Simplices in Unimodular Triangulations of the n-Cube

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Abstract

This article studies the simplices used in unimodular triangulations of the n-cube. Firstly, it studies the relationships between those simplices, and secondly, it studies those simplices themselves. The article includes a formula for the number of edges in the tight span of a unimodular triangulation of the n-cube. It also develops a constraint that identifies n-simplices of volume $1/n!$ with vertices in $[0,1]^n \cap \mathbb{Z}^n$, unique under symmetry.

1 Introduction

There are many open questions about triangulations of n-cubes. How many triangulations are there of the n-cube? How many triangulations are there that are unimodular or regular? How many n-simplices, unique under symmetry, can be used in triangulations of the n-cube?

These are important questions in themselves, and they also have applications to other areas of mathematics. For example, Gelfand et al. demonstrated a relationship between triangulations of the n-cube and the $2 \times ... \times 2$ hyperdeterminant [1], and Huggins et al. used the relationship to compuate a formula for the hyperdeterminant of format $2 \times 2 \times 2 \times 2$ [2].

This paper focuses on the simplices used in unimodular triangulations of the n-cube. Firstly, it studies how those simplices "fit together" by providing a formula for the edges in the tight span. In geometric terms, this number quantifies the number of $(n-1)$-dimensional faces in the triangulation shared by two n-simplices in the triangulation. Further exploration could yield results on the number of 2- or 3-cells in the tight span.

Secondly, it studies which simplices can be used in such triangulations. To start, the simplices must have volume $\frac{1}{n!}$. Also, many of these simplices are equivalent under symmetry, that is, one can use some composition of rotation, translation and reflection to get from one to another. For example, when $n = 3$, the standard simplex $\text{conv}\{0, e_1, e_2, e_3\}$ and the simplex $\text{conv}\left\{0, \begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}1\\0\\1\end{pmatrix}, \begin{pmatrix}1\\1\\0\end{pmatrix}\right\}$ are equivalent under symmetry. However, there are some that are unique under symmetry, such as the standard simplex and $\text{conv}\{0, e_1, e_2, e_1 + e_3\}$. This paper works towards answering the problem of how many n-simplices in the n-cube exist, unique under symmetry. To do this, it develops a graph theoretic representation of the simplices the respects equivalence under symmetry, and conjectures a criterion on that representation that identifies precisely those simplices in question.

2 Background

Below are a few relevant definitions. For additional details on polytopes and their geometry, consult the text [3] by Beck and Robins, from which a few of these definitions are taken.

Definition 2.1. *A* ***(convex) polytope*** *in* $\mathbb{R}^n$ *is the convex hull of finitely many points in* $\mathbb{R}^n$. *That is,* $conv\{v_1, ..., v_d\} = \{\sum_{i=1}^{d} \lambda_i v_i : \sum_{i=1}^{d} \lambda_i = 1, \lambda_i \geq 0\}$. *A* ***lattice polytope*** *has vertices only in* $\mathbb{Z}^n$.

Definition 2.2. *The* ***dimension*** *of a polytope* $\mathcal{P} \subset \mathbb{R}^n$ *is the dimension of the affine space* $\{x + \lambda(y-x) : x, y \in \mathcal{P}, \lambda \in \mathbb{R}\}$. $\mathcal{P}$ *is* ***full dimensional*** *if* $\dim \mathcal{P} = n$.

Definition 2.3. *A hyperplane* $H = \{x \in \mathbb{R}^n : a \cdot x = b\}$ *is a* ***supporting hyperplane*** *of* $\mathcal{P}$ *if* $\mathcal{P}$ *lies entirely on one side of* H. *That is,*

$$\mathcal{P} \subset \{x \in \mathbb{R}^n : a \cdot x \leq b\} \quad \text{or} \quad \mathcal{P} \subset \{x \in \mathbb{R}^n : a \cdot x \geq b\}$$

Definition 2.4. *A* ***face*** *of a polytope* $\mathcal{P}$ *of dimension* d *in* $\mathbb{R}^n$ *is a set of the form* $\mathcal{P} \cap H$ *for some supporting hyperplane* $H \subset \mathbb{R}^n$. *A* ***facet*** *is a face of dimension* $d-1$.

Definition 2.5. *A* ***d-simplex*** *in* $\mathbb{R}^n$ *is the convex hull of* $d+1$ *affinely independent points in* $\mathbb{R}^n$.

Definition 2.6. *A* ***triangulation*** $\mathcal{T}$ *of a full dimensional polytope* $\mathcal{P}$ *in* $\mathbb{R}^n$ *is a collection of* n*-simplices whose vertices are vertices of the polytope and that satisfies the following two properties:*

(UP)
$$\bigcup_{\Delta \in \mathcal{T}} \Delta = \mathcal{P}$$

(IP) *Given* $\Delta_1, \Delta_2 \in \mathcal{T}, \Delta_1 \cap \Delta_2$ *is a common face (possibly empty)*

Definition 2.7. *A triangulation of an* n*-dimensional polytope in* $\mathbb{R}^n$ *is* ***unimodular*** *if all its* n*-simplices are translations of linear transformations of the standard simplex* $conv\{0, e_1, ..., e_n\}$, *where the linear transformation's components are integers, and its determinant is* ± 1.

All n-simplices in a unimodular triangulation of a full dimensional lattice polytope in $\mathbb{R}^n$ have the same volume: $\frac{1}{n!}$. This is due to the fact that the determinant of the linear transformation is ± 1. For this reason, it becomes convenient to use the following term:

Definition 2.8. *The* ***normalized volume*** *of an* n*-simplex* Δ *in* $\mathbb{R}^n$ *is* $\frac{vol(\Delta)}{n!}$.

Accordingly, all n-simplices in a unimodular triangulation of an n-dimensional polytope in $\mathbb{R}^n$ have normalized volume one.

Definition 2.9. *Define the* ***adjacency matrix*** *of a multigraph* $G = (V, E)$ *where* $|V| = n$ *as the* $n \times n$ *matrix* (a_{ij}) *where* $a_{ij} = \begin{cases} 0 & i = j \\ \text{(edges between } v_i \text{ and } v_j) & i \neq j \end{cases}$.

3 Tight spans: How the Simplices "Fit Together"

Tight spans provide a convenient tool for studying the relationships between simplices in a triangulation.

Definition 3.1. *Define the* ***tight span*** *of a triangulation* $\mathcal{T} = \{\Delta_k\}_{k=1}^{n!}$ *of the* n*-cube as the simple graph with* $n!$ *vertices where vertex* i *and* j *share an edge if* Δ_i *and* Δ_j *share a facet.*

One can then use graph theory to identify properties of the tight span. These properties often translate to geometric properties of the traingulation. For example, the number of edges in the tight span quantifies the number of $(n-1)$-dimensional faces shared by two n-simplices in the triangulation. A cycle in the tight-span likewise identifies a geometric "cycle" of n-simplices, of sorts.

Firstly, we have the basic result that for each vertex v in the tight span, $\deg v \leq n+1$. This is because the vertex only has $n+1$ facets that could be shared with another simplex.

The lemma below aids in the proof that the number of edges in the tight span of unimodular triangulations of the n-cube is a function of n. A formula for this number is also found for arbitrary n.

Lemma 3.2. *Let* $\mathcal{T}$ *be a unimodular triangulation of* $[0,1]^n$*.* $\mathcal{T}$ *admits a unimodular triangulation of each of the cube's facets.*

Proof. This proof will show that, for each facet of $[0,1]^n$, there are $(n-1)!$ n-simplices in $\mathcal{T}$ with n vertices in the facet. For each of those n-simplices, take the $(n-1)$-simplex formed by the n vertices in the facet. Those $(n-1)$-simplices form a unimodular triangulation of the facet.

Without loss of generality, pick the facet $x_n = 0$. Assume there exist more than $(n-1)!$ n-simplices such that $x_n = 0$ for all vertices except one. Then, the simplices formed by disregarding the x_n-coordinate do not form a triangulation of $x_n = 0$ because there are too many of them, and thus they violate IP (Note: IP is defined in the definition of triangulation). Let $\Delta_{1,n}, \Delta_{2,n}$ be n-simplices that contain as facets "problematic " $(n-1)$-simplices $\Delta_{1,n-1}, \Delta_{2,n-1}$ in $x_n = 0$ that intersect in a face of dimension $n-1$. Pick $c = (c_1, ..., c_{n-1}, 0) = (c', 0) \in \mathbb{R}^n$ and $\epsilon > 0$ such that $B_\epsilon(c') = \{y \in \mathbb{R}^{n-1} : |y - c'| < \epsilon\}$ satisfies $\{(x,0) \in \mathbb{R}^{n-1} \times \mathbb{R} : x \in B_\epsilon(c')\} \subset \Delta_{1,n-1} \cap \Delta_{2,n-1}$. Then for $k > 0$ sufficiently small, the open prism $\mathcal{B}_{x',\epsilon,k} = \{(a,b) \in \mathbb{R}^{n-1} \times \mathbb{R} : a \in B_\epsilon(x'), b \in (0,k)\}$ is contained in the interior of $\Delta_{1,n} \cap \Delta_{2,n}$. So the common face is of dimension n, and this implies the contradiction that $\Delta_{1,n} = \Delta_{2,n}$.

Assume there are fewer than $(n-1)!$ such simplices. Then their corresponding $(n-1)$-simplices $\{\Delta_{k,n-1}\}$ violate (UP) for $x_n = 0$. By a similar manner, we can find an open prism such that $\mathcal{B}_{x,\epsilon,k} \subset [0,1]^n \cap (\cup_{\Delta \in \mathcal{T}} \Delta)^c$.

Given one of these $(n-1)!$ n-simplices Δ_n, the simplex formed by disregarding the x_n coordinate Δ_{n-1} must have volume $1/(n-1)!$, because $\text{vol}(\Delta_n) = \frac{1}{n}\text{vol}(\Delta_{n-1})$. □

Using this result, we prove the following theorem.

Theorem 3.3. *Let* $G = (V, E)$ *be a tight span of a unimodular triangulation of* $[0,1]^n$*.* $|E| = (n-1)!\binom{n}{2}$*.*

Proof. Each of the $n!$ simplices in the triangulation has $n+1$ facets of dimension $n-1$. Using the lemma, there are precisely $(n-1)!(2n)$ facets of dimension $n-1$ that are on the boundary of the cube, namely $(n-1)!$ for each of the $2n$ facets. The rest of the facets are common faces of two neighboring simplices. Thus, accounting for the fact that these facets are counted twice, we have:

$$\frac{(n!)(n+1)-(n-1)(2n)}{2} = (n-1)!\binom{n}{2}. \tag{1}$$

□

For all regular, unimodular triangulations of the 4-cube, the number of shared 2-faces and 1-faces is constant, as shown by Huggins et al. [2]. Moreover, these numbers match the number of 2- and 3-cells in the tight span examples provided by the same authors. Accordingly, we propose the following conjecture:

Conjecture 3.4. *The number of shared $n-k$ faces in a unimodular triangulation of the n-cube is a function of n and k, and each shared $n-k$ face corresponds to a k-cell in the tight span.*

This pattern might not hold in higher dimensions. Note that although these "shared faces" appear in multiple simplices, they are only counted once.

4 Which Simplices Can Be Used?

4.1 Multigraphs and Equivalence Under Symmetry

We know that the simplices used in unimodular triangulations of the n-cube have volume $1/n!$, but is it true that all n-simplices of such volume with vertices in $[0,1]^n \cap \mathbb{Z}^n$ are elements of at least one unimodular triangulation? For now, we stick to studying the set of n-simplices of such volume with vertices in $[0,1]^n \cap \mathbb{Z}^n$, assuming that such results will be relevant to unimodular triangulations.

Many of the simplices used in triangulations of the n-cube are identical up to symmetries of the cube. That is, one can use a composition of translations, reflections and rotations to get from one to another. Thus, it is convenient to find a representation of the simplices that respects this equivalence. Such a representation is defined below using a multigraph.

Definition 4.1. *Let x, y be elements of $[0,1]^n \cap \mathbb{Z}^n$. Define the* ***taxi-cab distance*** *of x, y as the minimum number of standard basis vectors that must be added to or subtracted from x to get y.*

Definition 4.2. *Given a polytope $\mathcal{P} = conv(x_1, ..., x_d)$ in $[0,1]^n \cap \mathbb{Z}^n$, define its* ***multigraph*** *$G = (V, E)$ as the multigraph with d vertices $v_1, ..., v_d$, where the number of edges between v_i and v_j is equal to the taxi-cab distance between x_i and x_j. Define the* ***characteristic polynomial*** *(resp.* ***eigenvalues****) of the polytope as the characteristic polynomial (resp. eigenvalues) of the adjacency matrix of its multigraph.*

Note: A key observation about polytopes with vertices in the unit n-cube is that the taxi-cab distance between two of such a polytope's vertices is equal to the square of their Euclidean distance. Such an observation is important in the case that this representation be generalized to polytopes with vertices not in the unit cube.

Because the operations that constitute our definition of symmetry—namely translation, reflection, and rotation—preserve distance, we have the following proposition and corollary:

Proposition 4.3. *Two polytopes are the same under symmetry if and only if their multigraphs are the same up to labeling of vertices.*

Corollary 4.3.1. *Given two polytopes in $[0,1]^n \cap \mathbb{Z}^n$, if their eigenvalues (resp. characteristic polynomial) are distinct, then they are not symmetries of each other.*

4.2 Multigraph Properties

This correspondence between polytopes in the n-cube and graph theory allows one to study the polytopes through their associated graphs. In higher dimensions, these tools become quite handy.

Notice that given a multigraph of a n-simplex, the multigraphs of its facets are given by its subgraphs with n vertices. Likewise, the multigraphs of the simplex's $(n-p)$-dimensional faces is given by its $(n-p+1)$-subgraphs. This relationship makes an interesting appearance in the characteristic polynomial of the multigraph.

Theorem 4.4. *Let Δ be an n-lattice simplex in $[0,1]^n$ with adjacency matrix A and characteristic polynomial $(-1)^{n+1}\lambda^{n+1} + k_n\lambda^n + ... + k_1\lambda + k_0$. Let $\mathcal{F} = \{f\}$ be the set of faces of Δ of dimension $\leq n-1$, and $\mathcal{F} = \mathcal{F}_{-1} \cup \mathcal{F}_0 \cup ... \cup \mathcal{F}_{n-1}$ partition the faces of $\mathcal{F}$ by dimension, with $\mathcal{F}_{-1}$ consisting only of the empty set. Then,*

$$\begin{aligned} k_0 &= \det A \\ -k_1 &= \sum_{f \in \mathcal{F}_{n-1}} \det A_f \\ &... \\ (-1)^q k_q &= \sum_{f \in \mathcal{F}_{n-q}} \det A_f \\ &... \\ k_n &= 0. \end{aligned} \tag{2}$$

Proof. Let A be the adjacency matrix of G, and let $A - \lambda I = (a_{ij})$. The characteristic polynomial of G is $p_G(\lambda) = \det(A - \lambda I) = \sum_{\sigma \in S_{n+1}} (-1)^\sigma a_{1\sigma(1)} ... a_{(n+1)\sigma(n+1)}$, where S_{n+1} is the symmetric group on $n+1$ elements, and $(-1)^\sigma := \begin{cases} 1 & \sigma \text{ is even} \\ -1 & \sigma \text{ is odd} \end{cases}$.

The coefficient k_n is the sum of terms that satisfy the condition that σ maps all elements except one to itself. But there are no such terms, since such maps do not exist in S_{n+1}.

The coefficient k_1 is the sum of terms that satisfy the condition that σ maps one and only one element to itself. Call the set of such permutations, where k is that element, $S_{n+1,k}$, and let

$\{A_{n-1,k}\}_{k=1}^{n+1}$ be the adjacency matrices of the $(n-1)$-dimensional faces. Then,

$$\begin{aligned}
k_1\lambda &= \sum_{k=1}^{n+1} \sum_{\sigma \in S_{n+1,k}} (-1)^\sigma a_{1\sigma(1)} \ldots a_{(n+1)\sigma(n+1)} \\
&= -\lambda \sum_{k=1}^{n+1} \sum_{\sigma \in S_{n+1,k}} (-1)^\sigma a_{1\sigma(1)} \ldots a_{(k-1)\sigma(k-1)} a_{(k+1)\sigma(k+1)} \ldots a_{(n+1)\sigma(n+1)} \\
&= -\lambda \sum_{k=1}^{n+1} \det A_{n-1,k}.
\end{aligned}$$

The proof for general q is similar: take the subset of S_{n+1} that maps q and only q elements to themselves, and partition that subset into subsets that map elements corresponding to non-vertices of the subgraph of a face to themselves. Then, factor out q copies of $-\lambda$, and recognize that the second sums correspond to determinants of A_{n-q}. Likewise, k_0 is obtained from permutations that map no elements to themselves, which is equal to the determinant of A since A has zeros along the diagonal. □

In a similar manner, we find a formula for the characteristic polynomial of a simplex in terms of the characteristic polynomials of its faces of smaller dimension.

Theorem 4.5. *Let Δ be an n-lattice simplex in $[0,1]^n$, and let $\mathcal{F} = \{f\}$ be the set of faces of Δ of dimension $\leq n-1$, including the empty set, which we assign the trivial dimension -1 and polynomial $p_\emptyset = 1$. Let A_Δ be the adjacency matrix of Δ. Then,*

$$p_\Delta(\lambda) = \det A_\Delta - \sum_{f \in \mathcal{F}} \lambda^{n-\dim f} p_f(\lambda) \tag{3}$$

Proof. Expressed differently, the earlier theorem states

$$p_\Delta(\lambda) = \sum_{q=0}^{n+1} (-1)^q \left(\sum_{f \in \mathcal{F}_{n-q}} \det A_f \right) \lambda^q.$$

Fix q. For all $f \in \mathcal{F}_{n-q}$, $\det A_f$ is counted (with sign):

$$\begin{array}{llll}
\binom{q}{q} \text{ time in} & (-1)^q p_\Delta(\lambda) & \text{as the coefficient of } \lambda^q \\
\ldots & \ldots & \ldots \\
\binom{q}{q-k} & (-1)^{q-k} \sum_{f \in \mathcal{F}_{n-k}} p_f(\lambda) & \lambda^{q-k} \\
\ldots & \ldots & \ldots \\
\binom{q}{0} & (-1)^0 \sum_{f \in \mathcal{F}_{n-q}} p_f(\lambda) & \lambda^0 \\
0 & (-1)^0 \sum_{\substack{f \in \mathcal{F}_{n-g} \\ g > q}} p_f(\lambda) & NA.
\end{array}$$

Then in

$$\sum_{f\in\mathcal{F}} p_f(\lambda)\lambda^{n-\dim f} = \lambda^{n+1}\left(\sum_{f\in\mathcal{F}_{-1}} p_f(\lambda)\right) + ... + \lambda\left(\sum_{f\in\mathcal{F}_{n-1}} p_f(\lambda)\right),$$

$\det A_f$ is counted (with sign) $\sum_{k=1}^{q}(-1)^{q-k}\binom{q}{q-k} = (-1)^{q+1}$ times as a coefficient of λ^q. The same can be said of $\sum_{f\in\mathcal{F}_{n-q}} \det A_f$. Furthermore, observe that $(-1)^{q+1}\sum_{f\in\mathcal{F}_{n-q}} \det A_f$ is the entire coefficient of λ^q, because for $g \in \mathcal{F}_{n-p}$ where $p \neq q$, $\det A_g$ is in the sum that is the coefficient of λ^p. As for the trivial cases, a single vertex v satisfies $\det A_v = 0$, and $\det A_\emptyset = 1$.

Thus, $\det A_\Delta - \sum_{f\in\mathcal{F}} p_f(\lambda)\lambda^{n-\dim f}$ is a polynomial in λ with $(-1)^q\sum_{f\in\mathcal{F}_{n-q}} \det A_f$ the coefficient of λ^q, for $q = 1, ..., n+1$, and $\det A_\Delta$ the sole constant term. By the earlier theorem, this is equal to $p_\Delta(\lambda)$. □

Moreover, analysis of the polynomial yields insight into other features of simplices of normalized volume, deliberated in the following subsection.

4.3 Multigraph Constraint for the Simplices

One significant open question is how many n-lattice simplices are possible in a unimodular triangulation of the n-cube, modulo equivalence under symmetry? One can answer this question by enumerating the possible $(n+1)\times(n+1)$ adjacency matrices, or identifying constraints on these matrices. Analysis of the characteristic polynomial suggests that $k_0 = \det A$ is a function of n, giving one such constraint. We have the following conjecture.

Conjecture 4.6. *Let $\mathcal{M}_n$ denote the set of all multigraphs on $n+1$ vertices of polytopes in the n-cube. There is a one-to-one correspondence between n-simplices in the n-cube with volume $1/n!$, unique under symmetry, and*

$$\{m \in \mathcal{M}_n : \det A_m = (-1)^n 2^{n-1} n\}. \tag{4}$$

The conjecture was checked for $n \leq 3$ and for several cases where $n = 4$, including in the non-regular triangulation given by de Loera [5]. This criterion provides a tighter bound for the number of "nice" simplices. For example, when $n = 3$, there are 6 multigraphs corresponding to lattice polytopes in the 3-cube, and only 3 that satisfy the property. Those satisfying the property are precisely the set of "nice" simplices.

We develop a criterion for proving this conjecture. Firstly, we note the relationship between the Cayley-Menger determinant and volume.

Definition 4.7. *Given an n-simplex Δ given by $n+1$ vectors $\{v_1, ..., v_{n+1}\}$ in $\mathbb{R}^n$, let $D :=$*

$$\det\begin{pmatrix} 0 & d(v_1,v_2)^2 & d(v_1,v_3)^2 & ... & d(v_1,v_{n+1})^2 \\ d(v_2,v_1)^2 & 0 & d(v_2,v_3)^2 & ... & d(v_2,v_{n+1})^2 \\ d(v_3,v_1)^2 & d(v_3,v_2)^2 & 0 & ... & d(v_3,v_{n+1})^2 \\ ... & ... & ... & ... & ... \\ d(v_{n+1},v_1)^2 & d(v_{n+1},v_2)^2 & ... & d(v_{n+1},v_n)^2 & 0 \end{pmatrix},$$

*where d is the Euclidean distance. Define the **Cayley-Menger determinant** as*

$$\det\begin{pmatrix} 0 & 1 \\ 1 & D \end{pmatrix}.$$

It is known that

$$\det \begin{pmatrix} 0 & 1 \\ 1 & D \end{pmatrix} = (-1)^{n+1} 2^n (n!) \mathrm{vol}_n(\Delta). \tag{5}$$

Observe that if Δ is an n-lattice simplex in the n-cube of normalized volume 1, and A is its adjacency matrix, then

$$\det \begin{pmatrix} 0 & 1 \\ 1 & D \end{pmatrix} = \det \begin{pmatrix} 0 & 1 \\ 1 & A \end{pmatrix} = (-1)^{n+1} 2^n. \tag{6}$$

Having noticed that this determinant is a function of n, one is faced with the problem of proving $\det A$ is a function of n.

The following identity of Silvester leads us further. If A, B, C, D are matrices with D invertible, it is known that $\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A - BD^{-1}C) \det D$ [6]. Applied in our case, if $A^{-1} = (b_{ij})$:

$$(-1)^{n+1} 2^n = \det \begin{pmatrix} 0 & 1 \\ 1 & A \end{pmatrix} = -\left(\sum_{i,j=1,\dots,n+1} b_{ij} \right) \det A. \tag{7}$$

This gives us the proposition:

Proposition 4.8. *To prove the conjecture, it suffices to show that for any adjacency matrix A of an n-lattice simplex in $[0,1]^n$ with $A^{-1} = (b_{ij})$, the simplex is of volume $1/n!$ if and only if*

$$-\left(\sum_{i,j=1,\dots,n+1} b_{ij} \right) = 2/n. \tag{8}$$

Thus, the conjecture motivates the study of other properties of this representation. For instance, the better one understands the inverse of the adjacency matrix, the closer one comes to proving the conjecture.

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