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On the characteristic of integral point sets in $\mathbb{E}^m$

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Abstract

We generalise the definition of the characteristic of an integral triangle to integral simplices and prove that each simplex in an integral point set has the same characteristic. This theorem is used for an efficient construction algorithm for integral point sets. Using this algorithm we are able to provide new exact values for the minimum diameter of integral point sets.

1 Introduction

Since the time of the Pythagoreans, mathematicians have considered geometrical objects with integral sides. Here we study sets of points in the Euclidean space $\mathbb{E}^m$ where the pairwise distances are integers. Although there is a long history for integral point sets, very little is known about integral point sets for dimension $m \geq 3$; see [3] for an overview.

Due to Heron the area of a triangle with side lengths a, b, and c is given by

$$A_\Delta = \frac{\sqrt{(a+b+c)(a+b-c)(a-b+c)(-a+b+c)}}{4}.$$

Thus we can write the area as $A_\Delta = q\sqrt{k}$ with a rational number q and a squarefree integer k. If $A_\Delta \neq 0$, the integer k is unique and is called the **characteristic** or the **index** of the triangle. This invariant receives its relevance from the following theorem [4].

Theorem 1 *The triangles spanned by each three non collinear points in a plane integral point set have the same characteristic.*

This theorem can be utilised to develop an efficient algorithm for the generation of plane integral point sets [5, 6]. Here we will generalise the definition of the characteristic of an integral triangle to integral simplices and prove an analogue to Theorem 1. Later on we will use this theorem to develop a generation algorithm for integral point sets in $\mathbb{E}^m$ and present some new numerical data.

2 Characteristic of integral simplices

Since the definition of the characteristic of an integral triangle depends on the area of a triangle, we consider the volume of an m-dimensional simplex for point sets in $\mathbb{E}^m$. Therefore we need the Cayley-Menger matrix of a point set.

Definition 2 *If $\mathcal{P}$ is a point set in $\mathbb{E}^m$ with vertices $v_0, v_1, \ldots, v_{n-1}$ and $C = (d_{i,j}^2)$ denotes the $n \times n$ matrix given by $d_{i,j}^2 = \|v_i - v_j\|_2^2$, the Cayley-Menger matrix $\hat{C}$ is obtained from C by bordering C with a top row $(0, 1, 1, \ldots, 1)$ and a left column $(0, 1, 1, \ldots, 1)^T$.*

We denote the determinant of $\hat{C}(\{v_0, v_1, \ldots, v_{n-1}\})$ by $CMD(\{v_0, v_1, \ldots, v_{n-1}\})$. If $n = m + 1$, the m-dimensional volume V_m of $\mathcal{P}$ is given by

$$V_m(\mathcal{P})^2 = \frac{(-1)^{m+1}}{2^m (m!)^2} \det(\hat{C}) \,.$$

This allows us to define the characteristic of an m-dimensional integral simplex to be the squarefree integer k in $V_m(\mathcal{P}) = q\sqrt{k}$ whenever $V_m(\mathcal{P}) \neq 0$ and $q \in \mathbb{Q}$. In order to prove the proposed theorem, we consider a special coordinate representation of integral simplices.

Lemma 3 *An integral m-dimensional simplex $\mathcal{S} = \{v_0', v_1', \ldots, v_m'\}$ with distance matrix $D = (d_{i,j})_{0 \le i,j \le m}$ and $V_m(\mathcal{S}) \neq 0$ can be transformed via an isometry into the coordinates*

$$\begin{aligned}
v_0 &= (0, 0, \ldots, 0),\\
v_1 &= (q_{1,1}\sqrt{k_1}, 0, 0 \ldots, 0),\\
v_2 &= (q_{2,1}\sqrt{k_1}, q_{2,2}\sqrt{k_2}, 0, \ldots, 0),\\
&\vdots\\
v_m &= (q_{m,1}\sqrt{k_1}, q_{m,2}\sqrt{k_2}, \ldots, q_{m,m}\sqrt{k_m}),
\end{aligned}$$

where k_i is the squarefree part of $\frac{V_i(v_0',v_1',\ldots,v_i')^2}{V_{i-1}(v_0',v_1',\ldots,v_{i-1}')^2}$, $q_{i,j} \in \mathbb{Q}$, and $q_{j,j}, k_j \neq 0$.

Proof. We can obviously set $v_0 = (0, 0, \ldots, 0)$ and since $d_{0,1} \in \mathbb{N}$ we can furthermore set $v_1 = (d_{0,1}\sqrt{k_1}, 0, 0, \ldots, 0)$ where $k_1 = \frac{V_1(v_0',v_1')}{V_0(v_0')} = 1$. Now we assume that we have already transformed $v_0', v_1', \ldots, v_{i-1}'$ into the stated coordinates. We set $v_i = (x_1, x_2, \ldots, x_m)$ with $x_j \in \mathbb{R}$. Since the points $v_0, v_1, \ldots, v_i$ span an i-dimensional hyperplane of $\mathbb{E}^m$ we can set $x_{i+1} = \ldots = x_m = 0$. For $j \le i$ we have

$$d_{j,i}^2 = \|v_j - v_i\|_2^2 = \sum_{h=1}^{j} (q_{j,h}\sqrt{k_h} - x_h)^2 + \sum_{h=j+1}^{i} x_h^2 \,.$$

For $0 < j < i$ we consider

$$d_{0,i}^2 - d_{j,i}^2 = \sum_{h=1}^{j} x_h^2 - (q_{j,h}\sqrt{k_h} - x_h)^2$$

where we can set $x_h = q_{i,h}\sqrt{k_h}$ for $h < j$ by induction, yielding

$$d_{0,i}^2 - d_{j,i}^2 = -q_{j,j}^2 k_h + 2q_{j,j}\sqrt{k_h}x_j + \sum_{h=1}^{j-1} 2q_{i,h}q_{j,h}k_h - q_{j,h}^2 k_h\,.$$

Thus

$$x_j = \frac{q_{j,j}^2 k_h + \sum\limits_{h=1}^{j-1}(q_{j,h}^2 k_h - 2q_{i,h}q_{j,h}k_h) + d_{0,i}^2 - d_{j,i}^2}{2q_{j,j}\sqrt{k_h}}$$

and we can write $x_j = q_{i,j}\sqrt{k_j}$ since $2q_{j,j}\sqrt{k_h} \neq 0$ due to induction. With this we have

$$d_{0,i}^2 = \sum_{h=1}^{i} x_h^2 = x_i^2 + \sum_{h=1}^{i-1} q_{i,h}^2 k_h.$$

Thus

$$x_i = \sqrt{d_{0,i}^2 - \sum_{h=1}^{i-1} q_{i,h}^2 k_h} = q_{i,i}\sqrt{k_i}\,.$$

We also have $q_{i,i}\sqrt{k_i} \neq 0$ since $v'_0, v'_1, \ldots, v'_i$ cannot lie in an $i-1$-dimensional hyperplane of $\mathbb{E}^m$ due to $V_m(v'_0, v'_1, \ldots, v'_m) \neq 0$. □

The k_j are associated to the characteristic $\text{char}(\mathcal{S}) = k$ in the following way

$$\text{char}(\mathcal{S}) = k = \text{squarefree part of } \prod_{j=1}^{m} k_j\,.$$

Theorem 4 *In an m-dimensional integral point set $\mathcal{P}$ all simplices $\mathcal{S} = \{v_0, v_1, \ldots, v_m\}$ with $V_m(\mathcal{S}) \neq 0$ have the same characteristic $\text{char}(S) = k$.*

PROOF. It suffices to prove that $\text{char}(\mathcal{S}_1) = \text{char}(\mathcal{S}_2)$ for two integral simplices $\mathcal{S}_1 = \{v_0, v_1, \ldots . v_m\}$ and $\mathcal{S}_2 = \{v_0, \ldots, v_{m-1}, v'_m\}$ with $V_m(\mathcal{S}_1), V_m(\mathcal{S}_2) \neq 0$. With the notations from Lemma 3 we have for the distance between v_m and v'_m,

$$\begin{aligned}
d(v_m, v'_m)^2 &= \sum_{i=1}^{m}(q_{m,i}\sqrt{k_i} - q'_{m,i}\sqrt{k'_i})^2 \\
&= \sum_{i=1}^{m}(q_{m,i}\sqrt{k_i} - q'_{m,i}\sqrt{k_i})^2 + (q_{m,m}\sqrt{k_m} - q'_{m,m}\sqrt{k'_m})^2 \\
&= \sum_{i=1}^{m-1}(q_{m,i} - q'_{m,i})^2 k_i + q_{m,m}^2 k_m - 2q_{m,m}q'_{m,m}\sqrt{k_m k'_m} + q'^2_{m,m}k'_m\,.
\end{aligned}$$

Thus $\sqrt{k_m, k'_m}$ has to be an integer. Because k_m and k'_m are squarefree integers $\neq 0$ we have $k_m = k'_m$ and so $\text{char}(\mathcal{S}_1) = \text{char}(\mathcal{S}_2)$. □

3 Construction of integral point sets

The key principle for a recursive construction of integral point sets consisting of n points is the combination of two integral point sets $\mathcal{P}_1 = \{v_0, \ldots, v_{n-2}\}$ and $\mathcal{P}_2 = \{v_0, \ldots, v_{n-3}, v_{n-1}\}$ consisting of $n-1$ points sharing $n-2$ points; see Figure 1. Here we describe an integral point set by a symmetric matrix $D = (d_{i,j})$

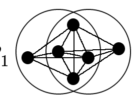

Figure 1: Combination of two integral point sets.

representing the distances between the points. Because not all symmetric matrices are realizable as distance matrices in $\mathbb{E}^m$ we need a generalisation of the triangle inequalities.

Theorem 5 ***(Menger [9])*** *A set of vertices $\{v_0, v_1, \ldots, v_{n-1}\}$ with pairwise distances $d_{i,j}$ is realizable in the Euclidean space $\mathbb{E}^m$ if and only if for all subsets $\{i_0, i_1, \ldots, i_{r-1}\} \subset \{0, 1, \ldots, n-1\}$ of cardinality $r \le m+1$,*

$$(-1)^r CMD(\{v_{i_0}, v_{i_1}, \ldots, v_{i_{r-1}}\}) \ge 0,$$

and for all subsets of cardinality $m+2 \le r \le n$,

$$(-1)^r CMD(\{v_{i_0}, v_{i_1}, \ldots, v_{i_{r-1}}\}) = 0\,.$$

Fortunately we do not need to check all these equalities and inequalities. Because the point sets $\mathcal{P}_1$ and $\mathcal{P}_2$ are realizable due to our construction strategy it suffices to check $(-1)^n CMD(\{v_0, v_1, \ldots, v_{n-1}\})$ [5].

To solve the equivalence problem for integral point sets we use a variant of orderly generation [1, 7, 8, 11]. For the required ordering we consider the upper right triangle matrix of D leaving out the diagonal,

$$\begin{pmatrix} d_{0,1} & d_{0,2} & \cdots & d_{0,n-1} \\ & d_{1,2} & \cdots & d_{1,n-1} \\ & & \ddots & \vdots \\ & & & d_{n-2,n-1} \end{pmatrix},$$

and read the entries column by column as a word

$$w(D) = (d_{0,1}, d_{0,2}, d_{1,2}, \ldots\ldots, d_{0,n-1}, \ldots, d_{n-2,n-1})\,.$$

With a lexicographical ordering on the words $w(D)$ we define

$$D_1 \succeq D_2 \quad \Longleftrightarrow \quad w(D_1) \succeq w(D_2)$$

for distance matrices D_1, D_2. We call a distance matrix $D = (d_{i,j})_{0\le i,j<n}$ **canonical** if

$$D \succeq (d_{\tau(i),\tau(j)}) \quad \forall \tau \in S_n\,.$$

By $\downarrow\! D$ we denote the distance matrix consisting of the first $n-1$ rows and columns of D. With this we call a distance matrix D **semi-canonical** if

$$\downarrow\! D \succeq \downarrow\!(d_{\tau(i),\tau(j)}) \quad \forall \tau \in S_n\,.$$

A canonical distance matrix is also semi-canonical. It is left to the reader to prove that each semi-canonical distance matrix D can be obtained by combining a canonical distance matrix D_1 and a semi-canonical distance matrix D_2; see Figure 1. Only the distance $d_{n-1,n-2}$ is not determined by the distances of D_1 and D_2. Here we consider two cases. If we combine two $(m'-1)$-dimensional simplices to get an m'-dimensional simplex Theorem 5 yields a biquadratic inequality for $d_{n-1,n-2}$. In the other case we can determine one or for $n = m+2$ at most two different coordinate representations of the n points similar to the proof of Lemma 3, calculate $d_{n-1,n-2}$, and check whether it is integral. We denote the sub routine doing this by *combine*(D_1, D_2). At first we provide an algorithm to generate m-dimensional integral simplices. Therefore we assume that for a given diameter Δ, this is the largest distance, we have two lists $\mathcal{L}_m^c$, $\mathcal{L}_m^s$ of the canonical and the semi-canonical $(m-1)$-dimensional integral simplices with diameter Δ which are ordered by $\prec$, respectively. The following algorithm determines the lists $\mathcal{L}_{m+1}^c$ and $\mathcal{L}_{m+1}^s$ of the m-dimensional integral simplices with diameter Δ ordered by $\prec$.

Algorithm 6
Input: $\mathcal{L}_m^c$, $\mathcal{L}_m^s$
Output: $\mathcal{L}_{m+1}^c$, $\mathcal{L}_{m+1}^s$
begin
    $\mathcal{L}_{m+1}^c = \emptyset, \quad \mathcal{L}_{m+1}^s = \emptyset$
    loop over $x \in \mathcal{L}_m^c$ **do**
        loop over $\mathcal{L}_m^s \ni y \preceq x$ **with** $\downarrow\! x = \downarrow\! y$ **do**
            loop over $z \in$ *combine*(x, y) **do**
                if z is canonical **then** $\mathcal{L}_{m+1}^c \longleftarrow z$ **end**
                if z is semi-canonical **then** $\mathcal{L}_{m+1}^s \longleftarrow z$ **end**
            end
        end
    end
end

Because an m-dimensional simplex is an m-dimensional point set consisting of $n = m+1$ points we can use Algorithm 6 to generate complete lists $\mathcal{M}_{m+1}^c$, $\mathcal{M}_{m+1}^s$ of the canonical and semi-canonical m-dimensional integral point sets with diameter Δ consisting of $m+1$ points, respectively. An m-dimensional point set is in semi-general position if no $m+1$ points are situated on an $(m-1)$-dimensional hyperplane. Using Theorem 4 we can give an algorithm to determine the lists $\mathcal{M}_n^c$ and $\mathcal{M}_n^s$ of the m-dimensional integral point sets in semi-general position consisting of n points with diameter Δ.

Algorithm 7
Input: $\mathcal{M}_{n-1}^c$, $\mathcal{M}_{n-1}^s$
Output: $\mathcal{M}_n^c$, $\mathcal{M}_n^s$
begin
  $\mathcal{M}_n^c = \emptyset, \quad \mathcal{M}_n^s = \emptyset$
  loop over $x \in \mathcal{M}_{n-1}^c$ **do**
    loop over $\mathcal{M}_{n-1}^s \ni y \preceq x$ **with** $\downarrow x = \downarrow y$ **and** $\mathrm{char}(x) = \mathrm{char}(y)$ **do**
      loop over $z \in$ *combine*(x, y) **do**
        if z is canonical **then** $\mathcal{M}_n^c \longleftarrow z$ **end**
        if z is semi-canonical **then** $\mathcal{M}_n^s \longleftarrow z$ **end**
      end
    end
  end
end

4 Improvements

To demonstrate the significance of Theorem 4 for an efficient enumeration algorithm for integral point sets we compare in Table 1 the number $\Psi(3, \Delta)$ of calls of *combine*(x, y) in Algorithm 7 for $m = 3$ and $n = 5$ to the number $\hat{\Psi}(3, \Delta)$ of calls of *combine*(x, y) without using Theorem 4. Additionally we give the number $\tilde{\alpha}(3, \Delta)$ of semi-canonical integral tetrahedrons with diameter Δ.

5 Minimum diameters

From the combinatorial point of view there is a natural interest in the minimum diameter $d(m, n)$ of m-dimensional integral point sets consisting of n points. By $\overline{d}(m, n)$ we denote the minimum diameter of m-dimensional integral point sets in semi-general position. If additionally no $m+2$ points lie on an m-dimensional sphere we denote the corresponding minimum diameter by $\dot{d}(m, n)$ and say the points are in general position. To check semi-general position we can use the Cayley-Menger matrix and test whether $V_m = 0$ or not. In the case of general position we have the following theorem.

Theorem 8 *Given $m+2$ points in $\mathbb{E}^m$, with pairwise distances $d_{i,j}$ and no $m+1$ points in an $m-1$-dimensional plane, lie on an m-dimensional sphere if and only if*

$$\begin{vmatrix} 0 & d_{0,1}^2 & \cdots & d_{0,m+1}^2 \\ d_{1,0}^2 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & d_{m,m+1}^2 \\ d_{m+1,0}^2 & \cdots & d_{m+1,m}^2 & 0 \end{vmatrix} = 0\,.$$

Δ	$\hat{\Psi}(3,\Delta)$	$\Psi(3,\Delta)$	$\tilde{\alpha}(3,\Delta)$	Δ	$\hat{\Psi}(3,\Delta)$	$\Psi(3,\Delta)$	$\tilde{\alpha}(3,\Delta)$
1	1	1	1	26	521610123	521589	356333
2	13	9	6	27	700065646	629939	428030
3	111	35	24	28	929489332	753113	510829
4	602	149	70	29	1222613496	832969	605970
5	2592	305	176	30	1592477593	1038224	714505
6	8833	770	380	31	2059062666	1145517	838646
7	26564	1379	754	32	2638060710	1439990	978820
8	68800	2761	1368	33	3357319548	1568195	1137638
9	162330	4182	2333	34	4241882219	1804079	1316239
10	353100	6660	3786	35	5323350205	2062374	1516567
11	719688	10254	5894	36	6638917601	2475320	1740591
12	1378977	16714	8839	37	8232016014	2613730	1990484
13	2526059	21902	12891	38	10148934902	3037708	2268149
14	4434103	30115	18289	39	12445587259	3430131	2575954
15	7490297	41250	25339	40	15183055989	4015829	2916089
16	12256818	59995	34436	41	18437914417	4224348	3291649
17	19551329	72315	46054	42	22280569281	4966748	3704516
18	30264028	96502	60474	43	26818516374	5278577	4158686
19	45952871	119896	78406	44	32132601503	6213243	4655277
20	68191989	162600	100277	45	38348410933	6821671	5198318
21	99420707	196490	126838	46	45598443859	7428904	5791458
22	142558111	245591	158772	47	54019488362	8057637	6437526
23	201289670	289672	196799	48	63756807373	9675353	7139157
24	279728968	388051	241672	49	75019979427	10055859	7901871
25	384663513	440140	294681	50	87968187078	11262298	8727553

Table 1: Number of calls of *combine*(x, y).

See [2, 10] for a proof.

We have implemented Algorithm 6 and Algorithm 7 and received the following values for minimum diameters; see also [3, 6, 10]. The values not previously known in the literature are emphasised.

$$\overline{d}(3,n)_{4\le n\le 7} = \dot{d}(3,n)_{4\le n\le 7} = 1, 3, 16, \mathbf{44}.$$

$$\overline{d}(4,n)_{5\le n\le 8} = 1, \mathbf{4}, \mathbf{11}, \mathbf{14}.$$

$$\dot{d}(4,n)_{5\le n\le 8} = 1, \mathbf{4}, \mathbf{7}, \mathbf{14}.$$

$$\overline{d}(5,n)_{6\le n\le 9} = \dot{d}(5,n)_{6\le n\le 9} = 1, \mathbf{4}, \mathbf{5}, \mathbf{8}.$$

To determine $d(m, n)$ we have to modify Algorithm 7 because not every $m + 1$ points of an m-dimensional pointset span an m-dimensional simplex. So we have to combine lower dimensional point sets with m-dimensional point sets. We leave the details to the reader and give only the results,

$$d(3,n)_{4\le n\le 23} = 1,3,4,8,13,\mathbf{16},17,\mathbf{17},\mathbf{17},\mathbf{56},\mathbf{65},\mathbf{77},\mathbf{86},\mathbf{99},\mathbf{112},\mathbf{133},\mathbf{154},\mathbf{195},\mathbf{212},\mathbf{228}.$$

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