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Hermite normal forms and δ-vectors

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ABSTRACT

Let $\delta(\mathcal{P}) = (\delta_0, \delta_1, \dots, \delta_d)$ be the δ-vector of an integral polytope $\mathcal{P} \subset \mathbb{R}^N$ of dimension d. Following previous work on the characterization of δ-vectors with $\sum_{i=0}^{d} \delta_i \leqslant 3$, all the possible δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$ are classified by means of simplices. We obtain our results by considering—by means of Hermite normal forms of square matrices—the classification of integral simplices with a given δ-vector $(\delta_0, \delta_1, \dots, \delta_d)$, where $\sum_{i=0}^{d} \delta_i \leqslant 4$.

1. introduction

1.1. Background on δ-vectors

Let $\mathcal{P} \subset \mathbb{R}^N$ be an integral polytope of dimension d and $\partial\mathcal{P}$ its boundary. Define the numerical functions $i(\mathcal{P}, n)$ and $i^*(\mathcal{P}, n)$ by setting

$$i(\mathcal{P}, n) = \left|n\mathcal{P} \cap \mathbb{Z}^N\right| \quad \text{and} \quad i^*(\mathcal{P}, n) = \left|n(\mathcal{P} - \partial\mathcal{P}) \cap \mathbb{Z}^N\right|.$$

Here $n\mathcal{P} = \{n\alpha\colon \alpha \in \mathcal{P}\}$ and $|X|$ is the cardinality of a finite set X. The systematic study of $i(\mathcal{P}, n)$ and $i^*(\mathcal{P}, n)$ originated in Ehrhart's work [1] carried out around 1955. In this work Ehrhart established the following fundamental properties: $i(\mathcal{P}, n)$ is a polynomial in n of degree d with $i(\mathcal{P}, 0) = 1$ which satisfies the reciprocity law

$$i^*(\mathcal{P}, n) = (-1)^d i(\mathcal{P}, -n) \tag{1.1}$$

for every integer $n > 0$. We say that $i(\mathcal{P}, n)$ is the *Ehrhart polynomial* of $\mathcal{P}$. An introduction to Ehrhart polynomials may be found in [8, pp. 235–241] and [2, Part II].

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We define the integer sequence $\delta_0, \delta_1, \delta_2, \ldots$ by

$$(1-\lambda)^{d+1}\left(1+\sum_{n=1}^{\infty} i(\mathcal{P}, n)\lambda^n\right) = \sum_{i=0}^{\infty} \delta_i \lambda^i. \tag{1.2}$$

In particular, $\delta_0 = 1$ and $\delta_1 = |\mathcal{P} \cap \mathbb{Z}^N| - (d+1)$. Thus, if $\delta_1 = 0$, then $\mathcal{P}$ is a simplex. The above facts together with a well-known result on generating functions (see [8, Corollary 4.3.1]) guarantee that $\delta_i = 0$ for every $i > d$. We say that the sequence

$$\delta(\mathcal{P}) = (\delta_0, \delta_1, \ldots, \delta_d)$$

which appears in (1.2) is the *δ-vector* of $\mathcal{P}$ and that the polynomial

$$\delta_{\mathcal{P}}(t) = \delta_0 + \delta_1 t + \cdots + \delta_d t^d$$

is the *δ-polynomial* of $\mathcal{P}$.

It follows from the reciprocity law (1.1) that

$$(1-\lambda)^{d+1}\left(\sum_{n=1}^{\infty} i^*(\mathcal{P}, n)\lambda^n\right) = \sum_{i=0}^{d} \delta_{d-i} \lambda^{i+1}.$$

In particular, $\delta_d = |(\mathcal{P} - \partial\mathcal{P}) \cap \mathbb{Z}^N|$. Each δ_i is nonnegative [9]. If $\delta_d \neq 0$, then $\delta_1 \leqslant \delta_i$ for every $1 \leqslant i < d$, see [3].

Let $s = \max\{i\colon\ \delta_i \neq 0\}$. In [10] Stanley showed that

$$\delta_0 + \delta_1 + \cdots + \delta_i \leqslant \delta_s + \delta_{s-1} + \cdots + \delta_{s-i}, \quad 0 \leqslant i \leqslant \lfloor s/2 \rfloor, \tag{1.3}$$

by using Cohen–Macaulay rings. The inequalities

$$\delta_{d-1} + \delta_{d-2} + \cdots + \delta_{d-i} \leqslant \delta_2 + \delta_3 + \cdots + \delta_i + \delta_{i+1}, \quad 1 \leqslant i \leqslant \lfloor (d-1)/2 \rfloor \tag{1.4}$$

appear in [3, Remark (1.4)].

1.2. Main result: characterization of δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$

One of the most fundamental problems of enumerative combinatorics is to find a combinatorial characterization of all vectors that can be realized as the δ-vector of some integral polytope. For example, restrictions like $\delta_0 = 1$, $\delta_i \geqslant 0$, (1.3) and (1.4) are necessary conditions for a vector to be a δ-vector of some integral polytope.

On the one hand, the complete classification of the δ-vectors for dimension 2 is essentially given by Scott [7], while the case where the dimension is at least 3 is unknown. In [4], on the other hand, the possible δ-vectors with $\sum_{i=0}^{d} \delta_i \leqslant 3$ are completely classified by the inequalities (1.3) and (1.4).

Theorem 1.1. *(See [4, Theorem 0.1].) Let $d \geqslant 3$. Given a sequence $(\delta_0, \delta_1, \ldots, \delta_d)$ of nonnegative integers, where $\delta_0 = 1$ and $\delta_1 \geqslant \delta_d$, which satisfies $\sum_{i=0}^{d} \delta_i \leqslant 3$, there exists an integral polytope $\mathcal{P} \subset \mathbb{R}^d$ of dimension d whose δ-vector coincides with $(\delta_0, \delta_1, \ldots, \delta_d)$ if and only if $(\delta_0, \delta_1, \ldots, \delta_d)$ satisfies all inequalities* (1.3) *and* (1.4)*.*

However, Theorem 1.1 is not true for $\sum_{i=0}^{d} \delta_i = 4$, see [4, Example 1.2]. In this paper, we will give the complete classification of the possible δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$, see Theorem 5.1 below. Moreover, similar to the case $\sum_{i=0}^{d} \delta_i \leqslant 3$, it turns out that all the possible δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$ can be chosen to correspond to integral simplices. Such a result does not hold when $\sum_{i=0}^{d} \delta_i = 5$, see Remark 5.3.

1.3. Approach: a classification of integral simplices with a given δ-vector

Let $\mathbb{Z}^{d\times d}$ denote the set of $d \times d$ integral matrices. Recall that a matrix $A \in \mathbb{Z}^{d\times d}$ is *unimodular* if $\det(A) = \pm 1$. Given integral polytopes $\mathcal{P}$ and $\mathcal{Q}$ in $\mathbb{R}^d$ of dimension d, we say that $\mathcal{P}$ and $\mathcal{Q}$ are *unimodularly equivalent* if there exists a unimodular matrix $U \in \mathbb{Z}^{d\times d}$ and an integral vector w such that $\mathcal{Q} = f_U(\mathcal{P}) + w$, where f_U is the linear transformation in $\mathbb{R}^d$ defined by U, i.e., $f_U(\mathbf{v}) = \mathbf{v}U$ for all $\mathbf{v} \in \mathbb{R}^d$. Clearly, if $\mathcal{P}$ and $\mathcal{Q}$ are unimodularly equivalent, then $\delta(\mathcal{P}) = \delta(\mathcal{Q})$. Conversely, given a vector $v \in \mathbb{Z}^{d+1}_{\geqslant 0}$, it is natural to ask for a description of all the integral polytopes $\mathcal{P}$ under unimodular equivalence, such that $\delta(\mathcal{P}) = v$.

In this paper, we will focus on the above problem for simplices with one vertex at the origin. In addition, we do not allow any shifts in the equivalence, i.e., integral polytopes $\mathcal{P}$ and $\mathcal{Q}$ of dimension d are equivalent if there exists a unimodular matrix U, such that $\mathcal{Q} = f_U(\mathcal{P})$. By considering the δ-vectors of all the integral simplices up to this equivalence, whose normalized volumes are 4, we obtain our main result, Theorem 5.1.

To discuss the representative under this equivalence of the integral simplices with one vertex at the origin, we consider Hermite normal forms.

Let $\mathcal{P} \subset \mathbb{R}^d$ be an integral simplex of dimension d with the vertices $\mathbf{0}, \boldsymbol{v}_1, \dots, \boldsymbol{v}_d$. Define $M(\mathcal{P}) \in \mathbb{Z}^{d\times d}$ to be the matrix with the row vectors $\boldsymbol{v}_1, \dots, \boldsymbol{v}_d$. Then we have the following connection between the matrix $M(\mathcal{P})$ and the δ-vector of $\mathcal{P}$: $|\det(M(\mathcal{P}))| = \sum_{i\geqslant 0} \delta_i$. In this setting, $\mathcal{P}$ and $\mathcal{P}'$ are equivalent if and only if $M(\mathcal{P})$ and $M(\mathcal{P}')$ have the same Hermite normal form. Here, the *Hermite normal form* of a nonsingular integral square matrix B is a unique nonnegative lower triangular matrix $A = (a_{ij}) \in \mathbb{Z}^{d\times d}_{\geqslant 0}$ such that $A = BU$ for some unimodular matrix $U \in \mathbb{Z}^{d\times d}$ and $0 \leqslant a_{ij} < a_{ii}$ for all $1 \leqslant j < i$, see [6, Chapter 4]. In other words, we can pick the Hermite normal form as the representative in each equivalence class and study the following

Problem 1.2. Given a vector $v \in \mathbb{Z}^{d+1}_{\geqslant 0}$, classify all possible $d \times d$ matrices $A \in \mathbb{Z}^{d\times d}$ which are in Hermite normal form with $\delta(\mathcal{P}) = (\delta_0, \delta_1, \dots, \delta_d) = v$, where $\mathcal{P} \subset \mathbb{R}^d$ is the integral simplex whose vertices are the row vectors of A together with the origin in $\mathbb{R}^d$.

1.4. Structure of this paper

In Section 2, we describe our approach to Problem 1.2. Concretely, we develop an algorithm to compute the δ-vector for any Hermite normal form A, see Theorem 2.1. This in fact results in a new way to compute the δ-vector for any integral simplex via its Hermite normal form. Our algorithm is very efficient for simplices with small volumes and prime volumes.

Based on this algorithm, as a by-product, we derive some conditions for Hermite normal forms to have "shifted symmetric" δ-vector, namely, $\delta_i = \delta_{d+1-i}$ for $1 \leqslant i \leqslant d$. We will discuss these conditions for two classes of Hermite normal forms in Section 3.

In Section 4, we apply Theorem 2.1 and obtain a solution to Problem 1.2 when $\sum_{i=0}^d \delta_i \leqslant 4$. Section 4.1 is devoted to studying the case $\sum_{i=0}^d \delta_i = 2$, Section 4.2 is $\sum_{i=0}^d \delta_i = 3$ and Section 4.3 is $\sum_{i=0}^d \delta_i = 4$.

Finally, in Section 5, as our main result, we show that the inequalities (1.3) and (1.4) with an additional condition will give all the possible δ-vectors with $\sum_{i=0}^d \delta_i = 4$. In this case, all the δ-vectors can be obtained by simplices, see Theorem 5.1.

2. An algorithm for the computation of the δ-vector of a simplex

In this section we introduce an algorithm for calculating the δ-vector of integral simplices arising from Hermite normal forms.

Let $M \in \mathbb{Z}^{d\times d}$. We write $\mathcal{P}(M)$ for the integral simplex whose vertices are the row vectors of M together with the origin in $\mathbb{R}^d$. We will present an algorithm to compute the δ-vector of $\mathcal{P}(M)$. To make the notation clear, we assume $d = 3$. The general case is completely analogous. Let A be the Hermite normal form of M. We have that $\{\mathcal{P}(M) \cap \mathbb{Z}^d\}$ is in bijection with $\{\mathcal{P}(A) \cap \mathbb{Z}^d\}$. By definition,

$$A = \begin{pmatrix} a_{11} & 0 & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

where each a_{ij} is a nonnegative integer.

For a vector $\lambda = (\lambda_1, \lambda_2, \lambda_3)$, consider

$$b(\lambda) := (\lambda_1, \lambda_2, \lambda_3)A = (a_{11}\lambda_1 + a_{21}\lambda_2 + a_{31}\lambda_3, a_{22}\lambda_2 + a_{32}\lambda_3, a_{33}\lambda_3).$$

Then it is clear that the set of interior points inside $\mathcal{P}(A)$ ($(\mathcal{P}(A) - \partial\mathcal{P}(A)) \cap \mathbb{Z}^3$) is in bijection with the set

$$\{(\lambda_1, \lambda_2, \lambda_3) \mid \lambda_i > 0,\ \lambda_1 + \lambda_2 + \lambda_3 < 1,\ b(\lambda) \in \mathbb{Z}^3\}.$$

We observe that for any $n \in \mathbb{N}$, $n(\mathcal{P}(A) - \partial\mathcal{P}(A)) \cap \mathbb{Z}^3$ is in bijection with

$$\{(\lambda_1, \lambda_2, \lambda_3) \mid \lambda_i > 0,\ \lambda_1 + \lambda_2 + \lambda_3 < n,\ b(\lambda) \in \mathbb{Z}^3\}.$$

We first consider all positive vectors λ satisfying $b(\lambda) \in \mathbb{Z}^3$. By the lower triangularity of the Hermite normal form, we can start from the last coefficient of $b(\lambda)$ and move forward. Let $\{r\}$ denote the fractional part of r. Then it is not hard to see that each vector λ has the following form:

$$\lambda_3 = \lambda_3^{k,k_3} := \frac{k}{a_{33}} + k_3,$$

$$\lambda_2 = \lambda_2^{jk,k_2} := \frac{j - \{a_{32}\lambda_3^k\}}{a_{22}} + k_2$$

and

$$\lambda_1 = \lambda_1^{ijk,k_1} := \frac{i - \{a_{21}\lambda_2^{jk} + a_{31}\lambda_3^k\}}{a_{11}} + k_1$$

for some nonnegative integers k_3, k_2, k_1, where $k \in \{1, 2, \dots, a_{33}\}$, $j \in \{1, 2, \dots, a_{22}\}$, $i \in \{1, 2, \dots, a_{11}\}$ and $\lambda_1^{ijk} = \lambda_1^{ijk,0}$, $\lambda_2^{jk} = \lambda_2^{jk,0}$, $\lambda_3^k = \lambda_3^{k,0}$. We call all the vectors λ with the same index (i, j, k) the *congruence class of* (i, j, k).

Now we consider the condition $\lambda_1 + \lambda_2 + \lambda_3 < n$ in the above bijection. As n increases, we wish to know when it is the first time that a congruence class (i, j, k) produces interior points inside $n\mathcal{P}(A)$. In other words, for a fixed (i, j, k) we want to find the smallest n such that $\lambda_1 + \lambda_2 + \lambda_3 < n$ with $\lambda_1, \lambda_2, \lambda_3 > 0$. It is clear that this happens when $k_1 = k_2 = k_3 = 0$ and

$$n = \lfloor \lambda_1^{ijk} + \lambda_2^{jk} + \lambda_3^k \rfloor + 1 =: s_{ijk},$$

where $\lfloor r \rfloor$ denotes the floor function.

Finally, when n grows larger than s_{ijk}, we want to consider how many interior points this fixed congruence class produces. Let $n = s_{ijk} + \ell$, so each interior point corresponds to a choice of $k_1 \geqslant 0$, $k_2 \geqslant 0$, $k_3 \geqslant 0$ in the formula of λ_1^{ijk,k_1}, λ_2^{ij,k_2} and λ_3^{i,k_3} such that $k_1 + k_2 + k_3 \leqslant \ell$. There are $\binom{d+\ell}{\ell}$ choices in total.

In summary, the following two facts hold for each congruence class (i, j, k), $k \in \{1, 2, \dots, a_{33}\}$, $j \in \{1, 2, \dots, a_{22}\}$, $i \in \{1, 2, \dots, a_{11}\}$:

(1) s_{ijk} is the smallest n such that this congruence class contributes interior points in the n-th dilation of $\mathcal{P}(A)$.
(2) In the $(s_{ijk} + \ell)$-th dilation of $\mathcal{P}(A)$, this congruence class contributes $\binom{d+\ell}{\ell}$ interior points.

The previous considerations imply the $d = 3$ instance of the following theorem. The general d case follows in analogous manner.

Theorem 2.1. *Let $\mathcal{P}(A)$ be a simplex of dimension d corresponding to a $d \times d$ matrix $A = (a_{ij}) \in \mathbb{Z}^{d\times d}$. Then the generating function for $i^*(\mathcal{P}(A), n)$ is given by*

$$\sum_{n=1}^{\infty} i^*\big(\mathcal{P}(A), n\big)t^n = (1-t)^{-(d+1)} \sum_{\substack{(i_1,\dots,i_d)\\ 1\leqslant i_j\leqslant a_{ij}}} t^{s_{i_1\cdots i_d}},$$

where

$$s_{i_1\cdots i_d} = \left\lfloor \sum_{k=1}^{d} \lambda_k^{i_k,i_{k+1},\dots,i_d} \right\rfloor + 1, \quad \textit{with } \lambda_d^{i_d} = \frac{i_d}{a_{dd}},$$

and

$$\lambda_k^{i_k,i_{k+1},\dots,i_d} = a_{kk}^{-1}\left(i_k - \left\{\sum_{h=k+1}^{d} a_{hk}\lambda_h^{i_h i_{h+1}\cdots i_d}\right\}\right), \quad \textit{for } 1 \leqslant k < d.$$

By the reciprocity law (1.1)*, we have*

$$\delta_{\mathcal{P}(A)}(t) = \sum_{\substack{(i_1,\dots,i_d)\\ 1\leqslant i_j\leqslant a_{ij}}} t^{d+1-s_{i_1\cdots i_d}}.$$

Example 2.2. Let A be the 4×4 matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 1 & 1 & 2 & 0\\ 1 & 0 & 1 & 3 \end{pmatrix}.$$

Then, for $1 \leqslant i \leqslant 2$ and $1 \leqslant j \leqslant 3$,

$$\lambda_2^{ij} = 1 - \big\{\lambda_3^{ij}\big\}, \qquad \lambda_1^{ij} = 1 - \big\{\lambda_3^{ij} + \lambda_4^{j}\big\},$$

where

$$\lambda_4^{j} = \frac{j}{3}, \qquad \lambda_3^{ij} = \frac{i - \{\lambda_4^{j}\}}{2}, \qquad \lambda_2^{ij} = 1 - \big\{\lambda_3^{ij}\big\}, \qquad \lambda_1^{ij} = 1 - \big\{\lambda_3^{ij} + \lambda_4^{j}\big\}.$$

From this we compute

$$s_{11} = 2, \qquad s_{21} = 3, \qquad s_{12} = 2, \qquad s_{22} = 3, \qquad s_{13} = 3, \qquad s_{23} = 5,$$

so that

$$\delta_{\mathcal{P}(A)}(t) = \sum_{i=1}^{3}\sum_{j=1}^{2} t^{d+1-s_{ij}} = 1 + 3t^2 + 2t^3,$$

and thus

$$\delta\big(\mathcal{P}(A)\big) = (1, 0, 3, 2, 0).$$

3. Shifted symmetric δ-vectors

In this section we define shifted symmetric δ-vectors and study when we have this property for some special Hermite normal forms. Results in this section are direct applications of the algorithm developed in the previous section, see Theorem 2.1. In [5], the second author studied shifted symmetric δ-vectors without using this algorithm.

We call a δ-vector *shifted symmetric* if $\delta_i = \delta_{d+1-i}$ for $1 \leqslant i \leqslant d$. For example, $(1, 1, 2, 2, 1, 2, 2, 1)$ is shifted symmetric.

The motivation for this definition is that it arises from the algorithm for the "one row" Hermite normal forms as discussed in Section 3.1. We will consider a special "one row" Hermite normal form in Section 3.2, which allows us to have better results.

3.1. "One row" Hermite normal forms

Consider all $d \times d$ matrices with positive determinant D and the following Hermite normal form.

$$A_D = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ a_1 & \cdots & a_{k-1} & D & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} \in \mathbb{Z}^{d \times d} \tag{3.1}$$

for some $k \in \{1, 2, \dots, d\}$, where $a_1, \dots, a_{k-1}$ are nonnegative integers smaller than D and all other entries are zero. Let d_j denote the number of j's among these a_ℓ's, for $j = 1, \dots, D-1$. Then we can simplify Theorem 2.1 for these "one row" Hermite normal forms.

Corollary 3.1. *Let $M \in \mathbb{Z}^{d \times d}$ with $\det(M) = D$ and $\mathcal{P}(M)$ be the corresponding integral simplex. If its Hermite normal form is of the form as in (3.1), then we have*

$$\delta_{\mathcal{P}(M)}(t) = \sum_{i=1}^{D} t^{d+1-s_i},$$

where

$$s_i = \left\lfloor \frac{i}{D} - \sum_{j=1}^{D-1} \left\{ \frac{ij}{D} \right\} d_j \right\rfloor + d. \tag{3.2}$$

Proof. Consider

$$b(\lambda) = (\lambda_1, \dots, \lambda_k, \dots, \lambda_d) A_D = (\lambda_1 + a_1\lambda_k, \dots, \lambda_{k-1} + a_{k-1}\lambda_k, D\lambda_k, \lambda_{k+1}, \dots, \lambda_d).$$

Using the notation from the proof of Theorem 2.1, we have, for $i = 1, 2, \dots, D$,

$$\lambda_k^i = \frac{i}{D}, \qquad \lambda_\ell^i = 1 - \left\{ a_\ell \frac{i}{D} \right\}, \quad \text{for } \ell = 1, \dots, k-1$$

and

$$\lambda_{k+1}^i = \dots = \lambda_d^i = 1.$$

Therefore, $s_i = 1 + \lfloor \lambda_1^i + \dots + \lambda_d^i \rfloor = \lfloor \frac{i}{D} - \sum_{j=1}^{D-1} \{\frac{ij}{D}\} d_j \rfloor + d$. $\square$

By using the above corollary, we deduce a symmetry property of the δ-vectors.

Proposition 3.2 *(Shifted symmetry for "one row"). For a matrix $M \in \mathbb{Z}^{d\times d}$ with Hermite normal form* (3.1), *we have $s_i + s_{D-i} = d+1$, for $i = 1, \ldots, D-1$, which implies $\delta_i = \delta_{d+1-i}$ by reciprocity, if and only if the following three conditions hold*:

(1) $\sum_{j=1}^{D-1} jd_j - 1$ *is coprime with* D;
(2) $d_j = 0$ *for all j which is not coprime with* D;
(3) $\sum_{j=1}^{D-1} d_j = d-1$.

Proof. Let us consider $s_i + s_{D-i}$. For an integer a, let $\bar{a}$ denote its residue class in $\mathbb{Z}/D\mathbb{Z}$. Then we have

$$\begin{aligned} s_i + s_{D-i} &= \left\lfloor \frac{i}{D} - \sum_{j=1}^{D-1}\left\{\frac{ij}{D}\right\}d_j \right\rfloor + \left\lfloor \frac{D-i}{D} - \sum_{j=1}^{D-1}\left\{\frac{(D-i)j}{D}\right\}d_j \right\rfloor + 2d \\ &= \left\lfloor \frac{i - \sum_{j=1}^{D-1}\overline{ij}d_j}{D} \right\rfloor + \left\lfloor \frac{D-i-\sum_{j=1}^{D-1}\overline{(D-i)j}d_j}{D} \right\rfloor + 2d. \end{aligned}$$

Since

$$\begin{cases} i - \sum_{j=1}^{D-1}\overline{ij}d_j \equiv i\left(1 - \sum_{j=1}^{D-1} jd_j\right) \pmod D, \\ D - i - \sum_{j=1}^{D-1}\overline{(D-i)j}d_j \equiv (D-i)\left(1 - \sum_{j=1}^{D-1} jd_j\right) \pmod D, \end{cases} \tag{3.3}$$

if the condition (1) is not satisfied, then one has

$$\begin{aligned} s_i + s_{D-i} &= \frac{D - \sum_{j=1}^{D-1}(\overline{ij} + \overline{(D-i)j})d_j}{D} + 2d \\ &= 2d + 1 - \sum_{j=1}^{D-1}\frac{\overline{ij} + \overline{(D-i)j}}{D}d_j \\ &\geqslant 2d + 1 - \sum_{j=1}^{D-1} d_j \geqslant d+2 > d+1 \end{aligned}$$

for some i with $1 \leqslant i \leqslant D-1$. Thus, the condition (1) is a necessary condition to have $s_i + s_{D-i} = d+1$ for all i. On the other hand, when the condition (1) is satisfied, again from (3.3), we have

$$\begin{aligned} s_i + s_{D-i} &= \frac{D - \sum_{j=1}^{D-1}(\overline{ij} + \overline{(D-i)j})d_j}{D} + 2d - 1 \\ &= 2d - \sum_{j=1}^{D-1}\frac{\overline{ij} + \overline{(D-i)j}}{D}d_j \\ &= 2d - \sum_{D\nmid ij} d_j. \end{aligned}$$

If the condition (2) is not satisfied, then we have

$$s_i + s_{D-i} = 2d - \sum_{D\nmid ij} d_j > d+1$$

for some i with $1 \leqslant i \leqslant D-1$. Hence, the condition (2) is also a necessary condition. In addition, if the condition (3) is not satisfied, then we have $s_i + s_{D-i} > d+1$. Thus, the condition (3) is also a necessary condition. On the other hand, when the conditions (1)–(3) are all satisfied, we have $s_i + s_{D-i} = D+1$ for all i. $\square$

The conditions of Proposition 3.2 are not very easy to check, so we consider a special case of Hermite normal forms (3.1).

3.2. "All $D-1$ one row" Hermite normal forms

Assume in addition that $d_{D-1} = d-1$ in Corollary 3.1, i.e., the Hermite normal form takes the form

$$\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ D-1 & D-1 & \cdots & D-1 & D \end{pmatrix}. \tag{3.4}$$

Then we have

Corollary 3.3 *(All $D-1$). For a matrix $M \in \mathbb{Z}^{d\times d}$ with Hermite normal form* (3.4), *we have*

$$\delta_{\mathcal{P}(M)}(t) = \sum_{i=1}^{D} t^{d+1-s_i}, \quad \textit{where } s_i = \left\lfloor \frac{id}{D} \right\rfloor + 1.$$

For the Hermite normal form (3.4), the conditions for shifted symmetry in Proposition 3.2 can be simplified.

Proposition 3.4 *(Shifted symmetry for "all $D-1$ one row"). Let $M \in \mathbb{Z}^{d\times d}$ with Hermite normal form* (3.4). *Then*

(1) $\delta_i = \delta_{d+1-i}$ *if and only if D and d are coprime.*
(2) *When $D = kd$, for $k \in \mathbb{N}$ and $k \geqslant 2$, the δ-vector is*

$$(1, \underbrace{k, \ldots, k}_{d-1}, k-1),$$

which is not shifted symmetric. But for $k = 2$, we have $\delta_k = \delta_{d-k}$ (i.e., it is Gorenstein).

4. Classification of Hermite normal forms with a given δ-vector

In this section we give another application of the algorithm Theorem 2.1. Consider Problem 1.2 with the assumption that the matrix $A \in \mathbb{Z}^{d\times d}$ has prime determinant, i.e., A is of the form (3.1), with only one general row. By Corollary 3.1, in order to classify all possible Hermite normal forms (3.1) with a given δ-vector $(\delta_0, \delta_1, \ldots, \delta_d)$, we need to find all nonnegative integer solutions $(d_1, d_2, \ldots, d_{D-1})$ with $d_1 + d_2 + \cdots + d_{D-1} \leqslant d-1$ such that

$$\#\{i\colon\ d+1-s_i = j,\ \text{for } i = 1, \ldots, D\} = \delta_j, \quad \text{for } j = 0, \ldots, d.$$

By Corollary 3.1, we can build equations with "floor" expressions for $(d_1, d_2, \ldots, d_{D-1})$. Removing the "floor" expressions, we obtain D linear equations of $(d_1, d_2, \ldots, d_{D-1})$ with different constant terms but the same $D \times D$ coefficient matrix M. Then we first find all integer solutions $(d_1, d_2, \ldots, d_{D-1})$ and check every candidate using the restrictions of nonnegativity and $d_1 + d_2 + \cdots + d_{D-1} \leqslant d-1$.

For $D = 2$ and 3, the coefficient matrix M is nonsingular, so we can write down the complete solutions, as presented in the first two subsections. For larger primes, the coefficient matrix becomes singular, so there are free variables in the integer solutions $(d_1, d_2, \ldots, d_{D-1})$, which make it very hard to simplify the final solutions after the test.

The idea is similar for Hermite normal forms with nonprime determinant. Instead of using Corollary 3.1, we need to use the formulas in Theorem 2.1. In Section 4.3, we will present the complete solution for $D = 4$.

4.1. A solution of Problem 1.2 when $\sum_{i=0}^{d} \delta_i = 2$

The goal of this subsection is to give a solution of Problem 1.2 when $\sum_{i=0}^{d} \delta_i = 2$, i.e., given a δ-vector $(\delta_0, \delta_1, \ldots, \delta_d)$ with $\sum_{i=0}^{d} \delta_i = 2$, we classify all the integral simplices with $(\delta_0, \delta_1, \ldots, \delta_d)$ arising from Hermite normal forms with determinant 2.

We consider all Hermite normal forms (3.1) with $D = 2$, where there are d_1 1's among the $a_1, \ldots, a_{k-1}$. Notice that the position of the row with a 2 does not affect the δ-vector, so the only variable is d_1. By Corollary 3.1, we have a formula for the δ-vector of this integral simplex $\mathcal{P}(A_2)$. Denote

$$k = 1 - \left\lfloor \frac{1 - d_1}{2} \right\rfloor.$$

Then one has $\delta_0 = \delta_k = 1$.

By this formula, we can characterize all Hermite normal forms with a given δ-vector. Let $\delta_0 = \delta_i = 1$. Then by solving the equation $i = 1 - \lfloor (1 - d_1)/2 \rfloor$, we obtain $d_1 = 2i - 2$ and $d_1 = 2i - 1$, both cases will give us the desired δ-vector.

Notice that there is a constraint on d_1 given by $0 \leqslant d_1 \leqslant d - 1$. Not all δ-vectors are obtained from simplices. But we can easily get the appropriate conditions on i and the corresponding d_1 as follows (by $d_1 \geqslant 0$, we have $i \geqslant 1$):

(1) If $i \leqslant d/2$, $d_1 = 2i - 2$ and $d_1 = 2i - 1$ both work, and these give all the matrices with this δ-vector.
(2) If $i = (d + 1)/2$, only $d_1 = 2i - 2 = d - 1$ works.
(3) If $i > (d + 1)/2$, there is no solution.

Now, this result has been obtained essentially in [4]. In fact, the inequality $i \leqslant (d + 1)/2$ means that the δ-vector satisfies (1.4).

4.2. A solution of Problem 1.2 when $\sum_{i=0}^{d} \delta_i = 3$

We consider all Hermite normal forms (3.1) with $D = 3$, where there are d_1 1's and d_2 2's among the $a_1, \ldots, a_{k-1}$. The position of the row with a 3 does not affect the δ-vector, so the only variables are d_1 and d_2. Also, by Corollary 3.1, we have $\delta_{\mathcal{P}(A_3)}(t) = 1 + t^{k_1} + t^{k_2}$, where

$$k_1 = 1 - \left\lfloor \frac{1 - d_1 - 2d_2}{3} \right\rfloor \quad \text{and} \quad k_2 = 1 - \left\lfloor \frac{2 - 2d_1 - d_2}{3} \right\rfloor.$$

Then by the formula, we can characterize all Hermite normal forms with a given δ-vector using arguments similar to $\sum_{i=0}^{d} \delta_i = 2$. Let $\delta_{\mathcal{P}(A_3)}(t) = 1 + t^i + t^j$. Set

$$i = 1 - \left\lfloor \frac{1 - d_1 - 2d_2}{3} \right\rfloor \quad \text{and} \quad j = 1 - \left\lfloor \frac{2 - 2d_1 - d_2}{3} \right\rfloor.$$

(Later reverse the role of i and j if $i \neq j$, in both equations and solutions.) The solutions for (d_1, d_2) are

$$d^{(1)} = \begin{cases} d_1 = 2j - i, \\ d_2 = 2i - j - 1, \end{cases} \qquad d^{(2)} = \begin{cases} d_1 = 2j - i - 1, \\ d_2 = 2i - j - 1 \end{cases} \quad \text{and} \quad d^{(3)} = \begin{cases} d_1 = 2j - i, \\ d_2 = 2i - j - 2. \end{cases}$$

Table 1
Characterizations for matrices of the form A_3.

$2j$	$2i$	$i+j$	solutions
$\geqslant i$	$\geqslant j+1$	$\leqslant d$	$d^{(1)}$
$\geqslant i+1$	$\geqslant j+1$	$\leqslant d+1$	$d^{(2)}$
$\geqslant i$	$\geqslant j+2$	$\leqslant d+1$	$d^{(3)}$

In addition, by the restriction on (d_1, d_2) that $d_1, d_2 \geqslant 0$ and $d_1 + d_2 \leqslant d - 1$, we have the characterizations shown in Table 1.

(1) If $2j \geqslant i$, $2i \geqslant j+1$ and $i+j \leqslant d$, then the solution $d^{(1)}$ will work and this gives all the matrices with this δ-vector.
(2) If $2j \geqslant i+1$, $2i \geqslant j+1$ and $i+j \leqslant d+1$, then the solution $d^{(2)}$ will work and this gives all the matrices with this δ-vector.
(3) If $2j \geqslant i$, $2i \geqslant j+2$ and $i+j \leqslant d+1$, then the solution $d^{(3)}$ will work and this gives all the matrices with this δ-vector.
(4) If $\{i, j\}$ in the given vector does not satisfy any of the above cases, there is no matrix with this vector as its δ-vector.

Again, this result has been obtained in [4]. In fact, for example, the inequality $2j \geqslant i$ means that (1.3) holds and the inequality $i+j \leqslant d+1$ means that (1.4) holds.

Notice that only the solution

$$d^{(2)} = \begin{cases} d_1 = d-1, \\ d_2 = 0 \end{cases}$$

works when $i = (d+2)/3$ and $j = (2d+1)/3$. This happens when $d \equiv 1 \pmod 3$ and there is only one matrix with $d_1 = d-1$ and $d_2 = 0$. Similarly, only the solution

$$d^{(3)} = \begin{cases} d_1 = 0, \\ d_2 = d-1 \end{cases}$$

works when $i = (2d+2)/3$ and $j = (d+1)/3$. This happens when $d \equiv 2 \pmod 3$ and again, there is only one matrix with $d_1 = 0$ and $d_2 = d-1$.

4.3. *A solution of Problem 1.2 when $\sum_{i=0}^{d} \delta_i = 4$*

When the determinant is 4, there are two cases of Hermite normal forms. One is the Hermite normal forms (3.1) with $D = 4$, where there are d_1 1's, d_2 2's and d_3 3's among the $a_1, \ldots, a_{k-1}$. The other hermit normal form takes the form

$$A_4' = \begin{pmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ \ast & \cdots & \ast & 2 & & & & & & & \\ & & & & 1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 1 & & & & \\ \dot{\ast} & \cdots & \dot{\ast} & \bar{\ast} & \dot{\ast} & \cdots & \dot{\ast} & 2 & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \end{pmatrix}, \tag{4.1}$$

where there are d_1 1's (resp. d_1' 1's) among $\ast$'s (resp. $\dot{\ast}$'s), there are e_1 1's (resp. e_1' 1's) among the $\ast$'s (resp. $\dot{\ast}$'s) of which the entry of the row of $\dot{\ast}$ (resp. $\ast$) in the same column is 0. Also, set $d_1'' = e_1 + e_1'$. (For example, a 6×6 Hermite normal form

Table 2
Characterizations for matrices of the form A_4.

$j+k$	$2j$	$i+j$	solutions
$\geqslant i+1$	$\leqslant i+k \leqslant d+1$	$\geqslant k+1$	$d^{(1)}$
$\geqslant i$	$\leqslant i+k \leqslant d+1$	$\geqslant k+2$	$d^{(2)}$
$\geqslant i$	$\leqslant i+k \leqslant d$	$\geqslant k+1$	$d^{(3)}$
$\geqslant i$	$\leqslant i+k-1 \leqslant d$	$\geqslant k+1$	$d^{(4)}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 2 \end{pmatrix}$$

is a matrix (4.1) with $d_1 = 2$, $d_1' = 3$, $e_1 = 1$, $e_1' = 2$, $d_1'' = 3$ and $\bar{*} = 1$.)

First, we consider the Hermite normal forms A_4. Then, by Corollary 3.1, we have $\delta_{\mathcal{P}(A_4)}(t) = 1 + t^{k_1} + t^{k_2} + t^{k_3}$, where

$$k_1 = 1 - \left\lfloor \frac{1 - d_1 - 2d_2 - 3d_3}{4} \right\rfloor, \qquad k_2 = 1 - \left\lfloor \frac{1 - d_1 - d_3}{2} \right\rfloor \quad \text{and}$$
$$k_3 = 1 - \left\lfloor \frac{3 - 3d_1 - 2d_2 - d_3}{4} \right\rfloor.$$

Let $\delta_{\mathcal{P}(A_4)}(t) = 1 + t^i + t^j + t^k$. We get three sets of equations:

$$i = 1 - \left\lfloor \frac{1 - d_1 - 2d_2 - 3d_3}{4} \right\rfloor, \qquad j = 1 - \left\lfloor \frac{1 - d_1 - d_3}{2} \right\rfloor \quad \text{and}$$
$$k = 1 - \left\lfloor \frac{3 - 3d_1 - 2d_2 - d_3}{4} \right\rfloor.$$

(Later replace the roles of i, j and k if any of the three are distinct.) The solutions for (d_1, d_2, d_3) are

$$d^{(1)} = \begin{cases} d_1 = -i + j + k - 1, \\ d_2 = i - 2j + k, \\ d_3 = i + j - k - 1, \end{cases} \qquad d^{(2)} = \begin{cases} d_1 = -i + j + k, \\ d_2 = i - 2j + k, \\ d_3 = i + j - k - 2, \end{cases}$$
$$d^{(3)} = \begin{cases} d_1 = -i + j + k, \\ d_2 = i - 2j + k, \\ d_3 = i + j - k - 1, \end{cases} \qquad d^{(4)} = \begin{cases} d_1 = -i + j + k, \\ d_2 = i - 2j + k - 1, \\ d_3 = i + j - k - 1. \end{cases}$$

In addition, by the restriction on (d_1, d_2, d_3) that $d_1, d_2, d_3 \geqslant 0$ and $d_1 + d_2 + d_3 \leqslant d - 1$, we have the characterizations shown in Table 2.

(1) If $j + k \geqslant i + 1$, $2j \leqslant i + k \leqslant d + 1$ and $i + j \geqslant k + 1$, then the solution $d^{(1)}$ will work and this gives all the matrices with this δ-vector.
(2) If $j + k \geqslant i$, $2j \leqslant i + k \leqslant d + 1$ and $i + j \geqslant k + 2$, then the solution $d^{(2)}$ will work and this gives all the matrices with this δ-vector.
(3) If $j + k \geqslant i$, $2j \leqslant i + k \leqslant d$ and $i + j \geqslant k + 1$, then the solution $d^{(3)}$ will work and this gives all the matrices with this δ-vector.
(4) If $j + k \geqslant i$, $2j + 1 \leqslant i + k \leqslant d + 1$ and $i + j \geqslant k + 1$, then the solution $d^{(4)}$ will work and this gives all the matrices with this δ-vector.
(5) If $\{i, j, k\}$ in the given vector does not satisfy any of the above cases, there is no matrix A_4 with this vector as its δ-vector.

Table 3
Characterizations for matrices of the form (4.1) with $\bar{*} = 0$.

i	j	k	$i+j$	$i+k$	$j+k$	$i+j+k$	solutions
$\leqslant \lfloor \frac{d}{2} \rfloor$	$\leqslant \lfloor \frac{d-1}{2} \rfloor$	$\geqslant 2$, $\leqslant \lfloor \frac{d+1}{2} \rfloor$	$\geqslant k$	$\geqslant j+2$	$\geqslant i+1$	$\leqslant d+1$	$d^{(1)}$
$\leqslant \lfloor \frac{d-1}{2} \rfloor$	$\leqslant \lfloor \frac{d}{2} \rfloor$	$\geqslant 2$, $\leqslant \lfloor \frac{d+1}{2} \rfloor$	$\geqslant k$	$\geqslant j+1$	$\geqslant i+2$	$\leqslant d+1$	$d^{(2)}$
$\leqslant \lfloor \frac{d-1}{2} \rfloor$	$\leqslant \lfloor \frac{d-1}{2} \rfloor$	$\leqslant \lfloor \frac{d}{2} \rfloor$	$\geqslant k$	$\geqslant j+1$	$\geqslant i+1$	$\leqslant d$	$d^{(3)}$
$\leqslant \lfloor \frac{d}{2} \rfloor$	$\leqslant \lfloor \frac{d}{2} \rfloor$	$\leqslant \lfloor \frac{d}{2} \rfloor$	$\geqslant k+1$	$\geqslant j+1$	$\geqslant i+1$	$\leqslant d+1$	$d^{(4)}$

Notice that only the solution

$$d^{(2)} = \begin{cases} d_1 = 0, \\ d_2 = 0, \\ d_3 = d-1 \end{cases}$$

works when $i = (3d+3)/4$, $j = (d+1)/2$ and $k = (d+1)/4$. This happens when $d \equiv 3 \pmod 4$ and there is only one matrix with $d_3 = d-1$. Similarly, only the solution

$$d^{(1)} = \begin{cases} d_1 = d-1, \\ d_2 = 0, \\ d_3 = 0 \end{cases}$$

works when $i = (d+3)/4$, $j = (d+1)/2$ and $k = (3d+1)/4$. This happens when $d \equiv 1 \pmod 4$ and again, there is only one matrix with $d_1 = d-1$.

Next, we consider the Hermite normal forms (4.1). However, we need to consider two cases, which are the cases where $\bar{*} = 0$ and $\bar{*} = 1$.

First, we consider the case with $\bar{*} = 0$. Notice that the variables are d_1, d_1' and d_1''. Obviously we cannot use Corollary 3.1, but we apply Theorem 2.1 directly. Thus we have $\delta_{\mathcal{P}(A_4')}(t) = 1 + t^{k_1} + t^{k_2} + t^{k_3}$, where

$$k_1 = \left\lfloor \frac{d_1+2}{2} \right\rfloor, \qquad k_2 = \left\lfloor \frac{d_1'+2}{2} \right\rfloor \quad \text{and} \quad k_3 = \left\lfloor \frac{d_1''+3}{2} \right\rfloor.$$

Let $\delta_{\mathcal{P}(A_4')}(t) = 1 + t^i + t^j + t^k$. We get three sets of equations:

$$i = \left\lfloor \frac{d_1+2}{2} \right\rfloor, \qquad j = \left\lfloor \frac{d_1'+2}{2} \right\rfloor \quad \text{and} \quad k = \left\lfloor \frac{d_1''+3}{2} \right\rfloor$$

or replace the role of i, j and k if i, j and k are distinct, in all equations and solutions. Since $d_1 + d_1' + d_1''$ is even, the solutions for (d_1, d_1', d_1'') are

$$d^{(1)} = \begin{cases} d_1 = 2i-2, \\ d_1' = 2j-1, \\ d_1'' = 2k-3, \end{cases} \qquad d^{(2)} = \begin{cases} d_1 = 2i-1, \\ d_1' = 2j-2, \\ d_1'' = 2k-3, \end{cases}$$

$$d^{(3)} = \begin{cases} d_1 = 2i-1, \\ d_1' = 2j-1, \\ d_1'' = 2k-2, \end{cases} \qquad d^{(4)} = \begin{cases} d_1 = 2i-2, \\ d_1' = 2j-2, \\ d_1'' = 2k-2. \end{cases}$$

In addition, by the restriction on (d_1, d_1', d_1'') that $0 \leqslant d_1 \leqslant d-2$, $0 \leqslant d_1' \leqslant d-2$, $0 \leqslant d_1'' \leqslant d-2$, $d_1 + d_1' + d_1'' \leqslant 2(d-2)$, $d_1'' \leqslant d_1 + d_1'$, $d_1' \leqslant d_1 + d_1''$ and $d_1 \leqslant d_1' + d_1''$, we have the characterizations shown in Table 3.

Table 4
Characterizations for matrices of the form (4.1) with $\bar{*} = 1$.

$2k$	$2i$	$2j$	$i+j$	$i+k$	$j+k$	solutions
$\geqslant j+3$, $\leqslant d+j+1$	$\geqslant j+2$, $\leqslant d+j$	$\leqslant d-1$	$\geqslant k$	$\geqslant 2j+2$, $\leqslant d+1$	$\geqslant i+1$	$d^{(1)}$
$\geqslant j+2$, $\leqslant d+j$	$\geqslant j+1$, $\leqslant d+j-1$	$\leqslant d-1$	$\geqslant k$	$\geqslant 2j+1$, $\leqslant d$	$\geqslant i+1$	$d^{(2)}$
$\geqslant j+3$, $\leqslant d+j+1$	$\geqslant j+1$, $\leqslant d+j-1$	$\leqslant d$	$\geqslant k$	$\geqslant 2j+1$, $\leqslant d+1$	$\geqslant i+2$	$d^{(3)}$
$\geqslant j+2$, $\leqslant d+j$	$\geqslant j+2$, $\leqslant d+j$	$\leqslant d$	$\geqslant k+1$	$\geqslant 2j+1$, $\leqslant d+1$	$\geqslant i+1$	$d^{(4)}$

(1) If $i \leqslant \lfloor d/2 \rfloor$, $j \leqslant \lfloor (d-1)/2 \rfloor$, $2 \leqslant k \leqslant \lfloor (d+1)/2 \rfloor$, $i+j+k \leqslant d+1$, $k \leqslant i+j$, $j+2 \leqslant i+k$ and $i+1 \leqslant j+k$, then the solution $d^{(1)}$ will work and this gives all the matrices with this δ-vector.
(2) If $i \leqslant \lfloor (d-1)/2 \rfloor$, $j \leqslant \lfloor d/2 \rfloor$, $2 \leqslant k \leqslant \lfloor (d+1)/2 \rfloor$, $i+j+k \leqslant d+1$, $k \leqslant i+j$, $j+1 \leqslant i+k$ and $i+2 \leqslant j+k$, then the solution $d^{(2)}$ will work and this gives all the matrices with this δ-vector.
(3) If $i, j \leqslant \lfloor (d-1)/2 \rfloor$, $k \leqslant \lfloor d/2 \rfloor$, $i+j+k \leqslant d$, $k \leqslant i+j$, $j+1 \leqslant i+k$ and $i+1 \leqslant j+k$, then the solution $d^{(3)}$ will work and this gives all the matrices with this δ-vector.
(4) If $i, j, k \leqslant \lfloor d/2 \rfloor$, $i+j+k \leqslant d+1$, $k+1 \leqslant i+j$, $j+1 \leqslant i+k$ and $i+1 \leqslant j+k$, then the solution $d^{(4)}$ will work and this gives all the matrices with this δ-vector.
(5) If $\{i, j, k\}$ in the given vector does not satisfy any of the above cases, there is no matrix (4.1), where $\bar{*} = 0$, with this vector as its δ-vector.

Next, we consider the case with $\bar{*} = 1$. By Theorem 2.1, we have $\delta_{\mathcal{P}(A_4')}(t) = 1 + t^{k_1} + t^{k_2} + t^{k_3}$, where

$$k_1 = 1 - \left\lfloor \frac{1 - d_1 - 2d_1''}{4} \right\rfloor, \qquad k_2 = 1 - \left\lfloor \frac{1 - d_1}{2} \right\rfloor \quad \text{and} \quad k_3 = 2 - \left\lfloor \frac{3 - d_1 - 2d_1'}{4} \right\rfloor.$$

Let $\delta_{\mathcal{P}(A_4')}(t) = 1 + t^i + t^j + t^k$. We get three sets of equations:

$$i = 1 - \left\lfloor \frac{1 - d_1 - 2d_1''}{4} \right\rfloor, \qquad j = 1 - \left\lfloor \frac{1 - d_1}{2} \right\rfloor \quad \text{and} \quad k = 2 - \left\lfloor \frac{3 - d_1 - 2d_1'}{4} \right\rfloor$$

or replace the roles of i, j and k if i, j and k are distinct. Since $d_1 + d_1' + d_1''$ is even, the solutions for (d_1, d_1', d_1'') are

$$d^{(1)} = \begin{cases} d_1 = 2j-1, \\ d_1' = 2k-j-3, \\ d_1'' = 2i-j-2, \end{cases} \qquad d^{(2)} = \begin{cases} d_1 = 2j-1, \\ d_1' = 2k-j-2, \\ d_1'' = 2i-j-1, \end{cases}$$
$$d^{(3)} = \begin{cases} d_1 = 2j-2, \\ d_1' = 2k-j-3, \\ d_1'' = 2i-j-1, \end{cases} \qquad d^{(4)} = \begin{cases} d_1 = 2j-2, \\ d_1' = 2k-j-2, \\ d_1'' = 2i-j-2. \end{cases}$$

In addition, by the restriction on (d_1, d_1', d_1'') that $0 \leqslant d_1 \leqslant d-2$, $0 \leqslant d_1' \leqslant d-2$, $0 \leqslant d_1'' \leqslant d-2$, $d_1 + d_1' + d_1'' \leqslant 2(d-2)$, $d_1'' \leqslant d_1 + d_1'$, $d_1' \leqslant d_1 + d_1''$ and $d_1 \leqslant d_1' + d_1''$, we have the characterizations shown in Table 4.

(1) If $j+3 \leqslant 2k \leqslant d+j+1$, $j+2 \leqslant 2i \leqslant d+j$, $2j \leqslant d-1$, $k \leqslant i+j$, $2j+2 \leqslant i+k \leqslant d+1$ and $i+1 \leqslant j+k$, then the solution $d^{(1)}$ will work and this gives all the matrices with this δ-vector.
(2) If $j+2 \leqslant 2k \leqslant d+j$, $j+1 \leqslant 2i \leqslant d+j-1$, $2j \leqslant d-1$, $k \leqslant i+j$, $2j+1 \leqslant i+k \leqslant d$ and $i+1 \leqslant j+k$, then the solution $d^{(2)}$ will work and this gives all the matrices with this δ-vector.

(3) If $j+3 \leqslant 2k \leqslant d+j+1$, $j+1 \leqslant 2i \leqslant d+j-1$, $2j \leqslant d$, $k \leqslant i+j$, $2j+1 \leqslant i+k \leqslant d+1$ and $i+2 \leqslant j+k$, then the solution $d^{(3)}$ will work and this gives all the matrices with this δ-vector.
(4) If $j+2 \leqslant 2k \leqslant d+j$, $j+2 \leqslant 2i \leqslant d+j$, $2j \leqslant d$, $k+1 \leqslant i+j$, $2j+1 \leqslant i+k \leqslant d+1$ and $i+1 \leqslant j+k$, then the solution $d^{(4)}$ will work and this gives all the matrices with this δ-vector.
(5) If $\{i, j, k\}$ in the given vector does not satisfy any of the above cases, there is no matrix (4.1) with this vector as its δ-vector.

Notice that only the solution

$$d^{(3)} = \begin{cases} d_1 = d-2, \\ d_1' = d-2, \\ d_1'' = 0 \end{cases}$$

works when $i = (d+2)/4$, $j = d/2$ and $k = (3d+2)/4$. This happens when $d \equiv 2 \pmod 4$ and there is only one matrix with $d_1 = d_1' = d-2$. Similarly, only the solution

$$d^{(4)} = \begin{cases} d_1 = d-2, \\ d_1' = 0, \\ d_1'' = d-2 \end{cases}$$

works when $i = 3d/4$, $j = d/2$ and $k = d/4+1$. This happens when $d \equiv 0 \pmod 4$ and again, there is only one matrix with $d_1 = d_1'' = d-2$.

5. The classification of the possible δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$

In this section we classify the possible δ-vectors with $\sum_{i=0}^{d} \delta_i = 4$ using results from Section 4.3.

Let $1 + t^{i_1} + t^{i_2} + t^{i_3}$ with $1 \leqslant i_1 \leqslant i_2 \leqslant i_3 \leqslant d$ be a δ-polynomial for some integral polytope and $(\delta_0, \delta_1, \ldots, \delta_d)$ the sequence of the coefficients of this polynomial, where it is clear that $\delta_0 = 1$ and $\sum_{i=0}^{d} \delta_i = 4$. Assume that $(\delta_0, \delta_1, \ldots, \delta_d)$ satisfies the inequalities (1.3), (1.4) and $\delta_1 \geqslant \delta_d$, which are necessary conditions to be a possible δ-vector. Then (1.3) and (1.4) lead into the following inequalities that (i_1, i_2, i_3) satisfies

$$i_3 \leqslant i_1 + i_2, \qquad i_1 + i_3 \leqslant d+1 \quad \text{and} \quad i_2 \leqslant \lfloor (d+1)/2 \rfloor. \tag{5.1}$$

Finally, the classification of possible δ-vectors of integral polytopes with $\sum_{i=0}^{d} \delta_i = 4$ is given by the following

Theorem 5.1. *Let $1 + t^{i_1} + t^{i_2} + t^{i_3}$ be a polynomial with $1 \leqslant i_1 \leqslant i_2 \leqslant i_3 \leqslant d$. Then there exists an integral polytope $\mathcal{P} \subset \mathbb{R}^d$ of dimension d whose δ-polynomial equals $1 + t^{i_1} + t^{i_2} + t^{i_3}$ if and only if (i_1, i_2, i_3) satisfies* (5.1) *and the additional condition*

$$2i_2 \leqslant i_1 + i_3 \quad \text{or} \quad i_2 + i_3 \leqslant d+1. \tag{5.2}$$

Moreover, all these polytopes can be chosen to be simplices.

Proof. There are four cases: (1) $i_1 = i_2 = i_3$, (2) $i_1 < i_2 = i_3$, (3) $i_1 = i_2 < i_3$, (4) $i_1 < i_2 < i_3$. We will show that in each case (5.1) together with (5.2) are the necessary and sufficient conditions for $1 + t^{i_1} + t^{i_2} + t^{i_3}$ to be the δ-polynomial of some integral polytope.

(1) Assume $i_1 = i_2 = i_3 = \ell$. By the inequalities (5.1), we have $1 \leqslant \ell \leqslant \lfloor (d+1)/2 \rfloor$. Set $i = j = k = \ell$. We have

$$j + k \geqslant i + 1, \qquad 2j \leqslant i + k \leqslant d+1 \quad \text{and} \quad i + j \geqslant k + 1. \tag{5.3}$$

Thus, by our result on the classification in the case of a matrix of the form A_4 (Table 2, the solution $d^{(1)}$), there exists an integral simplex whose δ-vector is of the form $(1, 0, \ldots, 0, 3, 0, \ldots, 0)$.

On the other hand, if there exists an integral polytope with this δ-vector, then (5.1) holds since it is a necessary condition. In this case, both inequalities in (5.2) hold.

(2) Assume $\ell = i_1 < i_2 = i_3 = \ell'$. By (5.1), we have $1 \leqslant \ell < \ell' \leqslant \lfloor (d+1)/2 \rfloor$. Let $j = \ell$ and $i = k = \ell'$. Then the inequalities (5.3) hold. Thus there exists an integral simplex whose δ-vector is $(1, 0, \dots, 0, 1, 0, \dots, 0, 2, 0, \dots, 0)$.

On the other hand, if there exists an integral polytope with this δ-vector, then we have (5.1) and $i_2 + i_3 \leqslant d + 1$ follows from $i_2 \leqslant \lfloor (d+1)/2 \rfloor$.

(3) Assume $\ell = i_1 = i_2 < i_3 = \ell'$. Set $i = \ell'$ and $j = k = \ell$. Then it follows from (5.1) that

$$j + k \geqslant i, \qquad 2j + 1 \leqslant i + k \leqslant d + 1 \quad \text{and} \quad i + j \geqslant k + 1.$$

Thus, by our result (Table 2, the solution $d^{(4)}$), there exists an integral simplex whose δ-vector is $(1, 0, \dots, 0, 2, 0, \dots, 0, 1, 0, \dots, 0)$.

On the other hand, if there exists an integral polytope with this δ-vector, then (5.1) holds. In this case, both inequalities in (5.2) hold.

(4) Assume $1 \leqslant i_1 < i_2 < i_3 \leqslant d$. Suppose $2i_2 \leqslant i_1 + i_3$ holds. Set $i = i_3$, $j = i_2$ and $k = i_1$. Then we have $j + k = i_1 + i_2 \geqslant i_3 = i$, $2j = 2i_2 \leqslant i_1 + i_3 = i + k \leqslant d + 1$ and $i + j = i_2 + i_3 \geqslant 2i_2 + 1 \geqslant 2i_1 + 3 > i_1 + 2 = k + 2$. Thus, by our result (Table 2, the solution $d^{(2)}$), there exists an integral simplex whose δ-vector is $(1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0)$.

Suppose $i_2 + i_3 \leqslant d + 1$ holds. Set $i = i_3$, $j = i_1$ and $k = i_2$. Then we have $j + k = i_1 + i_2 \geqslant i_3 = i$, $2j = 2i_1 < i_2 + i_3 = i + k \leqslant d + 1$ and $i + j = i_1 + i_3 \geqslant i_1 + i_2 + 1 \geqslant i_2 + 2 = k + 2$. Thus, by our result (Table 2, the solution $d^{(2)}$), there exists an integral simplex whose δ-vector is $(1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0)$.

On the other hand, assume the contrary of (5.2): both $2i_2 > i_1 + i_3$ and $i_2 + i_3 > d + 1$ hold. We claim that there exists no integral polytope $\mathcal{P}$ with this δ-vector. First we want to show that if there exists such a polytope, it must be a simplex. Note that the δ-vector satisfies (5.1). Suppose $i_1 = 1$. It then follows from (5.1) and $i_2 + i_3 > d + 1$ that $i_2 = (d+1)/2$ and $i_3 = (d+3)/2$. However, this contradicts (1.4). Therefore $i_1 > 1$, and thus $\delta_1 = 0$. By the explanation after Eq. (1.2), $\mathcal{P}$ must be a simplex. Now we can apply our characterization results for simplices.

If we set $j = i_3$, then $2j = 2i_3 > i_1 + i_2 = i + k$. If we set $j = i_2$, then $2j = 2i_2 > i_1 + i_3 = i + k$. If we set $j = i_1$, then $i + k = i_2 + i_3 > d + 1$. In any case there does not exist a Hermite normal form A_4 whose δ-polynomial coincides with $1 + t^{i_1} + t^{i_2} + t^{i_3}$.

Moreover, since $i + j + k = i_1 + i_2 + i_3 > i_2 + i_3 > d + 1$, there does not exist a Hermite normal form (4.1) with $\bar{*} = 0$ whose δ-polynomial coincides with $1 + t^{i_1} + t^{i_2} + t^{i_3}$.

In addition, if we set $j = i_3$, then $2j = 2i_3 > i_1 + i_2 = i + k$. If we set $j = i_2$, then $2j = 2i_2 > i_1 + i_3 = i + k$. If we set $j = i_1$, then $i + k = i_2 + i_3 > d + 1$. Thus there does not exist a Hermite normal form (4.1) with $\bar{*} = 1$ whose δ-polynomial coincides with $1 + t^{i_1} + t^{i_2} + t^{i_3}$. $\square$

Examples 5.2. (a) We consider the integer sequence $(1, 0, 1, 1, 0, 1, 0)$. Then one has $i_1 = 2$, $i_2 = 3$, $i_3 = 5$ and $d = 6$. Since (1.3) and (1.4) are satisfied and $2i_2 \leqslant i_1 + i_3$ holds, there is an integral polytope whose δ-vector coincides with $(1, 0, 1, 1, 0, 1, 0)$ by Theorem 5.1. In fact, let $M \in \mathbb{Z}^{6 \times 6}$ be the Hermite normal form A_4 with $(d_1, d_2, d_3) = (0, 1, 4)$ or $(0, 0, 5)$. Then we have $\delta(\mathcal{P}(M)) = (1, 0, 1, 1, 0, 1, 0)$.

(b) There is no integral polytope with its δ-vector $(1, 0, 1, 0, 1, 1, 0, 0)$ since we have $2i_2 > i_1 + i_3$ and $i_2 + i_3 > d + 1$, although this integer sequence satisfies (1.3) and (1.4). (This example is described in [4, Example 1.2] as a counterexample of [4, Theorem 0.1] for the case where $\sum_{i=0}^{d} \delta_i = 4$.) However, there exists an integral polytope with its δ-vector $(1, 0, 1, 0, 1, 1, 0, 0, 0)$ since $i_2 + i_3 = d + 1$ holds.

Remark 5.3. From the above proof, we can see that when $\sum_{i=0}^{d} \delta_i = 4$, all the possible δ-vectors can be obtained by simplices. This is also true for all δ-vectors with $\sum_{i=0}^{d} \delta_i \leqslant 3$, from the proof of [4, Theorem 0.1]. However, when $\sum_{i=0}^{d} \delta_i = 5$, the δ-vector $(1, 3, 1)$ cannot be obtained from any simplex, while it is a possible δ-vector of an integral polygon. In fact, suppose that $(1, 3, 1)$ can be obtained from a simplex. Since $\min\{i\colon \delta_i \neq 0,\ i > 0\} = 1$ and $\max\{i\colon \delta_i \neq 0\} = 2$, one has $\min\{i\colon \delta_i \neq 0,\ i > 0\} = 3 - \max\{i\colon \delta_i \neq 0\}$, which implies that the assumption of [5, Theorem 2.3] is satisfied. Thus the δ-vector must be shifted symmetric, a contradiction.

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