 3420 22 40 23 0441 1800 32 10 12	0441 1800 33 10 11
04412520312011	04412520323011	0441 2610 22 20 11	04412610322011
04412610323011	04412520323011 $04412700332021$	0441 2010 22 20 11 0441 3420 22 40 21	05221710321011
01112010020011	07712100002021	0771 0720 22 40 21	0022 1110 02 10 11

05221800321012	05221800331011	05222520312021	05222520323011
05222610323011	06030900310161	12511710312011	12512520323011
13321710312011	13321710322011	13322520314011	13322520323011
13322610323012	23042520314021	02802600222011	02802600232021
02803410223021	02803410224021	03612600222011	03612600232011
03613410223011	03613410224022	03613500233011	04422600222013
04422600222022	04422600232022	04423410223011	04423410223023
04423500233013	05232600222021	05232600232021	05233410224021
06042600222041	12523410224022	13333410224021	14143410224021
02814300134012	02814300134021	03624300134011	03624300134021
04434300134013	04434300134021	05244300134021	02826000046041
03636000046021	03636000046061	04446000046083	

The letters a, b and c appearing in this list represent the integers 10, 11 and 12. We label the 327 types of three-dimensional metrics as Type 13, Type 14, ..., Type 339, in the order in which they appear in this list. Whenever the string does not end in a 1 then that string refers to more than one type.

For instance, the first underlined string refers to Type 32 and Type 33. For both of these types, the three-dimensional cell in  $T_d$  is a triangular prism, hence R = (2, 3, 0, 0). The next invariant B = (0, 9, 4, 0) says that the two-dimensional part of  $T_d$  consists of nine quadrangles and four pentagons. Types 34 through 38 share these characteristics. What distinguishes Types 32-33 from Types 34-38 is the number of cubic generators in the Stanley-Reisner ideal. The relevant vectors  $C = (c_5, c_6)$  in the table entries are 01, 11 and 21. The tight spans of Type 32 and 33 are depicted in Figure 2. The location of the four pentagons relative to the six exterior segments of the figure shows that these two types are non-isomorphic.

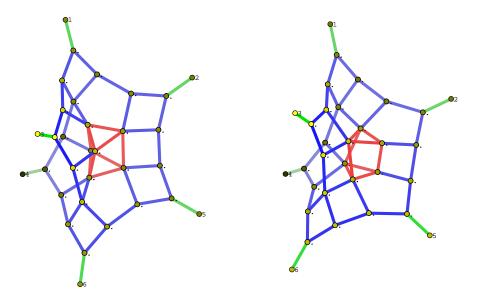


Figure 2: The tight spans of the metrics # 32 and # 33

The second underlined string in the long list is Type 66. Its 3-cell is a cube (hence

R = 0600), and its 2-dimensional part consists of twelve quadrangles (hence B = 0c00). This is the unique generic metric which is *split-decomposable* (hence S = 63) in the sense of [1]. It corresponds to the quadratic Gröbner bases (hence C = 00) and the *thrackle triangulation* described in [3, §2]. It has the symmetry group of a regular hexagon (hence g = 12) and it is uniquely characterized by R and B (hence t = 1). Its tight span is the logo for the conference on *Phylogenetic Combinatorics* which was held in Uppsala, Sweden, in July 2004, http://www.lcb.uu.se/pca04/.

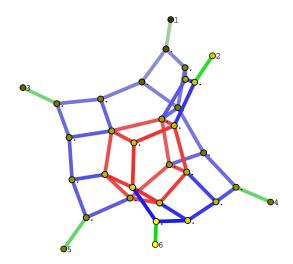


Figure 3: The tight span of the metric # 131

The third underlined string represents a class of four types, namely, Types 131, 132, 133 and 134. In each of these four cases, the 3-dimensional cell is a pentagonal prism (hence R = 0520), the two-dimensional part consists of nine quadrangles and two pentagons (hence B = 0920), and the Gröbner basis is quadratic (hence C = 00). Figure 3 shows one of these tight spans.

### 4 The 14 Non-regular Triangulations

Theorem 4.2 in [3] states that the hypersimplex  $\Delta(n, 2)$  has non-regular triangulations for  $n \geq 9$ . In this section we strengthen this result as follows.

**Theorem 3** The second hypersimplex  $\Delta(n, 2)$  admits non-regular triangulations if and only if  $n \geq 6$ . There are precisely 14 symmetry classes of non-regular triangulations of  $\Delta(6, 2)$ .

It can be shown by explicit computations that all triangulations of  $\Delta(4, 2)$  and  $\Delta(5, 2)$  are regular. In what follows we list the 14 non-regular triangulations of  $\Delta(6, 2)$ . Each of them can be lifted to a non-regular triangulation of  $\Delta(n, 2)$  for  $n \ge 7$  using the technique described at the end of [3, §4].

Each non-regular triangulation  $\Delta$  has a dual polyhedral cell complex T. This complex T shares all the combinatorial properties of a tight span  $T_d$ , but it cannot be realized as the complex of bounded faces of a polyhedron  $P_d$ . We call T the *abstract tight span* dual to  $\Delta$ .

We use the labels Type 340, Type 341, ..., Type 353 to denote the 14 non-regular triangulations  $\Delta$  of  $\Delta(6, 2)$ . In each case we describe the abstract tight span T. The first four of the 14 abstract tight spans are two-dimensional. They can be characterized by means of the invariants in Section 2:

Type 340: (0, 12, 3), 1, 1 Type 341: (0, 12, 3), 1, 2 Type 342: (0, 12, 3), 6, 0 Type 343: (1, 10, 4), 4, 1

The remaining ten abstract tight spans have a unique three-dimensional cell. We characterize them using the invariants (R, B, S, C, g) of Section 3:

Type 344: (4, 0, 0, 0), (0, 8, 6, 0), (4, 0), (0, 0), 4 Type 345: (0, 4, 4, 0), (0, 8, 2, 0), (4, 0), (0, 0), 4 Type 346: (0, 4, 4, 0), (2, 4, 4, 0), (4, 0), (4, 0), 2 Type 347: (0, 4, 4, 0), (2, 4, 4, 0), (4, 0), (2, 0), 4 Type 348: (0, 4, 4, 0), (2, 4, 4, 0), (4, 0), (2, 0), 4 Type 349: (0, 4, 4, 0), (2, 4, 4, 0), (4, 0), (6, 0), 8 Type 350: (0, 3, 6, 0), (2, 5, 2, 0), (3, 0), (2, 0), 2 Type 351: (0, 3, 6, 0), (2, 5, 2, 0), (3, 0), (4, 0), 2 Type 352: (0, 2, 8, 0), (2, 6, 0, 0), (2, 2), (2, 0), 4 Type 353: (0, 0, 12, 0), (6, 0, 0, 0), (0, 4), (6, 0), 24.

Type # 353 is the most symmetric one among triangulations  $\Delta$  of  $\Delta(6, 2)$ . The corresponding abstract tight span T is a beautiful object, namely, it is a dodecahedron with six triangles and six edges attached, as shown in Figure 4. The Stanley-Reisner ideal corresponding to the dodecahedral type # 353 is generated by 30 quadrics and 6 cubics. The quadrics in this ideal are

 $\begin{array}{l} x_{12}x_{35}, x_{12}x_{36}, x_{12}x_{45}, x_{12}x_{46}, x_{12}x_{56}, x_{13}x_{24}, x_{13}x_{26}, x_{13}x_{45}, \\ x_{13}x_{46}, x_{13}x_{56}, x_{14}x_{23}, x_{14}x_{26}, x_{14}x_{35}, x_{14}x_{36}, x_{14}x_{56}, x_{15}x_{23}, \\ x_{15}x_{24}, x_{15}x_{26}, x_{15}x_{36}, x_{15}x_{46}, x_{23}x_{45}, x_{23}x_{46}, x_{23}x_{56}, x_{24}x_{35}, \\ x_{24}x_{36}, x_{24}x_{56}, x_{26}x_{35}, x_{26}x_{45}, x_{35}x_{46}, x_{36}x_{45}. \end{array}$ 

The twelve variables  $x_{ij}$  appearing in this list can be identified with the edges of an octahedron. The 30 quadrics are precisely the pairs of disjoint edges of the octahedron. We note that these quadratic generators (and hence the global structure of the tight span) are also shared by the last six types (334, 335, 336, 337, 338, 339) in the table of Section 3. The simplicial complex represented by these 30 quadrics is (essentially) the boundary of the truncated octahedron (with the six square faces regarded as tetrahedra).

Now, each of the Types 334, 335, 336, 337, 338, 339 and 353 has six cubic generators in its ideal. The choice of these cubic generators amounts to subdividing each of the six square faces of the truncated octahedron with one of its two diagonals. Type 353 arises from the most symmetric choice of these diagonals. The six cubics in the ideal for Type 353 are

 $\underline{x_{34}}x_{12}x_{26}, \underline{x_{34}}x_{15}x_{56}, \underline{x_{16}}x_{23}x_{35}, \underline{x_{16}}x_{24}x_{45}, \underline{x_{25}}x_{13}x_{14}, \underline{x_{25}}x_{36}x_{46}.$ 

The underlined variables are the non-edges of the octahedron.

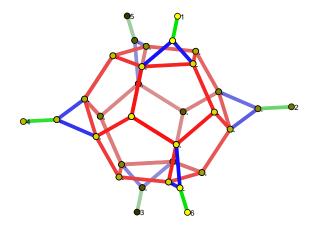


Figure 4: The dodecahedral (abstract) tight span # 353

The abstract tight span T has the following geometric description. The polytope dual to the truncated octahedron is gotten from the 3-cube by subdividing each of the six facets with a new vertex (thus creating  $6 \times 4 = 24$  edges) and then erasing the 12 edges of the cube. Consider the six 4-valent vertices we just introduced. Each of them can be replaced by two trivalent vertices with a new edge in-between. If this replacement is done in the most symmetric manner then the result is a dodecahedron. Finally, we glue a triangle and an edge on each of the six new edges. The result is Figure 4.

### 5 Prime Metrics and Minimal Subdivisions

Koolen, Moulton and Tönges [12] classified all the *prime metrics* for n = 6. These are the rays in the metric fan  $MF_6$ . There are 14 symmetry classes:

 $\begin{array}{ll} 1/5 \ {\rm Split:} \ d = (0,0,0,0,1,0,0,0,1,0,0,1,0,1,1)\\ 2/4 \ {\rm Split:} \ d = (1,1,0,1,1,0,1,0,0,1,0,0,1,1,0)\\ 3/3 \ {\rm Split:} \ d = (0,0,1,1,1,0,1,1,1,1,1,1,0,0,0)\\ {\rm Prime} \ P_1: \ d = (1,1,1,2,2,2,2,1,2,2,1,2,1,1)\\ {\rm Prime} \ P_2: \ d = (1,1,1,2,2,2,2,1,1,2,1,1,1,1,2)\\ {\rm Prime} \ P_3: \ d = (1,1,1,2,2,2,2,1,1,2,1,1,1,1,2)\\ {\rm Prime} \ P_4: \ d = (1,1,1,1,2,1,1,1,1,1,1,1,1,2,1,1)\\ {\rm Prime} \ P_5: \ d = (1,2,2,2,4,3,3,3,3,2,2,2,4,2,2)\\ {\rm Prime} \ P_6: \ d = (1,1,2,3,3,2,3,2,2,3,2,2,1,1,2)\\ \end{array}$ 

Prime  $P_7$ : d = (1, 1, 1, 2, 2, 2, 2, 1, 1, 2, 1, 1, 2, 1, 2)Prime  $P_8$ : d = (1, 2, 2, 4, 4, 3, 3, 3, 3, 4, 2, 2, 2, 2, 4)Prime  $P_9$ : d = (1, 1, 1, 2, 3, 2, 2, 1, 2, 2, 1, 2, 3, 2, 1)Prime  $P_{10}$ : d = (0, 1, 1, 1, 2, 1, 1, 1, 2, 2, 2, 1, 2, 1, 1)Prime  $P_{11}$ : d = (0, 1, 1, 2, 2, 1, 1, 2, 2, 2, 1, 1, 1, 1, 2)

Our computations provide an independent verification of the correctness and completeness of the results in [12]. Namely, we computed the cone in the metric fan corresponding to each of the 339 metrics. For each cone we computed (using POLYMAKE [10]) the facets and the extreme rays of the cone. And it turned out that the extreme rays we found are precisely the 14 types listed above. All the facets and extreme rays of the 339 types of maximal cones in the metric fan  $MF_6$  are posted at

### bio.math.berkeley.edu/SixPointMetrics

Our computations lead to the following result.

**Proposition 4** If  $f_i$  is the number of types of maximal cones in the metric fan  $MF_6$  with *i* facets and  $e_j$  is the number with *j* extreme rays then

$$(f_{15}, f_{16}, \dots, f_{21}) = (197, 42, 63, 18, 8, 10, 1) (e_{15}, e_{16}, \dots, e_{24}) = (197, 60, 28, 19, 20, 2, 5, 2, 1, 5).$$

In particular, the metric fan  $MF_6$  has 197 types of simplicial cones.

Proposition 4 shows that the largest number of facets of any cone is 21, attained by only one type, and the largest number of extreme rays is 24, attained by five types. The next two examples concern the extremal cases.

**Example 5** Type 12 is the last metric listed in the table of Section 2. Its cone in the metric fan is described by the following 21 linear inequalities:

$$\begin{aligned} d_{12} + d_{25} &\geq d_{15}, \quad d_{13} + d_{36} \geq d_{16}, \quad d_{45} + d_{46} \geq d_{56}, \\ d_{25} + d_{45} &\geq d_{24}, \quad d_{36} + d_{46} \geq d_{34}, \quad d_{12} + d_{13} \geq d_{23}, \\ d_{26} + d_{34} &\geq d_{24} + d_{36}, \quad d_{15} + d_{26} \geq d_{16} + d_{25}, \quad d_{14} + d_{23} \geq d_{13} + d_{24}, \\ d_{14} + d_{56} &\geq d_{16} + d_{45}, \quad d_{16} + d_{35} \geq d_{15} + d_{36}, \quad d_{24} + d_{35} \geq d_{25} + d_{34}, \\ d_{14} + d_{23} &\geq d_{12} + d_{34}, \quad d_{14} + d_{56} \geq d_{15} + d_{46}, \quad d_{26} + d_{34} \geq d_{23} + d_{46}, \\ d_{24} + d_{35} &\geq d_{23} + d_{45}, \quad d_{15} + d_{26} \geq d_{12} + d_{56}, \quad d_{16} + d_{35} \geq d_{13} + d_{56}, \\ d_{15} + d_{23} + d_{34} + d_{56} \geq d_{16} + d_{24} + 2d_{35}, \\ d_{16} + d_{23} + d_{24} + d_{56} \geq d_{15} + 2d_{26} + d_{34}, \\ d_{15} + d_{16} + d_{24} + d_{34} \geq 2d_{14} + d_{23} + d_{56}. \end{aligned}$$

None of these 21 inequalities is redundant. This cone has 19 extreme rays: the six 1/5 splits, six 2/4 splits, three rays of type  $P_6$ , three rays of type  $P_7$ , and a unique ray of type  $P_2$ , namely, (1, 1, 1, 2, 2, 2, 2, 1, 1, 2, 1, 1, 1, 1, 2).

The six 1/6-splits are among the extreme rays of every cone in the metric fan  $MF_6$ . In the next example, we only list the other extreme rays.

**Example 6** The five types of cones in  $MF_6$  with 24 extreme rays are # 7, # 26, # 337, # 338, and # 339. Only # 7 corresponds to a two-dimensional tight span. The following 18 vectors are extreme rays of this cone:

2/4 split : (101111000111000)	2/4 split : (100011110001011)
2/4 split : (011111111000000)	2/4 split : (010011001110011)
$P_2:(111222211211112)$	$P_6:(121333222311222)$
$P_6:(122233312221213)$	$P_6:(211333311222222)$
$P_6:(212233221312213)$	$P_7:(111222211211212)$
$P_8:(221444322322334)$	$P_8:(222344412432323)$
$P_8:(222344432412323)$	$P_8:(223444322322314)$
$P_{10}:(111222011211112)$	$P_{10}:(111222211011112)$
$P_{10}:(111022211211112)$	$P_{10}:(111222211211110)$

The other four types with 24 extreme rays are three-dimensional, and each of them has three-dimensional prime metrics among its extreme rays. For instance, the following 18 vectors are extreme rays of the cone # 338:

3/3 split : (110010110110011)	3/3 split : (101011010101101)
3/3 split : (010111011100110)	3/3 split : (001110111111000)
$P_1:(111122221221211)$	$P_4:(111121111211111)$
$P_5:(322243331422222)$	$P_5:(222142232432323)$
$P_5:(122243333422222)$	$P_5:(222342232432321)$
$P_9:(221232121321121)$	$P_9:(121131222311222)$
$P_9:(112132122322112)$	$P_9:(212231221312211)$
$P_{11}:(111122221221011)$	$P_{11}:(111122221201211)$
$P_{11}:(111120221221211)$	$P_{11}:(111122021221211)$

The corresponding lists for all 339 types appear on our website.

It is instructive to draw the tight spans of the eleven prime metrics. Four of them are actually three-dimensional. For instance, the metric  $P_4$  has the structure of an octahedron. Please compare Figure 5 with [12, Figure 1].

	# vertices	# edges	# polygons	# 3-cells
$P_1:$	6	9	4	0
$P_2$ :	7	15	9	0
$P_3$ :	6	10	6	1
$P_4$ :	10	20	12	1
$P_5$ :	11	20	11	1
$P_6$ :	7	11	5	0
$P_7:$	11	20	10	0
$P_8:$	11	19	9	0
$P_{9}:$	7	12	7	1
$P_{10}:$	5	7	3	0
$P_{11}:$	5	7	3	0

For each of the 11 prime metrics, we list the f-vector of their tight span:

The metrics  $P_1, \ldots, P_9$  each have six *trivial vertices* in their tight span. The list of non-trivial vertices given in [12, Table 1] is consistent with our list above. The prime metrics  $P_{10}$  and  $P_{11}$  are improper in the sense that two points have distance zero.

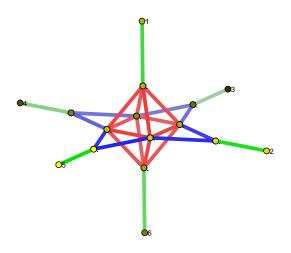


Figure 5: The tight span of the metric  $P_4 + (1, 1, ..., 1)$ 

**Remark 7** The tight spans of the prime metrics  $P_3$ ,  $P_4$ ,  $P_5$ ,  $P_9$  have a 3-dimensional cell, while the tight spans of the other seven are 2-dimensional.

The metric fan  $MF_6$  defines an incidence relation between the prime metrics and the generic metrics. This leads to a finer invariant for distinguishing among the 339 types of generic types. This invariant is the vector  $(S, P) = (s_2, s_3, p_1, p_2, \ldots, p_{11})$  where  $p_i$  is the number of extreme rays of type  $P_i$  which lie on the corresponding cone. This invariant resolves about half of the clusters which had been left unresolved by the earlier invariants.

**Example 8** The three two-dimensional types # 9, # 10 and # 11, all have the same invariants R = (2, 8, 5), g = 2 and c = 4 in the list of Section 2. They are distinguished by the new invariant  $(S, P) = (s_2, s_3, p_1, p_2, \ldots, p_{11})$ 

Type 9 has (S, P) = (4, 0, 0, 1, 0, 0, 0, 2, 1, 2, 0, 2, 0). Type 10 has (S, P) = (5, 0, 0, 1, 0, 0, 0, 1, 2, 2, 0, 2, 0). Type 11 has (S, P) = (5, 0, 0, 1, 0, 0, 0, 2, 2, 2, 0, 2, 0).

**Example 9** The last three three-dimensional types # 337, # 338 and # 339 all have the same invariants (f, R, B, S, C) in the big table of Section 3. They are distinguished by the new invariant  $(S, P) = (s_2, s_3, p_1, p_2, \dots, p_{11})$ 

Type 337 has (S, P) = (0, 4, 0, 0, 1, 1, 4, 0, 0, 0, 4, 0, 4). Type 338 has (S, P) = (0, 4, 1, 0, 0, 1, 4, 0, 0, 0, 4, 0, 4). Type 339 has (S, P) = (0, 4, 1, 0, 1, 0, 4, 0, 0, 0, 4, 0, 4).

We close this section with a remark aimed at experts in polytope theory. The metric fan is the secondary fan of the hypersimplex  $\Delta(6, 2)$ , hence it is the normal fan of the secondary polytope  $\Sigma(\Delta(6, 2))$ . Following [2], the vertices of the secondary polytope correspond to the regular triangulations of  $\Delta(6, 2)$ , and the facets of the secondary polytope correspond to minimal regular subdivisions of  $\Delta(6, 2)$ . For instance, Figure 5 is the dual picture to a regular subdivision of  $\Delta(6, 2)$  into 10 five-dimensional polytopes.

The results described in this section provide the vertex-facet incidence matrix of the secondary polytope  $\Sigma(\Delta(6,2))$ . In particular, the classification result of Koolen, Moulton and Tönges [12] can be restated as follows.

**Corollary 10** Up to the action of the symmetric group on  $\{1, 2, 3, 4, 5, 6\}$ , the secondary polytope  $\Sigma(\Delta(6, 2))$  has precisely 14 facets.

# 6 Visualization of Tight Spans in POLYMAKE

POLYMAKE is a software package developed by Ewgenij Gawrilow and Michael Joswig for studying polytopes and polyhedra [10]. It allows us to define a polyhedron by a set of either inequalities or vertices and computes numerous properties of the polyhedron. We implemented a client program to POLYMAKE for visualizing the tight span  $T_d$  of a given metric d. In short, our program does the following to produce the figures in this paper:

- 1. Compute all faces of the polyhedron  $P_d$  from the given metric d.
- 2. Build the tight span  $T_d$  by extracting the bounded faces of  $P_d$ .
- 3. Spring-embed the 2-skeleton of  $T_d$  in 3-space using POLYMAKE's spring embedder and display it using JAVAVIEW.
- 4. Label the points corresponding to the finite set (the "taxa") on which the metric is defined. In our case, the set of labels is  $\{1, 2, 3, 4, 5, 6\}$ .

The program was developed by the second author with the assistance of Michael Joswig and Julian Pfeifle. The code can be downloaded at

### www.math.berkeley.edu/~jyu/.

The figures above only show the combinatorial properties of the tight span and, because of the projection and the spring embedder, the edge lengths seen here do not represent the actual edge lengths in the tight span.

The pictures produced by our software are different from the output produced by the software SPLITSTREE [8]. SPLITSTREE is a program that can, among other things, compute and visualize the split-decompositions of metrics (see [1, 8]). It decomposes an input metric into a sum of splits plus a *split-prime* metric that cannot be further decomposed into splits. SPLITSTREE outputs a planar graph representing the split-decomposable part of the input metric, where sets of parallel edges represent splits.

When a metric is split-decomposable, then the tight span is a cubical complex, and the output from SPLITSTREE agrees with our visualization with a few edges removed to make it planar. The edges output by SPLITSTREE are scaled to be metrically accurate. By contrast, our implementation does not preserve the edge lengths. Among the 339 generic metrics on six points, only one type (namely, Type # 66) is split-decomposable. For all other 338 types, the picture produced by our program contains more refined combinatorial information than the output of SPLITSTREE.

The split-decomposition theory of Bandelt and Dress [1] has the following interpretation in terms of the metric fan. The 31 splits are among the extreme rays of the metric fan. Consider the *induced subfan* of  $MF_6$  on the 31 splits. A key result in [1] states that this subcomplex is simplicial, i.e., all cones in this subfan are spanned by linearly independent vectors. Now consider any metric d, for instance, one of our 339 generic metrics, and let C be the cone of the metric fan  $MF_6$  containing d in its relative interior. The intersection of C with the induced subfan of split-decomposable metrics is a simplicial face F of C. It follows that d can be written uniquely as a sum of a vector d' in F and a positive combination of extreme rays of C not in F. The output of SPLITSTREE is the edge graph of the tight span of d'.

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# References

- H.-J. Bandelt and A. Dress: A canonical decomposition theory for metrics on a finite set, Advances in Mathematics 92 (1992) 47–105.
- [2] L. Billera, P. Filliman and B. Sturmfels: Constructions and complexity of secondary polytopes, Advances in Mathematics 83 (1990) 155–179.
- [3] J. De Loera, B. Sturmfels and R. Thomas: Gröbner bases and the triangulations of the second hypersimplex, *Combinatorica* 15 (1995) 409–423.
- [4] A. Deza, K. Fukuda, T. Misutani and C. Vo: On the face lattice of the metric polytope, *Lecture Notes in Computer Science* 2866, Springer-Verlag, Berlin, (2003) 118–128.
- [5] M. Deza and M. Laurent: Geometry of Cuts and Metrics, Algorithms and Combinatorics, 15, Springer-Verlag, Berlin, 1997.
- [6] A. Dress: Trees, tight extensions of metric spaces, and the cohomological dimension of certain groups, Advances in Mathematics 53 (1984) 321–402.
- [7] A. Dress, K. Huber and V. Moulton: Totally split-decomposable metrics of combinatorial dimension two, Annals of Combinatorics 8 (2001) 99–112.
- [8] A. Dress, D. Huson and V. Moulton: Analyzing and visualizing sequence and distance data using SplitsTree. *Discrete Appl. Math.* **71** (1996) 95–109.
- [9] M. Dutour: Cut and Metric Cones, Classification of facets and extreme rays for  $n \le 8$  posted at http://www.liga.ens.fr/~dutour/CUT\_MET/CutMetricCones.html.
- [10] E. Gawrilow and M. Joswig: Polymake: a framework for analyzing convex polytopes. em Polytopes – Combinatorics and Computation (Oberwolfach, 1997), 43–73, DMV Sem., 29, Birkhäuser, Basel, 2000.
- [11] K. Polthier, S. Khadem, E. Preuss, and U. Reitebuch: JAVAVIEW: Interactive 3D Geometry and Visualization, www.javaview.de.
- [12] J. Koolen, V. Moulton and U. Tönges: A classification of the six-point prime metrics, European Journal of Combinatorics 21 (2000) 815–829.
- [13] J. Rambau: TOPCOM: triangulations of point configurations and oriented matroids. *Mathematical Software* (Beijing, 2002), 330–340, World Sci. Publishing, River Edge, NJ, 2002.