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Enumeration of Integral Tetrahedra

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Abstract

We determine the numbers of integral tetrahedra with diameter d up to isomorphism for all $d \leq 1000$ via computer enumeration. Therefore we give an algorithm that enumerates the integral tetrahedra with diameter at most d in $O(d^5)$ time and an algorithm that can check the canonicity of a given integral tetrahedron with at most 6 integer comparisons. For the number of isomorphism classes of integral 4×4 matrices with diameter d fulfilling the triangle inequalities we derive an exact formula.

1 Introduction

Geometrical objects with integral side lengths have fascinated mathematicians for ages. A very simple geometric object is the m-dimensional simplex. Recently an intriguing bijection between m-dimensional simplices with edge lengths in $\{1, 2\}$ and the partitions of $m+1$ was discovered [2]. So far, for m-dimensional simplices with edge lengths in $\{1, 2, 3\}$ no formula is known and exact numbers are obtained only up to $m = 13$ [9]. Let us more generally denote by $\alpha(m, d)$ the number of non-isomorphic m-dimensional simplices with edge lengths in $\{1, \ldots, d\}$ where at least one edge has length d. We also call d the diameter of the simplex. The known results, see i.e., [9], are, besides some exact numbers,

$$\begin{aligned}
\alpha(1, d) &= 1, \\
\alpha(2, d) &= \left\lfloor \frac{d+1}{2} \right\rfloor \left\lfloor \frac{d+2}{2} \right\rfloor = \left\lfloor \frac{(d+1)^2}{4} \right\rfloor, && \text{[A002620]} \\
\alpha(m, 1) &= 1, \\
\alpha(m, 2) &= p(m+1) - 1, && \text{[A000065]}
\end{aligned}$$

where $p(m+1)$ denotes the number of partitions [A000041] of $m+1$. The aim of this article is the determination of the number of non-isomorphic integral tetrahedra $\alpha(3,d)$.

Besides an intrinsic interest in integral simplices, their study is useful in field of integral point sets. These are sets of n points in the m-dimensional Euclidean space $\mathbb{E}^m$ with pairwise integral distances. Applications for this combinatorial structure involving geometry and number theory are imaginable in radio astronomy (wave lengths), chemistry (molecules), physics (energy quantums), robotics, architecture, and other fields, see [3] for an overview. We define the largest occurring distance of an integral point set $\mathcal{P}$ as its diameter. From the combinatorial point of view there is a natural interest in the determination of the minimum possible diameter $d(m,n)$ for given parameters m and n [3, 4, 5, 7, 9, 10, 11, 12, 14, 16]. In most cases exact values of $d(m,n)$ are obtained by an exhaustive enumeration of integral point sets with diameter $d \leq d(m,n)$. A necessary first step for the enumeration of m-dimensional integral point sets is the enumeration of m-dimensional integral simplices. Hence there is a need for an efficient enumeration algorithm.

Another application of integral tetrahedra concerns geometric probabilities. Suppose you are given a symmetric 3×3 matrix Δ_2 with entries being equi-distributed in $[0,1]$ and zeros on the main diagonal. The probability $\mathcal{P}_2$ that Δ_2 is the distance matrix of a triangle in the Euclidean metric can be easily determined to be $\mathcal{P}_2=\frac{1}{2}$. As a generalization we ask for the probability $\mathcal{P}_m$ of a similar defined $(m+1)\times(m+1)$ matrix Δ_m being the distance matrix of an m-dimensional simplex in the Euclidean metric. To analyze the question for $m=3$ we consider a discretization and obtain $\mathcal{P}_3=\lim\limits_{d\to\infty}\frac{4\cdot\alpha(3,d)}{d^5}$.

Our main results are the determination of $\alpha(3,d)$ for $d\leq 1000$,

Theorem 1. *The number $\hat{\alpha}_{\leq}(d,3)$ of symmetric 4×4 matrices with entries in $\{1,\dots,d\}$ fulfilling the triangle inequalities is given by*

$$\hat{\alpha}_{\leq}(d,3)=\begin{cases}\frac{17d^6+425d^4+1628d^2}{2880}, & \text{if } d\equiv 0 (\text{mod } 2);\\ \frac{17d^6+425d^4+1763d^2+675}{2880}, & \text{if } d\equiv 1 (\text{mod } 2).\end{cases}$$

If we additionally request a diameter of exactly d we have

$$\hat{\alpha}(d,3)=\begin{cases}\frac{34d^5-85d^4+680d^3-962d^2+1776d-960}{960} & \text{if } d\equiv 0 (\text{mod } 2);\\ \frac{34d^5-85d^4+680d^3-908d^2+1722d-483}{960} & \text{if } d\equiv 1 (\text{mod } 2).\end{cases}$$

Theorem 2.

$$0.090\leq\mathcal{P}_3\leq 0.111,$$

and the enumeration algorithms of Section 4 and Section 5, which allows us to enumerate integral tetrahedra with diameter at most d in time $O(d^5)$ and to check a 4×4-matrix for canonicity using at most 6 integer comparisons.

2 Number of integral tetrahedra

Because a symmetric 4×4-matrix with zeros on the diagonal has six independent non-zero values there are d^6 labeled integral such matrices with diameter at most d. To obtain the number $\overline{\alpha}_{\leq}(d,3)$ of unlabeled matrices we need to apply the following well known Lemma:

Lemma 3. *(Cauchy-Frobenius, weighted form)*
Given a group action of a finite group G on a set S and a map $w : S \longrightarrow R$ from S into a commutative ring R containing $\mathbb{Q}$ as a subring. If w is constant on the orbits of G on S, then we have, for any transversal $\mathcal{T}$ of the orbits:

$$\sum_{t\in\mathcal{T}} w(t) = \frac{1}{|G|}\sum_{g\in G}\sum_{s\in S_g} w(s)$$

where S_g denotes the elements of S being fixed by g, i.e.

$$S_g = \{s \in S | s = gs\}\,.$$

For a proof, notation and some background we refer to [6]. Applying the lemma yields:

Lemma 4.

$$\overline{\alpha}_{\le}(d,3) = \frac{d^6 + 9d^4 + 14d^2}{24}$$

and

$$\overline{\alpha}(d,3) = \overline{\alpha}_{\le}(d,3) - \overline{\alpha}_{\le}(d-1,3) = \frac{6d^5 - 15d^4 + 56d^3 - 69d^2 + 70d - 24}{24}.$$

As geometry is involved in our problem we have to take into account some properties of Euclidean spaces. In the Euclidean plane $\mathbb{E}^2$ the possible occurring triples of distances of triangles are completely characterized by the triangle inequalities. In general there is a set of inequalities using the so called Cayley-Menger determinant to characterize whether a given symmetric $(m+1)\times(m+1)$ matrix with zeros on the diagonal is a distance matrix of an m-dimensional simplex [13]. For a tetrahedron with distances $\delta_{i,j}$, $0 \le i \le j < 4$, the inequality

$$CMD_3 = \begin{vmatrix} 0 & \delta_{0,1}^2 & \delta_{0,2}^2 & \delta_{0,3}^2 & 1 \\ \delta_{1,0}^2 & 0 & \delta_{1,2}^2 & \delta_{1,3}^2 & 1 \\ \delta_{2,0}^2 & \delta_{2,1}^2 & 0 & \delta_{2,3}^2 & 1 \\ \delta_{3,0}^2 & \delta_{3,1}^2 & \delta_{3,2}^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} > 0 \qquad (1)$$

has to be fulfilled besides the triangle inequalities.

In the first step we exclusively consider the triangle inequalities for $m = 3$ and count the number $\hat{\alpha}_{\le}(d,3)$ of non-isomorphic symmetric 4×4 matrices with entries in $\{1,\ldots,d\}$ fulfilling the triangle inequalities.

Proof of Theorem 1.
Counting labeled symmetric 4×4 matrices with entries in $\{1,\ldots,d\}$ fulfilling the triangle inequalities is equivalent to determining integral points in a six-dimensional polyhedron. Prescribing the complete automorphism group results in some further equalities and an application of the inclusion-exclusion principle. Thus, after a lengthy but rather easy computation we can apply Lemma 3 and obtain

$$24\hat{\alpha}_{\le}(d,3) = 3\cdot\left\lceil\frac{4d^4+5d^2}{12}\right\rceil + 6\cdot\frac{37d^4 - 18d^3 + 20d^2 - 21d + (36d^2+42)\left\lceil\frac{d}{2}\right\rceil}{96}$$

$$+\left\lceil\frac{34d^6+55d^4+136d^2}{240}\right\rceil+6\cdot\left(d^2-d\left\lceil\frac{d}{2}\right\rceil+\left\lceil\frac{d}{2}\right\rceil^2\right)+8\cdot\left(d^2-d\left\lceil\frac{d}{2}\right\rceil+\left\lceil\frac{d}{2}\right\rceil^2\right),$$

which can be modified to the stated formulas. □

d	$\alpha(d,3)$	d	$\alpha(d,3)$	d	$\alpha(d,3)$	d	$\alpha(d,3)$	d	$\alpha(d,3)$
1	1	26	305861	51	8854161	76	65098817	120	639349793
2	4	27	369247	52	9756921	77	69497725	140	1382200653
3	16	28	442695	53	10732329	78	74130849	160	2695280888
4	45	29	527417	54	11783530	79	79008179	180	4857645442
5	116	30	624483	55	12916059	80	84138170	200	8227353208
6	254	31	735777	56	14133630	81	89532591	220	13251404399
7	516	32	861885	57	15442004	82	95198909	240	20475584436
8	956	33	1005214	58	16845331	83	101149823	260	30554402290
9	1669	34	1166797	59	18349153	84	107392867	280	44260846692
10	2760	35	1348609	60	19957007	85	113942655	300	62496428392
11	4379	36	1552398	61	21678067	86	120807154	320	86300970558
12	6676	37	1780198	62	23514174	87	127997826	340	116862463817
13	9888	38	2033970	63	25473207	88	135527578	360	155526991341
14	14219	39	2315942	64	27560402	89	143409248	380	203808692441
15	19956	40	2628138	65	29783292	90	151649489	400	263399396125
16	27421	41	2973433	66	32145746	91	160268457	420	336178761892
17	37062	42	3353922	67	34657375	92	169272471	440	424224122232
18	49143	43	3773027	68	37322859	93	178678811	460	529820175414
19	64272	44	4232254	69	40149983	94	188496776	480	655468974700
20	82888	45	4735254	70	43145566	95	198743717	500	803900006590
21	105629	46	5285404	71	46318399	96	209427375	520	978079728301
22	133132	47	5885587	72	49673679	97	220570260	540	1181221582297
23	166090	48	6538543	73	53222896	98	232180129	560	1416796092768
24	205223	49	7249029	74	56969822	99	244275592	580	1688540496999
25	251624	50	8019420	75	60926247	100	256866619	600	2000468396580

Table 1: Number $\alpha(d,3)$ of integral tetrahedra with diameter d - part 1.

In addition to this proof we have verified the stated formula for $d \le 500$ via a computer enumeration. We remark that $\frac{\hat{\alpha}_{\le}(d,3)}{\overline{\alpha}_{\le}(d,3)}$ and $\frac{\hat{\alpha}(d,3)}{\overline{\alpha}(d,3)}$ tend to $\frac{17}{120}=0.141\overline{6}$ if $d\to\infty$. Moreover we were able to obtain an exact formula for $\hat{\alpha}(d,3)$ because the Cayley-Menger determinant

$$CMD_2=\begin{vmatrix} 0 & \delta_{0,1}^2 & \delta_{0,2}^2 & 1\\ \delta_{1,0}^2 & 0 & \delta_{1,2}^2 & 1\\ \delta_{2,0}^2 & \delta_{2,1}^2 & 0 & 1\\ 1 & 1 & 1 & 0\end{vmatrix}$$

for dimension $m=2$ can be written as

$$CMD_2=-(\delta_{0,1}+\delta_{0,2}+\delta_{1,2})(\delta_{0,1}+\delta_{0,2}-\delta_{1,2})(\delta_{0,1}-\delta_{0,2}+\delta_{1,2})(-\delta_{0,1}+\delta_{0,2}+\delta_{1,2}).$$

Thus $CMD_2 < 0$ is equivalent to the well known linear triangle inequalities $\delta_{0,1} + \delta_{0,2} > \delta_{1,2}$, $\delta_{0,1}+\delta_{1,2} > \delta_{0,2}$ and $\delta_{0,2}+\delta_{1,2} > \delta_{0,1}$. Unfortunately for $m \geq 3$ the Cayley-Menger determinant is irreducible [1] and one cannot simplify $(-1)^{m+1}CMD_m > 0$ into a set of inequalities of lower degree. So we are unable to apply the same method to derive an analytic formula for $\alpha(d,3)$.

d	$\alpha(d,3)$	d	$\alpha(d,3)$	d	$\alpha(d,3)$
620	2356880503873	760	6523288334629	900	15192308794063
640	2762373382787	780	7428031732465	920	16957109053082
660	3221850132593	800	8430487428682	940	18882231158104
680	3740530243895	820	9538364312059	960	20978358597822
700	4323958989350	840	10759766492473	980	23256639532080
720	4978017317882	860	12103204603044	1000	25728695195597
740	5708932993276	880	13577602128303		

Table 2: Number $\alpha(d,3)$ of integral tetrahedra with diameter d - part 2.

Lemma 5. *We have $\alpha(3,d) \in \Omega(d^5)$, $\alpha(3,d) \in O(d^5)$, $\alpha_{\leq}(3,d) \in \Omega(d^6)$, and $\alpha_{\leq}(3,d) \in O(d^6)$.*

Proof. The upper bounds are trivial since they also hold for symmetric matrices with integer values at most d and zeros on the diagonal. For the lower bounds we consider six-tuples $\delta_{0,1} \in [d, d(1-\varepsilon))$, $\delta_{0,2} \in [d(1-\varepsilon), d(1-2\varepsilon))$, $\delta_{1,2} \in [d(1-2\varepsilon), d(1-3\varepsilon))$, $\delta_{0,3} \in [d(1-3\varepsilon), d(1-4\varepsilon))$, $\delta_{1,3} \in [d(1-4\varepsilon), d(1-5\varepsilon))$, and $\delta_{2,3} \in [d(1-5\varepsilon), d(1-6\varepsilon))$. For each ε there are $\Omega(d^6)$ non-isomorphic matrices. If ε is suitable small then all these matrices fulfill the triangle conditions and inequality 1. $\square$

In general we have $\alpha_{\leq}(m,d) \in \Omega(d^{m(m+1)/2})$, $\alpha_{\leq}(m,d) \in O(d^{m(m+1)/2})$, $\alpha(m,d) \in \Omega(d^{m(m+1)/2-1})$, and $\alpha(m,d) \in O(d^{m(m+1)/2-1})$.

In Section 4 and Section 5 we give an algorithm to obtain $\alpha(d,3)$ via implicit computer enumeration. Some of these computed values are given in Table 1 and Table 2. For a complete list of $\alpha(d,3)$ for $d \leq 1000$ we refer to [8]. This amounts to

$$\alpha_{\leq}(1000,3) = 4299974867606266 \approx 4.3 \cdot 10^{15}.$$

3 Bounds for $\mathcal{P}_3$

In this section we give bounds for the probability $\mathcal{P}_3$ that Δ_3 is the distance matrix of a tetrahedron in the 3-dimensional Euclidean space $\mathbb{E}^3$, where Δ_3 is a symmetric 4×4 matrix with zeros on the main diagonal and the remaining entries being equi-distributed in $[0,1]$. Therefore we consider a discretization. Let d be a fixed number. We consider the d^6 six-dimensional cubes $\mathcal{C}_{i_1,\dots,i_6} := \times_{j=1}^{6}\left[\frac{i_j}{d}, \frac{i_j+1}{d}\right] \subseteq [0,1]^6$. For every cube $\mathcal{C}$ it is easy to decide whether every point of $\mathcal{C}$ fulfills the triangle conditions, no points of $\mathcal{C}$ fulfill the triangle conditions, or both cases occur. For inequality 1 we have no explicit test but we are able to compute a lower bound $\underline{CMD_3}(\mathcal{C})$ and an upper bound $\overline{CMD_3}(\mathcal{C})$, so that we have

$$\underline{CMD_3}(\mathcal{C}) \leq CMD_3(x) \leq \overline{CMD_3}(\mathcal{C}) \text{ for all } x \in \mathcal{C}.$$

Thus for some cubes $\mathcal{C}$ we can decide that all $x \in \mathcal{C}$ correspond to a tetrahedron. We denote this case by $\Xi(\mathcal{C}) = 1$. If no $x \in \mathcal{C}$ corresponds to a tetrahedron we set $\Xi(\mathcal{C}) = -1$. In all other cases we define $\Xi(\mathcal{C}) = 0$. With this we obtain for all $d \in \mathbb{N}$ the following bounds:

Lemma 6.

$$\sum_{\mathcal{C}\,:\,\Xi(\mathcal{C})=1} \frac{1}{d^6} \leq \mathcal{P}_3 \leq 1 - \sum_{\mathcal{C}\,:\,\Xi(\mathcal{C})=-1} \frac{1}{d^6}.$$

Thus we have a method to obtain bounds on $\mathcal{P}_3$ using computer calculations. For the actual computation we use two further speed ups. We can take advantage of symmetries and use an adaptive strategy: We start with a small value of d and subdivide cubes $\mathcal{C}$ with $\Xi(\mathcal{C}) = 0$ recursively into 8 smaller cubes. After a computer calculation we obtain

$$0.090 \leq \mathcal{P}_3 \leq 0.111,$$

which proves Theorem 2. Clearly Theorem 2 can be improved by simply letting the computers work for a longer time or by using a computing cluster, but the convergence of our approach seems to be rather slow. An enhanced check whether a cube C fulfills inequality (1) would be very useful.

Good estimates for $\mathcal{P}_3$ can be obtained by considering the values $\alpha(3, d)$ in the following way. At first we consider the probability $\tilde{\mathcal{P}}_3$ being defined as $\mathcal{P}_3$ where additionally $\delta_{0,1} = 1$.

Lemma 7.

$$\tilde{\mathcal{P}}_3 = \mathcal{P}_3.$$

Proof. The problem of determining $\mathcal{P}_3$ or $\tilde{\mathcal{P}}_3$ is an integration problem. Due to symmetry we only need to consider the domain where $\delta_{0,1}$ is the maximum. For every $\delta_{0,1} \in (0, 1]$ there is a probability $p(\delta_{0,1})$ that $\delta_{0,1}, \ldots, \delta_{2,3}$ are distances of a tetrahedron where $\delta_{0,2}, \ldots, \delta_{2,3} \in (0, \delta_{0,1}]$ are equi-distributed random variables. Since $p(\delta_{0,1})$ is constant we can conclude the stated equation. □

Lemma 8.

$$\mathcal{P}_3 = \lim_{d\to\infty} \frac{4 \cdot \alpha(d, 3)}{d^5}.$$

Proof. We consider a modified version of the algorithm described above to obtain exact bounds on $\tilde{\mathcal{P}}_3$. As already mentioned, the triangle inequalities alone define a five-dimensional polyhedron. Since determinants are continuous $CMD_3 = 0$ defines a smooth surface and so the volume of all cubes $\mathcal{C}$ with $\Xi(\mathcal{C}) = 0$ converges to zero. Thus substituting $\Xi(\mathcal{C})$ by the evaluation of Ξ in an arbitrary corner of $\mathcal{C}$ yields the correct value for $\tilde{\mathcal{P}}_3 = \mathcal{P}_3$ for $d \to \infty$. Since there are at most $O(d^4)$ six-tuples $(d, i_2, \ldots, i_6)$, $i_j \in \{1, \ldots, d\}$ with non-trivial automorphism group we can factor out symmetry and conclude the stated result. □

Using Lemma 4 and Theorem 1 we can modify this to

$$\mathcal{P}_3 = \lim_{d\to\infty} \frac{\alpha(d,3)}{\overline{\alpha}(d,3)} \le \lim_{d\to\infty} \frac{\hat{\alpha}(d,3)}{\overline{\alpha}(d,3)} = \frac{17}{120} = 0.141\overline{6}.$$

Heuristically we observe that the finite sequence $\left(\frac{\alpha(d,3)}{\overline{\alpha}(d,3)}\right)_{1\le d\le 1000}$ is strictly decreasing. So the following values might be seen as a good estimate for $\mathcal{P}_3$:

$$\begin{aligned}
\frac{\alpha(600,3)}{\overline{\alpha}(600,3)} &= \frac{2000468396580}{19359502966749} \approx 0.103333,\\
\frac{\alpha(800,3)}{\overline{\alpha}(800,3)} &= \frac{8430487428682}{81665192828999} \approx 0.103232, \text{ and}\\
\frac{\alpha(1000,3)}{\overline{\alpha}(1000,3)} &= \frac{25728695195597}{249377330461249} \approx 0.103172.
\end{aligned}$$

4 Orderly generation of integral tetrahedra

Our strategy to enumerate integral tetrahedra is to merge two triangles along a common side. In Figure 1 we have depicted the two possibilities in the plane to join two triangles $(0, 1, 2)$ and $(0, 1, 3)$ along the side $\overline{01}$. If we rotate the triangle $(0, 1, 3)$ in the 3-dimensional space from the position on the left in Figure 1 to the position on the right we obtain tetrahedra and the distance $\delta_{2,3}$ forms an interval $[l, u]$. The restriction to integral tetrahedra is fairly easy.

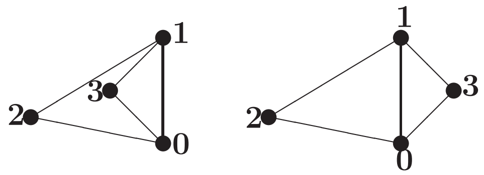

Figure 1: Joining two triangles.

Let us consider the example $\delta_{0,1} = 6$, $\delta_{0,2} = \delta_{1,2} = 5$, $\delta_{0,3} = 4$, and $\delta_{1,3} = 3$. Solving $CMD_3 = 0$ over the positive real numbers yields that the configuration is a tetrahedron iff $\delta_{2,3} \in \left(\frac{\sqrt{702-24\sqrt{455}}}{6}, \frac{\sqrt{702+24\sqrt{455}}}{6}\right) \approx (2.297719304, 5.806934304)$. Thus there are integral tetrahedra for $\delta_{2,3} \in \{3, 4, 5\}$. In general we denote such a set of tetrahedra by

$$\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3} \in [l, r].$$

This notation permits to implicitly list $\Omega(d^6)$ integral tetrahedra in $O(d^5)$ time.

All integral tetrahedra can be obtained in this manner. So an enumeration method is to loop over all suitable pairs of integral triangles and to combine them. We will go into detail in a while. Before that we have to face the fact that our enumeration method may construct pairs of isomorphic tetrahedra. Looking at Table 1 we see that storing all along the way constructed non-isomorphic integral tetrahedra in a hash table is infeasible. Here we use the concept of orderly generation [15] which allows us to decide independently for each single constructed discrete structure if we have to take or to reject it. Therefore we have to define a canonical form of an integral tetrahedron. Here we say that a tetrahedron $\mathcal{T}$ with side lengths $\delta_{i,j}$ is canonical if for the lexicographic ordering of vectors $\succeq$,

$$(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3}) \succeq (\delta_{\tau(0),\tau(1)}, \ldots, \delta_{\tau(2),\tau(3)})$$

holds for all permutation τ of the points $0, 1, 2, 3$. We describe the algorithmic treatment of a canonicity function $\chi(\mathcal{T}) \mapsto \{true, false\}$ which decides whether a given integral tetrahedron $\mathcal{T}$ is canonical in Section 5. We have the following obvious lemma:

Lemma 9. *If* $\chi(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3}) = true$ *and* $\chi(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3} + 1) = false$ *then* $\chi(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3} + n) = false$ *for all* $n \geq 1$.

Thus for given $\delta_{0,1}$, $\delta_{0,2}$, $\delta_{1,2}$, $\delta_{0,3}$, and $\delta_{1,3}$ the possible values for $\delta_{2,3}$ which correspond to a canonical tetrahedron form an interval $[\hat{l}, \hat{u}]$. Clearly, the value of $\chi(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3})$ has to be evaluated for $\delta_{2,3} \in \{\delta_{i,j} - 1, \delta_{i,j}, \delta_{i,j} + 1 \mid (i, j) \in \{(0, 1), (0, 2), (1, 2), (0, 3), (1, 3)\}\}$ only. Thus we can determine the interval $[\hat{l}, \hat{u}]$ using $O(1)$ evaluations of $\chi(\mathcal{T})$.

Algorithm 1. Orderly generation of integral tetrahedra
Input: Diameter d
Output: A complete list of canonical integral tetrahedra with diameter d
begin
  $\delta_{0,1} = d$
  for $\delta_{0,2}$ **from** $\left\lfloor \frac{d+2}{2} \right\rfloor$ **to** d **do**
    for $\delta_{1,2}$ **from** $d + 1 - \delta_{0,2}$ **to** $\delta_{0,2}$ **do**
      for $\delta_{0,3}$ **from** $d + 1 - \delta_{0,2}$ **to** $\delta_{0,2}$ **do**
        for $\delta_{1,3}$ **from** $d + 1 - \delta_{0,3}$ **to** $\delta_{0,2}$ **do**
          Determine the interval $[\hat{l}, \hat{u}]$ *for* $\delta_{2,3}$
          print $\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, [\hat{l}, \hat{u}]$
        end
      end
    end
  end
end

We leave it as an exercise for the reader to prove the correctness of Algorithm 1 (see [15] for the necessary and sufficient conditions of an orderly generation algorithm). Since we will see in the next section that we can perform $\chi(\mathcal{T})$ in $O(1)$ the runtime of Algorithm 1 is $O(d^4)$. By an obvious modification Algorithm 1 returns a complete list of all canonical integral tetrahedra with diameter at most d in $O(d^5)$ time.

We remark that we have implemented Algorithm 1 using Algorithm 2 for the canonicity check. For the computation of $\alpha(800, 3)$ our computer needs only 3.3 hours which is really fast compared to the nearly 3 hours needed for a simple loop from 1 to $\alpha(800, 3)$ on the same machine. Due to the complexity of $O(d^4)$ for suitable large d the determination of $\alpha(d, 3)$ will need less time than the simple loop from 1 to $\alpha(d, 3)$.

5 Canonicity check

In the previous section we have used the canonicity check $\chi(\mathcal{T})$ as a black box. The straight forward approach to implement it as an algorithm is to run over all permutations $\tau \in S_4$ and to check whether $(\delta_{0,1}, \dots, \delta_{2,3}) \succeq (\delta_{\tau(0),\tau(1)}, \dots, \delta_{\tau(2),\tau(3)})$. This clearly leads to running time $O(1)$ but is too slow for our purpose. It may be implemented using $24 \cdot 6 = 144$ integer comparisons. Here we can use the fact that the tetrahedra are generated by Algorithm 1. So if we arrange the comparisons as in Algorithm 2 at most 6 integer comparisons suffice.

Algorithm 2. Canonicity check for integral tetrahedra generated by Algorithm 1
Input: $\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3}$
Output: $\chi(\delta_{0,1}, \delta_{0,2}, \delta_{1,2}, \delta_{0,3}, \delta_{1,3}, \delta_{2,3})$

begin
  if $\delta_{0,1} = \delta_{0,2}$ **then**
    if $\delta_{0,2} = \delta_{1,2}$ **then**
      if $\delta_{0,3} < \delta_{1,3}$ **then return** $false$
      else
        if $\delta_{1,3} < \delta_{2,3}$ **then return** $false$ **else return** $true$
      end
    else
      if $\delta_{1,3} < \delta_{2,3}$ **then return** $false$
      else
        if $\delta_{0,1} = \delta_{0,3}$ **then**
          if $\delta_{1,2} < \delta_{1,3}$ **then return** $false$ **else return** $true$ **end**
        else
          if $\delta_{0,1} > \delta_{1,3}$ **then return** $true$
          else
            if $\delta_{1,2} < \delta_{0,3}$ **then return** $false$ **else return** $true$ **end**
          end
        end
      end
    end
  else
    if $\delta_{0,2} = \delta_{1,2}$ **then**
      if $\delta_{0,1} < \delta_{2,3}$ **or** $\delta_{0,3} < \delta_{1,3}$ **then return** $false$ **else return** $true$ **end**
    else
      if $\delta_{0,2} = \delta_{1,3}$ **then**
        if $\delta_{0,3} > \delta_{1,2}$ **or** $\delta_{0,1} < \delta_{2,3}$ **then return** $false$ **else return** $true$ **end**
      else
        if $\delta_{0,2} = \delta_{0,3}$ **then**
          if $\delta_{1,2} < \delta_{1,3}$ **or** $\delta_{0,1} \leq \delta_{2,3}$ **then return** $false$ **else return** $true$ **end**
        else
          if $\delta_{0,3} > \delta_{1,2}$ **then**
            if $\delta_{0,1} \leq \delta_{2,3}$ **then return** $true$ **else return** $false$ **end**
          else

if $\delta_{0,1} < \delta_{2,3}$ **then return** $true$ **else return** $false$ **end**
end
end
end
end
end
end

To prove the correctness of Algorithm 2 we consider all vectors $(\delta_{0,1}, \ldots, \delta_{2,3})$ with $\delta_{i,j} \in \{0, \ldots, 5\}$, $\delta_{0,1} \geq \delta_{0,2} \geq \delta_{1,2}$, $\delta_{0,2} \geq \delta_{0,3}$, and $\delta_{0,2} \geq \delta_{1,3}$. It suffices to show that Algorithm 2 returns the correct value for this finite set of vectors since these inequalities are fulfilled by Algorithm 1 and also necessary for $\chi(\mathcal{T}) = true$. Algorithm 2 can be considered as a binary decision tree. It might be a task to optimize this type of binary decision tree in the worst or in the average case.

6 Dimensions $\mathbf{m \geq 4}$

Clearly the question for bounds for P_m arises also for $m \geq 4$. But non-trivial answers seem out of reach by our approach. So far we have no efficient equivalent of Algorithm 2 at hand and the number $\alpha(4, d)$ of integral 4-dimensional simplices with diameter d is $\Omega\left(d^9\right)$. We give the known values of $\alpha(4, d)$ in Table 6.

d	$\alpha(d,4)$	d	$\alpha(d,4)$	d	$\alpha(d,4)$	d	$\alpha(d,4)$
1	1	14	12957976	27	4716186332	40	162007000505
2	6	15	24015317	28	6541418450	41	202323976907
3	56	16	42810244	29	8970194384	42	251321436143
4	336	17	73793984	30	12168243592	43	310607982160
5	1840	18	123240964	31	16344856064	44	382002253424
6	7925	19	200260099	32	21748894367	45	467627887530
7	29183	20	317487746	33	28688094208	46	569910996879
8	91621	21	492199068	34	37529184064	47	691631229557
9	256546	22	747720800	35	48713293955	48	835911697430
10	648697	23	1115115145	36	62769489452	49	1006370948735
11	1508107	24	1634875673	37	80321260053	50	1207047969441
12	3267671	25	2360312092	38	102108730634	51	1442539675756
13	6679409	26	3358519981	39	128999562925	52	1718015775541

Table 3: Number $\alpha(d, 4)$ of integral 4-dimensional simplices with diameter $1 \leq d \leq 52$.

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