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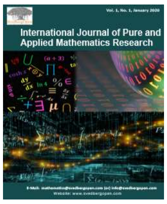

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Coordinate Permutation-Invariant Unit N-Simplexes in $\mathbb{R}^N$

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Abstract

A unit N-simplex is a regular N-dimensional simplex whose $N+1$ vertices lie on the unit sphere in $\mathbb{R}^N$. The equidistant vertices are spread evenly over the sphere, and thus are useful in applications that require a representative sample of points on a sphere (such as N-dimensional integration). It is always possible to choose coordinate axes such that the set of vertices is invariant under all permutations of the coordinates. This paper gives two different mathematical constructions of coordinate permutation invariant unit N-simplexes in N-dimensional space. The first construction method involves translation followed by rotation in $N+1$-dimensional space, while the second requires only a single translation in N-dimensional space. The development of these constructions will begin with a unit 2-simplex (i.e., equilateral triangle) in $\mathbb{R}^2$, with visualizations in GeoGebra. These arguments are then generalized to the N-dimensional case for any integer $N \geq 2$. The constructions also provide a simple derivation for the formula for the length of the edges of a unit N-simplex, from which may be derived the angle between any two vertex vectors. These constructions and their applications involve an interesting mixture of geometry, algebra, and analysis. The GeoGebra visualizations for 2- and 3-dimensional simplexes are available online. For readers who want to cut to the chase, formulas for unit N-simplex vertices and edge lengths are summarized in the last section.

Keywords: *Simplex, Permutation, Coordinates, Invariance, Numerical integration, GeoGebra*

1. Definition and Examples of N-Simplexes

In mathematics, a simplex is a multidimensional generalization of a triangle. For example, a 2-simplex in $\mathbb{R}^2$ is a triangle and a 3-simplex in $\mathbb{R}^3$ is a tetrahedron.

A simplex is characterized by its vertices. For example, a 2-dimensional simplex (i.e., triangle) has three vertices. The line segments joining these vertices are the edges of the simplex. The simplex also has an interior, defined mathematically as the set of convex combinations of the vertices. In this paper, only the vertices and edges will be considered.

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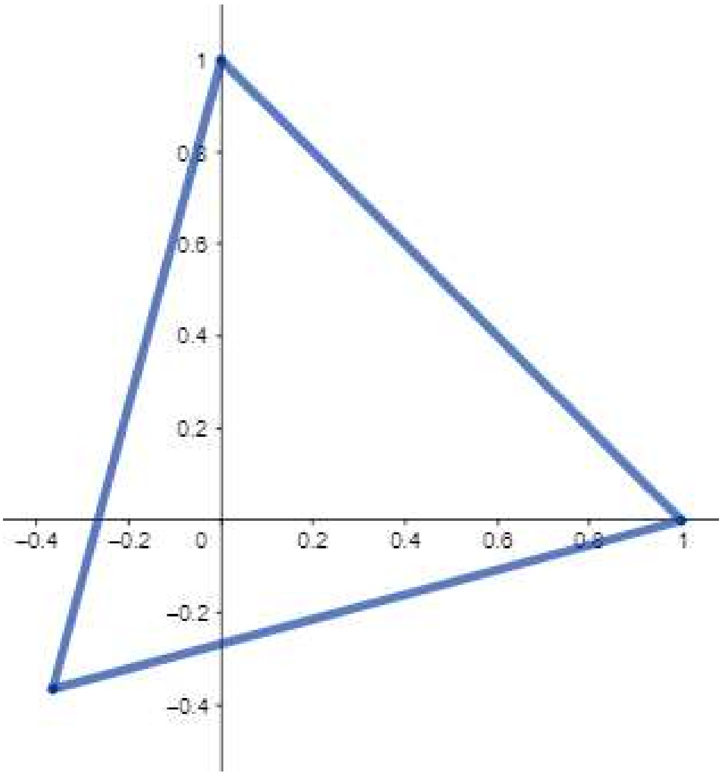

Figure 1: A 2-Simplex in R2. A GeoGebra Construction Can be Found at Anderson (2015)

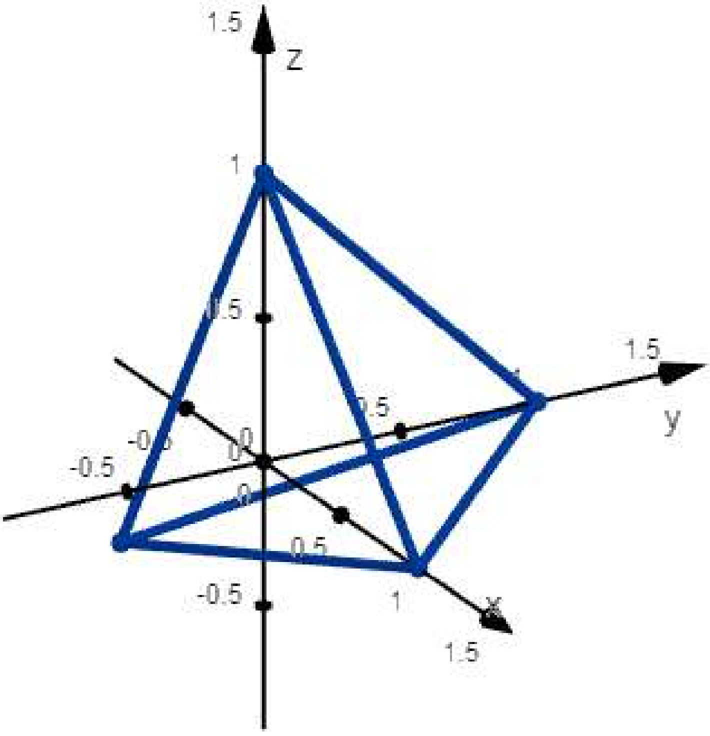

Figure 2: A 3-Simplex in R3. A GeoGebra Construction Can be Found at Anderson (2015)

In general, any three points in two or more dimensions will form a simplex, unless they are collinear. Similarly, any four points in will form a three dimensional simplex for three or more dimensions, unless they are coplanar. The same concept holds for $N+1$ points in N or more dimensions.

2. Applications of Simplexes

Simplexes have many uses in theoretical and computational mathematics. In the field of computer graphics, simplexes have aided in visualization algorithms for studying data. This has allowed for smoother animation, even in dimensions higher than three (Bhaniramka *et al.*, 2000). Simplexes have also been utilized to extend computer graphics in a domain with a higher dimension for scientific visualization problems (Hanson, 1994).

In general, simplexes can be used to divide up arbitrary polytopes (i.e., N-dimensional objects with flat sides). This process is called *triangulation*. Triangulations are important in representing complicated geometry by piecewise simple geometry (Lee and Santos, 2017). In particular, simplexes are often used in the Finite Element Method (FEM), which computes numerical solutions to partial differential equations in complicated regions. FEM works by breaking the region up into small geometrical "elements", and then piecing back together the solutions found for individual elements. Quite often, the elements used in FEM are simplexes (Hecht, 2021).

Another application of simplexes is the Nelder-Mead Simplex algorithm. This algorithm utilizes a moving N-simplex to perform a direct search method for the user to find the minimum or maximum of a function of N variables (Olsson and Nelson, 2012).

Simplexes have even been found to be useful in the medical field. In the structural connectivity of the nervous system within the brain, there are higher-order simplicial complexes located in the core network around hubs. A simplicial complex is a collection of simplexes of various dimensions (Friedman, 2012). The discovery of these sets of simplexes may help in learning the complex, higher-order neural connections in in the brain (Andjelkovic *et al.*, 2020).

In this paper, the primarily interest is in regular simplexes inscribed in the unit sphere. Such simplexes are useful in numerical integration in higher dimensions, in case where the function to be integrated is spherically symmetric (Wang *et al.*, 2014) (in fact, this was the original motivation for this research).

3. Regular and Standard Simplexes

A regular simplex is a simplex with all edges having the same length. For example, an equilateral triangle is a regular 2-simplex. For higher dimensions, a N-simplex consists of $N + 1$ vertices joined by edges such that every vertex is the same distance from every other vertex.

Consider for instance the standard basis vectors $\vec{e}_1 = [1,0,0]$, $\vec{e}_2 = [0,1,0]$, and $\vec{e}_3 = [0,0,1]$ in $\mathbb{R}^3$. The distance between any two basis vectors (i.e., length of an edge) is always $\sqrt{2}$. It follows that these unit vectors form a regular 2-simplex. This will be referred to as the *standard 2-simplex*. In general, the standard N-simplex is created by taking the standard basis vectors in $\mathbb{R}^{N+1}$. For any $N \geq 2$, the length of any edge of a standard N-simplex is always $\sqrt{2}$.

4. Coordinate Permutation Symmetry of Sets in $\mathbb{R}^N$

It is visually evident that standard 2- and 3-simplexes are highly symmetrical objects. In mathematics, symmetries are always associated with groups. In this section, one group associated with the symmetries of the standard N-simplex will be discussed. This group is the group of *permutations*.[1]

Intuitively, a permutation of a set is a rearrangement of the elements of the set. Permutations are usually denoted by Greek letters ϕ (phi), σ (sigma), μ (mu), etc. The primary focus about permutations will be on S_N, which is the set of all permutations on the set $\{1, ..., N\}$. Mathematically speaking, an element of S_N is a bijection from $\{1, ..., N\} \to \{1, ..., N\}$. For example, consider the permutation $1 \to 3, 3 \to 5, 5 \to 7, 7 \to 1$ in S_7. This permutation rearranges $\{1, ..., 7\}$ to $\{3, 2, 5, 4, 7, 6, 1\}$.

The set S_N of all permutations on the set $\{1, ..., N\}$ is a group, where the group operation corresponds to composition of permutations. Recall that the conditions of a group operation are that it must be closed and associative, there must be an identity element, and every element must have an inverse. It would be a good idea at this point to convince (or remind) yourself that composition of permutations satisfies these properties.[2]

---

[1] It just so happens that the group of permutations is of fundamental importance in group theory. In fact, it turns out that via a simple relabeling of elements it is possible to turn every finite group into a subgroup of a permutation group. This fantastic result is called *Cayley's Theorem* (see Chapter 17 of Hill and Thron, 2021).

[2] For an elementary reference on permutations and groups, including definitions, examples, and properties, see Chapters 11-12 of Hill and Thron (2021).

S_N was described as the set of rearrangements of the numbers {1, ..., N}, but the same rearrangements may be applied to any set of N objects. For example, given 15 billiard balls numbered 1-15 placed in a row, then any permutation in S_N produces a corresponding rearrangement of the balls. This is one example of permutations in *acting* on a set (in this case, the set of billiard balls).[3]

In this paper, S_N will be acting on vectors in $\mathbb{R}^N$ by rearranging the coordinates. In other words, when a permutation in S_N is applied to a vector in $\mathbb{R}^N$, it produces a rearranged vector. For example, when the permutation $1 \to 3$, $2 \to 2$, $3 \to 1$ is applied to the coordinates of the vector [5, 12, 13], the resulting vector is [13, 12, 5]. Visually, this is like plotting the same vector in x, y, z space but with the x and z axes interchanged.

More generally, let ϕ be a permutation on {1, ..., N}. Define the *action* of ϕ on a point $\vec{x} = [x_1, ..., x_N]$ in $\mathbb{R}^N$ by $\phi([x_1, ..., x_N]) = [x_{\phi(1)}, ..., x_{\phi(N)}]$.

This idea of permutation action can be extended so that it also applies to sets of vectors, not just individual vectors. For example, let ϕ be the permutation $1 \to 3$, $2 \to 1$, $3 \to 2$ in S_3. Then ϕ acts on the set {[1, 2, 3], [4, 5, 6], [7, 8, 9]} by acting on each vector in the set. This produces a new set of vectors:

$$\{\phi([1,2,3]), \phi([4,5,6]), \phi([7,8,9])\} = \{[3,1,2], [6,4,5], [9,7,8]\}$$

A *transposition* is a permutation that only interchanges two numbers. One example in S_5 would be the function that takes $1 \to 4$ and $4 \to 1$, and leaves 2, 3, and 5 unchanged. If the transposition is applied to vectors in $\mathbb{R}^N$, then two of the coordinates would be exchanged. Consider, for example, the set of vectors $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ in $\mathbb{R}^3$, which are the vertices of the standard simplex in three dimensions. Interchanging any two coordinates of any vertex of the simplex maps back to another vertex in the set. It is not hard to see that the same thing will be true for the standard simplex in any dimension. Therefore, transposition of coordinates for a standard N-simplex preserves the simplex. Another way of saying this is that the simplex is *invariant* under interchange of coordinates.

This algebraic operation of switching coordinates also has a geometrical interpretation. Switching coordinates and affects only the m^{th} and n^{th} vertex of the standard simplex. All the other vertices have the same m- and n-coordinates, so switching them does not do anything. The conclusion is that the algebraic operation of exchanging the coordinates m and n is equivalent to the geometric operation of reflecting the simplex. This can also be generalized for higher-dimensional standard simplexes as well.

It is a fact that all permutations are expressible as a composition of transpositions (Section 11.6, Hill and Thron, 2012). Thus applying any permutation to the coordinates of the vertices of the standard simplex will result in exactly the same simplex. It can be summarized by saying that the standard simplex is *invariant under coordinate permutations*. This is a very useful property for many applications. However, the standard N-simplex also has some drawbacks. First of all, although the standard N-simplex has N+1 points, it is really a N-dimensional object (e.g., the 2-simplex is 2-dimensional, even though it has 3 points). So the standard N-simplex is a representation in a higher dimension than necessary. The other disadvantage is that the standard N-simplex is not centered at $\vec{0}$. If the standard simplex is moved to the origin, then all vertices of the simplex will lie on a single sphere centered at $\vec{0}$, which is a useful property. This is the motivation to find a way to "move" the standard simplex into a lower dimension and re-center it, without destroying the symmetry under coordinate permutations.

For the succeeding discussion, the following three key facts about how permutations act on vectors and sets of vectors in $\mathbb{R}^N$ are essential:

Fact A: *Permutations act linearly on vectors in* $\mathbb{R}^N$. Mathematically, this can written this as:

$$\phi(b \cdot \vec{v} + c \cdot \vec{w}) = b \cdot \phi(\vec{v}) + c \cdot \phi(\vec{w})$$

for any $\phi \in S_N$, real numbers b and c, and vectors $\vec{v}$, $\vec{w} \in \mathbb{Z}^N$. In particular, if $\vec{w} = \vec{1}$ (the vector consisting of N 1's), then $\phi(c \cdot \vec{w}) = c \cdot \vec{w}$.

[3] The fact that groups act on sets has profound and far-reaching consequences. For example, most of modern physics is built on this simple fact. For an introduction to group actions in general, as well as some beautiful examples of applications, see Chapter 17, Hill and Thron (2017).

Fact B: *Adding* $c \cdot \vec{1}$ *to every vector in a permutation-invariant set gives another set that is still permutation-invariant.* For example, the set $\left\{\vec{e}_1 - \frac{1}{3}\vec{1}, \vec{e}_2 - \frac{1}{3}\vec{1}, \vec{e}_3 - \frac{1}{3}\vec{1}\right\} = \left\{\left[\frac{2}{3}, \frac{-1}{3}, \frac{-1}{3}\right], \left[\frac{-1}{3}, \frac{2}{3}, \frac{-1}{3}\right], \left[\frac{-1}{3}, \frac{-1}{3}, \frac{2}{3}\right]\right\}$ is still invariant under coordinate permutations.

Fact B follows directly from Fact A as follows. Given $\{\vec{v}_1, \vec{v}_2, ..., \vec{v}_k\} \subset \mathbb{R}^N$ and any permutation $\phi \in S_N$:

$$\phi\left(\vec{v}_k + c \cdot \vec{1}\right) = \phi\left(\vec{v}_k\right) + \phi\left(c \cdot \vec{1}\right)$$

$$= \phi\left(\vec{v}_k\right) + c \cdot \vec{1}$$

Fact C: *The union of any two permutation-invariant subsets of* $\mathbb{R}^N$ *is also a permutation-invariant subset.* The proof of this is left as an exercise for the reader.

In the following, two different ways to construct *N*-simplexes in *N*-dimensional space that are symmetric under coordinate permutations and centered at the origin are demonstrated. These simplexes will then be rescaled so they can be inscribed in the unit *N*-sphere and will be referred to as unit *N*-simplexes. In order to better visualize the process, standard 2-simplexes in three dimensions will be constructed first. The same procedure can then be applied to arbitrary *N*-simplexes in $N+1$ dimensions.

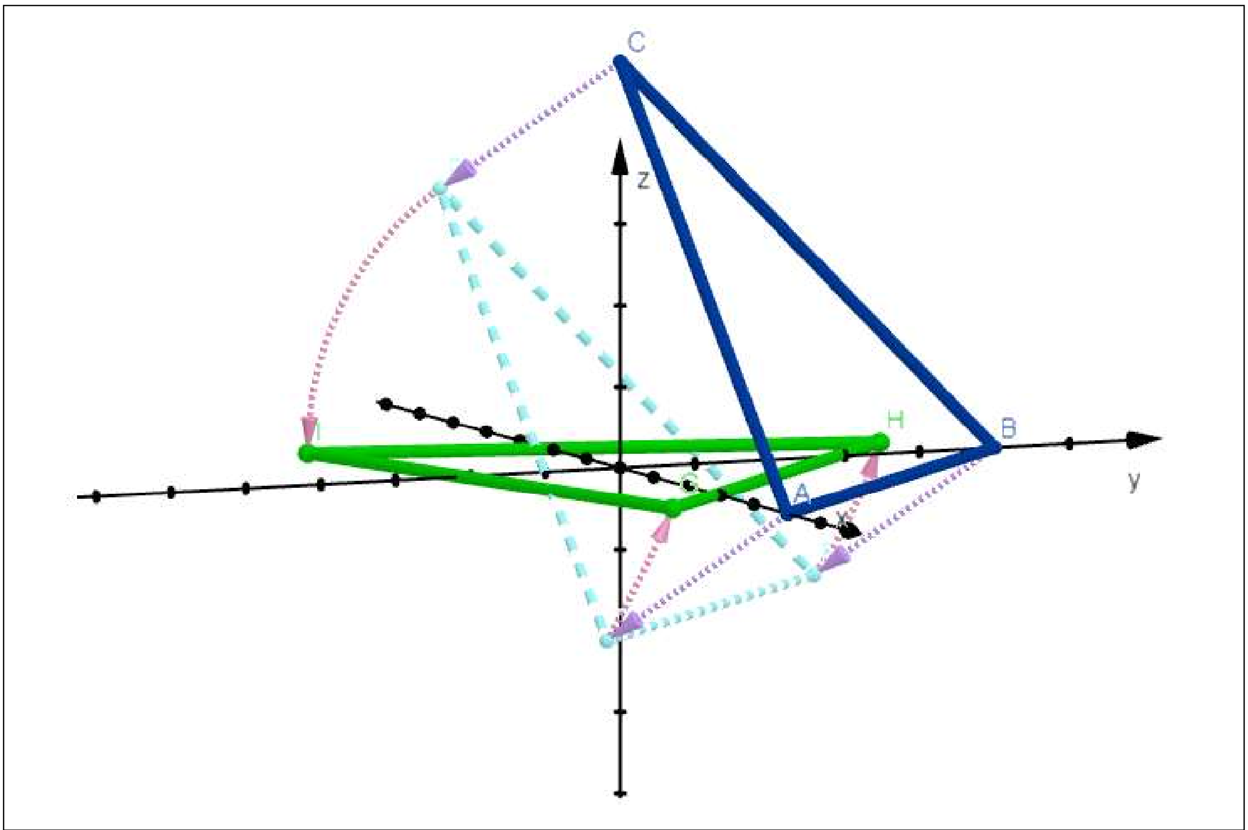

Figure 3: Translation and Rotation of 2-Simplex. A Rotatable GeoGebra Construction Can be Found at Anderson (2015)

5. Construction of a Permutation-Symmetric 2-Simplex Using Rotation and Translation in $\mathbb{R}^3$

The standard basis vectors $\vec{e}_1, \vec{e}_2$, and $\vec{e}_3$ form a 2-dimensional simplex in $\mathbb{R}^3$. The centroid can be calculated as the average of these three: $\frac{1}{3}\left(\vec{e}_1 + \vec{e}_2 + \vec{e}_3\right) = \frac{1}{3} \cdot \vec{1}$.

The centroid is then translated to the origin, which is achieved by the transformation $\vec{x} \to \vec{x} - \frac{1}{3} \cdot \vec{1}$. Applying the same transformation to the vertices yields the new vertices:

$$\vec{u}_1 = \vec{e}_1 - \frac{1}{3}\cdot\vec{1} = \left[\frac{2}{3} - \frac{1}{3} - \frac{1}{3}\right]$$

$$\vec{u}_2 = \vec{e}_2 - \frac{1}{3}\cdot\vec{1} = \left[-\frac{1}{3}, \frac{2}{3} - \frac{1}{3}\right]$$

$$\vec{u}_3 = \vec{e}_3 - \frac{1}{3}\cdot\vec{1} = \left[-\frac{1}{3} - \frac{1}{3}, \frac{2}{3}\right] \quad ...(1)$$

Note that the vectors $\vec{u}_1$, $\vec{u}_2$ and $\vec{u}_3$ are coordinate permutation invariant. This follows directly from **Fact B** in the previous section.

The 2-simplex now lies in the plane $x_1 + x_2 + x_3 = 0$. The vector $\vec{1} = [1, 1, 1]$ is perpendicular to the 2 dimensional simplex that is now centered at the origin. This perpendicular vector, $\vec{1}$, and the vector $\vec{e}_3$ are coplanar. To rotate the simplex into $\mathbb{R}^2$, the vector $\vec{1}$ must be rotated into $\vec{e}_3$. This corresponds to a rotation in the plane containing the two vectors $\vec{1}$ and $\vec{e}_3$.

At this point, whether or not this rotation preserves the coordinate permutation symmetry in $\mathbb{R}^2$ should be investigated further. The algebraic proof is given in Section 7, but for now an intuitive geometrical argument will be provided. The rotation that is being used is defined in terms of the two vectors $\vec{1}$ and $\vec{e}_3$. These vectors both lie in the plane $x_1 = x_2$. So if the x_1 and x_2 axes are exchanged, there is no effect on any of the points in the plane, or on the rotation of the vectors in the plane. On the other hand, any vector that is perpendicular to the plane $x_1 = x_2$ is not affected by the rotation. Therefore, it makes no difference whether a perpendicular vector is reflected before or after the rotation: the outcome is the same. Since every vector in $\mathbb{R}^3$ can be written as a vector in the plane plus a perpendicular vector, it follows that the reflection can come first followed by the rotation, or vice versa: the result remains the same. Since the original (unrotated) simplex is not changed by the reflection $x_1 = x_2$, it follows that the rotated simplex is similarly unchanged. This gives the sought after coordinate permutation symmetry.

To find the equations for this rotation, an orthogonal basis for the plane $x_1 = x_2$ is needed. By looking at the dot product, it is observed that $[1, 1, 0] = \vec{1} - \vec{e}_3$ is orthogonal to $\vec{e}_3$. Thus the two vectors $\vec{w}_1 = \vec{e}_3$ and $\vec{w}_2 = \frac{1}{\sqrt{2}}[1, 1, 0]$ produce the orthonormal basis.

Next, the angle of rotation, denoted by θ, needs to be characterized. This is just the angle between [1, 1, 1] and $\vec{w}_1$. From the dot product formula, $\cos(\theta) = \frac{1}{\sqrt{3}}$ is calculated, which implies that $\sin(\theta) = \sqrt{\frac{2}{3}}$.

The rotation of $\vec{w}_1$ and $\vec{w}_2$ through an angle θ produces the new vectors $\vec{w}_1{}' = -\sin(\theta)\vec{w}_2 + \cos(\theta)\vec{w}_1$ and $\vec{w}_2{}' = \cos(\theta)\vec{w}_2 + \sin(\theta)\vec{w}_1$. Substituting in the known angles produces: $\vec{w}_1{}' = -\sqrt{\frac{2}{3}}\vec{w}_2 + \frac{1}{\sqrt{3}}\vec{w}_1$ and $\vec{w}_2{}' = \frac{1}{\sqrt{3}}\vec{w}_2 + \sqrt{\frac{2}{3}}\vec{w}_1$. It follows that:

$$\vec{w}_1{}' = \frac{1}{\sqrt{3}}[-1, -1, 1]; \ \vec{w}_2{}' = \frac{1}{\sqrt{6}}[1, 1, 2]$$

The three vertices $\{\vec{u}_1, \vec{u}_2, \vec{u}_3\}$ may be rotated by finding their components along the two orthonormal vectors $\vec{w}_1$ and $\vec{w}_2$, and then replacing $\vec{w}_1$ and $\vec{w}_2$ with $\vec{w}_1{}'$ and $\vec{w}_2{}'$ respectively. We'll do $\vec{u}_1$ first. Projecting $\vec{u}_1$ onto $\vec{w}_1$ gives:

$$\vec{u}_1 = \left[\frac{2}{3}, -\frac{1}{3}, 0\right] - \frac{1}{3}\vec{w}_1$$

Projecting the result onto $\vec{w}_2$ gives:

$$\vec{u}_1 = \left[\frac{1}{2}, -\frac{1}{2}, 0\right] + \frac{\sqrt{2}}{6}\vec{w}_2 - \frac{1}{3}\vec{w}_1$$

One may easily double-check that the first vector on the right-hand side is perpendicular to the other two. Making the replacement $\vec{w}_j \to \vec{w}_j{}'$ for $j = 1, 2$, it is found that $\vec{u}_1$ rotates to $\vec{u}_1{}'$, where:

$$\vec{u}_1{}' = \left[\frac{1}{2}, -\frac{1}{2}, 0\right] + \frac{\sqrt{2}}{6}\vec{w}_2{}' - \frac{1}{3}\vec{w}_1{}' = \left[\frac{3+\sqrt{3}}{6}, \frac{-3+\sqrt{3}}{6}, 0\right] \quad ...(2)$$

In similar fashion, the other two vertices can be calculated:

$$\vec{u}_2{}' = \left[-\frac{1}{2}, \frac{1}{2}, 0\right] + \frac{\sqrt{2}}{6}\vec{w}_2{}' - \frac{1}{3}\vec{w}_1{}' = \left[\frac{-3+\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}, 0\right]$$

$$\vec{u}_3{}' = -\frac{\sqrt{2}}{3}\vec{w}_2{}' + \frac{2}{3}\vec{w}_1{}' = \left[-\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}, 0\right] \quad ...(3)$$

Thus, the three vertices of the 2-simplex in $\mathbb{R}^2$ are $\left[\frac{3+\sqrt{3}}{6}, \frac{-3+\sqrt{3}}{6}\right]$, $\left[\frac{-3+\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}\right]$ and $\left[-\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}\right]$.

The vertices can then be normalized so they lie on the unit sphere. This is achieved by dividing each vertex by its magnitude. For 2-simplexes, all three vertices have magnitude $\sqrt{\frac{2}{3}}$. So multiplying the vertices by $\sqrt{\frac{3}{2}}$ produces normalized vertices with magnitude 1:

$$\vec{v}_1 = \sqrt{\frac{3}{2}}\left[\frac{3+\sqrt{3}}{6}, \frac{-3+\sqrt{3}}{6}\right] = \left[\frac{\sqrt{6}+\sqrt{2}}{4}, \frac{-\sqrt{6}+\sqrt{2}}{4}\right]$$

$$\vec{v}_2 = \sqrt{\frac{3}{2}}\left[\frac{-3+\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}\right] = \left[\frac{-\sqrt{6}+\sqrt{2}}{4}, \frac{\sqrt{6}+\sqrt{2}}{4}\right]$$

$$\vec{v}_3 = \sqrt{\frac{3}{2}}\left[-\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}\right] = \left[-\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right] \quad ...(4)$$

At this point, it should be checked that the new simplex $\{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$ is still permutation invariant. It turns out IT IS, but the situation has changed a little bit. The simplex consists of two permutation-invariant sets instead of one: $\{\vec{v}_3\}$ by itself and $\{\vec{v}_1, \vec{v}_2\}$.

As a bonus, this construction gives a formula for the length of the edges of the simplex that is inscribed in the unit sphere. The edges of the standard simplex all have length $\sqrt{2}$, which follows directly from the Pythagorean theorem. This length does not change during translation or rotation, and is multiplied by $\sqrt{\frac{3}{2}}$ during the normalization of the vertices. Therefore, the length of the edges of the unit simplex in $\mathbb{R}^2$ is $\sqrt{\frac{3}{2}} \cdot \sqrt{2} = \sqrt{3}$. The angle α between vertex vectors can also be calculated:

$$\sin(\alpha/2) = \frac{\sqrt{3}}{2} \Rightarrow \alpha = \frac{2\pi}{3} \quad ...(5)$$

6. Creation of a Permutation-Symmetric 2-Simplex Using Translation in $\mathbb{R}^2$

It is also possible to construct a $\vec{0}$ -centered coordinate permutation symmetric 2-simplex directly in $\mathbb{R}^2$. First, notice that $\{\vec{e}_1, \vec{e}_2\}$ is a permutation invariant set in $\mathbb{R}^2$. How about the third vertex? It must be equally distant from $\vec{e}_1$ and $\vec{e}_2$, so it lies on the perpendicular bisector, which is the line $x_1 = x_2$. The third vertex thus has the form $[a, a]$, therefore only the value of a needs to be found. The distance between $\vec{e}_1$ and $\vec{e}_2$ is calculated to be $\sqrt{2}$. So the distance between $\vec{e}_2$ and $[a, a]$ must also be $\sqrt{2}$. Using the distance formula, it is found:

$$\sqrt{2}=\sqrt{a^2+(a-1)^2}\Rightarrow a=\frac{1\pm\sqrt{3}}{2} \qquad \text{...(6)}$$

The negative sign for a is chosen to obtain the correct orientation so as to more easily center the simplex at the origin (Figure 2).

Happily, the set $\{[a, a]\}$ is also permutation invariant. It follows from **Fact C** that $\{\vec{e}_1, \vec{e}_2, [a, a]\}$ is a permutation invariant set.

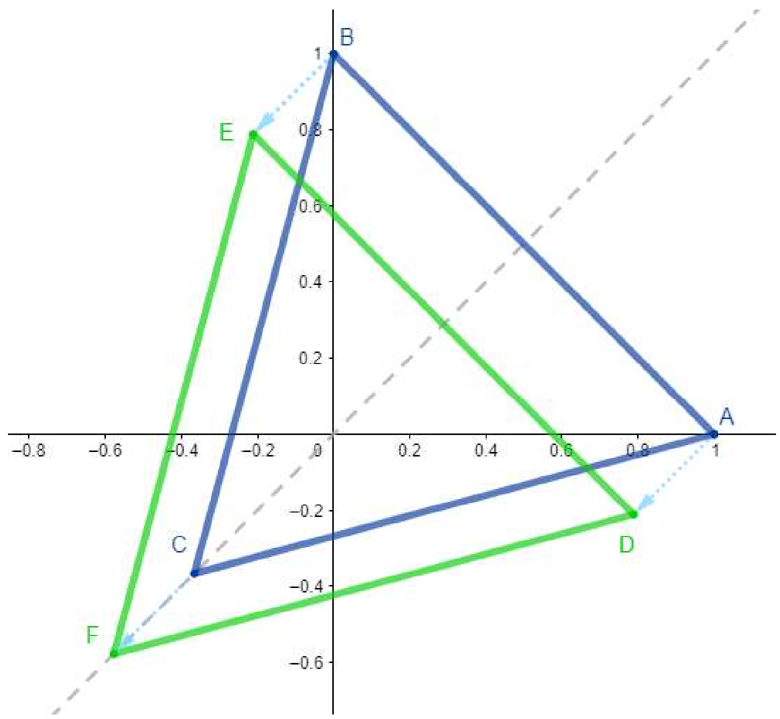

Figure 4: Creation of a Permutation-Symmetric 2-Simplex by Using Translationmethod. A GeoGebra Construction Can be Found at Anderson (2015)

Now this 2-simplex is translated so the centroid is at $\vec{0}$ by the transformation $\vec{x}\to\vec{x}-\vec{c}$, where $\vec{c}=\frac{1}{3}\left(\vec{e}_1+\vec{e}_2+[a, a]\right)=\left[\frac{3-\sqrt{3}}{6}, \frac{3-\sqrt{3}}{6}\right]$. Applying this transformation to the vertices gives the new vertices:

$$\vec{u}_1=\vec{e}_1-\vec{c}=\left[\frac{3+\sqrt{3}}{6}, \frac{-3+\sqrt{3}}{6}\right]$$

$$\vec{u}_2=\vec{e}_2-\vec{c}=\left[\frac{-3+\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}\right]$$

$$\vec{u}_3=\left[\frac{1-\sqrt{3}}{2}, \frac{1-\sqrt{3}}{2}\right]-\vec{c}=\left[-\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{3}\right] \qquad \text{...(7)}$$

These agree with $\vec{u}_1$, $\vec{u}_2$, $\vec{u}_3$ in Section [sec:2simRot]. So after normalization, the results are the same set of vectors $\{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$ as before.

7. Creation of a Permutation-Symmetric N-Simplex Using Translation and Rotation in $\mathbb{R}^{N+1}$

In this section, the construction in Section 5 will be generalized to construct a unit N-simplex in $\mathbb{R}^N$ centered at $\vec{0}$ by translating and rotating the standard N-simplex in N+1 dimensions.

In $N+1$ dimensions, the standard N-simplex has vertices $\{\vec{e}_1, \vec{e}_2, ..., \vec{e}_{N+1}\}$. As previously remarked, this is a permutation-invariant set. The centroid of this simplex is the average of these basis vectors:

$$Centroid = \frac{1}{N+1}\left[\vec{e}_1 + ... + \vec{e}_{N+1}\right] = \frac{1}{N+1}\vec{1} \quad ...(8)$$

As done previously the centroid is translated to the origin $\vec{0}$, using the transformation $\vec{x} \to \vec{x} - \frac{1}{N+1}\vec{1}$. Applying the same transformation to the vertices gives the new vertices:

$$\vec{u}_1 = \vec{e}_1 - \frac{1}{N+1}\vec{1} = \frac{1}{N+1}\left[N, -1, ..., -1\right]$$

$$\vec{u}_2 = \vec{e}_2 - \frac{1}{N+1}\vec{1} = \frac{1}{N+1}\left[-1, N, ..., -1\right]$$

$$\vdots$$

$$\vec{u}_{N+1} = \vec{e}_{N+1} - \frac{1}{N+1}\vec{1} = \frac{1}{N+1}\left[-1, ..., -1, N\right] \quad ...(9)$$

According to **Fact B**, these new vertices also form a coordinate permutation-invariant set.

Next, find a vector that is perpendicular to the N-dimensional simplex that is now centered at the origin. The N-simplex lies in the plane $x_1 + x_2 + ... + x_N = 0$, therefore the vector $\vec{1} = [1, 1, ..., 1]$ is perpendicular to a plane of the simplex. This perpendicular vector and the vector $\vec{e}_{N+1}$ lie in a plane. To rotate the simplex into $\mathbb{R}^N$, the vector $\vec{1}$ needs to be rotated so that it lies along $\vec{e}_{N+1}$. This corresponds to a rotation in the plane containing the two vectors. To find the equations for this rotation, an orthogonal basis for this plane is needed. $[1, ..., 1, 0] = \vec{1} - \vec{e}_{N+1}$ is orthogonal to $\vec{e}_{N+1}$ and also lies in the same plane. It follows that an orthonormal basis of the plane of rotation is:

$$\vec{w}_1 = \frac{1}{\sqrt{N}}\left[1, ..., 1, 0\right]$$

$$\vec{w}_2 = \vec{e}_{N+1} \quad ...(10)$$

Note also that both of these vectors are invariant under S_N acting on the first N coordinates.

The cosine of the angle between $\vec{1}$ and $\vec{w}_2$ is $\cos(\theta) = \frac{1}{\sqrt{N+1}}$, which implies that $\sin(\theta) = \sqrt{\frac{N}{N+1}}$.

The rotation of $\vec{w}_1$ and $\vec{w}_2$ through a counterclockwise angle θ produces the new vectors:

$$\vec{w}_1{}' = \cos(\theta)\vec{w}_1 + \sin(\theta)\vec{w}_2$$

$$\vec{w}_2{}' = -\sin(\theta)\vec{w}_2 + \cos(\theta)\vec{w}_1 \quad ...(11)$$

Substituting in the sine and cosine values gives:

$$\vec{w}_1{}' = \frac{1}{\sqrt{N+1}}\vec{w}_1 + \sqrt{\frac{N}{N+1}}\vec{w}_2 = \frac{1}{\sqrt{N(N+1)}}\left[1, ..., 1, N\right]$$

$$\vec{w}_2{}' = \sqrt{\frac{N}{N+1}}\vec{w}_1 + \frac{1}{\sqrt{N+1}}\vec{w}_2 = \frac{1}{\sqrt{N+1}}\left[-1, ..., -1, 1\right] \quad ...(12)$$

Now the N vertices, $\vec{u}_1, ..., \vec{u}_N$, are rotated by finding their components along the two orthonormal vectors $\vec{w}_1$ and $\vec{w}_2$, and replacing them with $\vec{w}_1{}'$ and $\vec{w}_2{}'$, respectively.

Let's begin with $\vec{u}_1 = \frac{1}{N+1}\left[N, -1, ..., -1\right]$, and write $\vec{u}_1$ as a linear combination of $\vec{w}_1$, $\vec{w}_2$, and a vector that is perpendicular to $\vec{w}_1$ and $\vec{w}_2$. Projecting $\vec{u}_1$ onto $\vec{w}_2$ gives:

$$\vec{u}_1 = \frac{1}{N+1}\left[N, -1, ..., -1, 0\right] - \frac{1}{N+1}\vec{w}_2 \qquad ...(13)$$

Projecting the result onto $\vec{w}_1$ gives:

$$\vec{u}_1 = \frac{1}{N}\left[N, -1, -1, ..., -1, 0\right] + \frac{1}{\sqrt{N}\left(N+1\right)}\vec{w}_1 - \frac{1}{N+1}\vec{w}_2$$

$$= \vec{e}_1 - \frac{1}{N}\left[1, ..., 1, 0\right] + \frac{1}{N+1}\left(\frac{\vec{w}_1}{\sqrt{N}} - \vec{w}_2\right) \qquad ...(14)$$

Since $\vec{w}_1$ and $\vec{w}_2$ rotate into $\vec{w}_1'$ and $\vec{w}_2'$, respectively, it follows that $\vec{u}_1$ rotates to $\vec{u}_1'$, where:

$$\vec{u}_1' = \vec{e}_1 - \frac{1}{N}\left[1, ..., 1, 0\right] + \frac{1}{N+1}\left(\frac{\vec{w}_1'}{\sqrt{N}} - \vec{w}_2'\right) \qquad ...(15)$$

Applying the same rotation to $\vec{u}_2, \ldots, \vec{u}_N$ gives:

$$\left\{\vec{u}_1', ..., \vec{u}_N'\right\} = \left\{\vec{e}_1, ..., \vec{e}_N\right\} - \frac{1}{N}\left[1, ..., 1, 0\right] + \frac{1}{N+1}\left(\frac{\vec{w}_1'}{\sqrt{N}} - \vec{w}_2'\right) \qquad ...(16)$$

To obtain the final vertex, it is noted that:

$$\vec{u}_{N+1} = -\frac{\sqrt{N}}{N+1}\vec{w}_1 + \frac{1}{N+1}\vec{w}_2 = -\frac{N}{N+1}\left(\frac{\vec{w}_1}{\sqrt{N}} - \vec{w}_2\right) \qquad ...(17)$$

which gives:

$$\vec{u}_{N+1}' = -\frac{N}{N+1}\left(\frac{\vec{w}_1'}{\sqrt{N}} - \vec{w}_2'\right) \qquad ...(18)$$

The rotation has been chosen so that the $N+1'$ th component of all vectors is 0. Therefore the last component of all vectors can be disregarded, so just the first N components are considered. Notice that the vector $\frac{1}{N+1}\left(\frac{\vec{w}_1'}{\sqrt{N}} - \vec{w}_2'\right)$ appears in both (16) and (18). Considering only the first N components, it can be rewritten as:

$$\vec{w}_1' = \frac{1}{\sqrt{N\left(N+1\right)}}\vec{1}$$

$$\vec{w}_2' = \frac{-1}{\sqrt{N+1}}\vec{1} \qquad ...(19)$$

so that

$$\frac{1}{N+1}\left(\frac{\vec{w}_1'}{\sqrt{N}} - \vec{w}_2'\right)\frac{-1}{N\sqrt{N+1}}\vec{1} \qquad ...(20)$$

Taking only the first N components of the $\vec{u}_j'$ vectors gives:

$$\{\vec{u}_1', \ldots, \vec{u}_N'\} = \{\vec{e}_1, \ldots, \vec{e}_N\} - \frac{1}{N}\vec{1} + \frac{1}{N+1}\left(\frac{N+1}{N\sqrt{N+1}}\vec{1}\right)$$

$$= \{\vec{e}_1, \ldots, \vec{e}_N\} - \frac{1}{N}\left(1 - \frac{1}{\sqrt{N+1}}\right)\vec{1} \qquad \text{...(21)}$$

and

$$\vec{u}_{N+1}' = \frac{-N}{N+1}\left(\frac{N+1}{N\sqrt{N+1}}\vec{1}\right)$$

$$= \frac{-1}{\sqrt{N+1}}\vec{1} \qquad \text{...(22)}$$

From **Facts B and C**, it follows immediately that $\{\vec{u}_1', \ldots, \vec{u}_{N+1}'\}$ is a coordinate permutation invariant set in $\mathbb{R}^N$!

It remains to put all of the vertices on the unit *N*-sphere. All vertices are equidistant from the origin, which is the centroid of the simplex. Therefore, the distance from just one vertex to the origin can be divided by all the vertices to yield a unit *N*-simplex. Clearly $\vec{u}_{N+1}'$ is the easiest to work with: the distance is $\sqrt{\frac{N}{N+1}}$. Dividing all vertices by this distance yields the vertices of the unit *N*-simplex:

$$\vec{v}_j = \sqrt{\frac{N+1}{N}}\left(\vec{e}_j - \frac{1}{N}\left(1 - \frac{1}{\sqrt{N+1}}\right)\vec{1}\right),\ j = 1, \ldots, N$$

$$= \sqrt{\frac{N+1}{N}}\vec{e}_j - \frac{1}{N\sqrt{N}}\left(\sqrt{N+1} - 1\right)\vec{1},\ j = 1, \ldots, N$$

$$\vec{v}_{N+1} = \sqrt{\frac{N+1}{N}}\left(\frac{-1}{\sqrt{N+1}}\vec{1}\right)$$

$$= \frac{-1}{\sqrt{N}}\vec{1} \qquad \text{...(23)}$$

The edge lengths of this unit simplex can be found in the same fashion as the 2-simplex in Section 5. All the distances between vertices of the original *N*-simplex are $\sqrt{2}$, as for the 2-simplex. The edge lengths for the unit simplex are re-scaled by the multiplicative factor $\sqrt{\frac{N+1}{N}}$. This implies the unit simplex edge lengths are equal to $\sqrt{\frac{N+1}{N}}\sqrt{2} = \sqrt{\frac{2(N+1)}{N}}$. From this, the angle α between vertex vectors can be found, since

$$\sin(\alpha/2) = \sqrt{\frac{(N+1)}{2N}} \Rightarrow \cos(\alpha) = \frac{-1}{N} \qquad \text{...(24)}$$

8. Creation of a Permutation-Symmetric *N*-Simplex Using Translation in $\mathbb{R}^N$

In $\mathbb{R}^3$, a 3-simplex can be created similarly to a 2-simplex in $\mathbb{R}^2$, as shown in Figure 5. The fourth vertex is found on the $x = y = z$ line using the distance formula, and then the four vertices translated parallel to $\vec{1}$ so that the 3-simplex is centered at the origin. This is represented in the graph in Figure 5.

The generalization to *N* dimensions is straightforward. As before, the process begins with the basis vectors in $\mathbb{R}^N$. The $N+1'^{\text{th}}$ vertex, $a\,.\,\vec{1}$, can be obtained by utilizing the equality of the distances between vertices, which is known to be $\sqrt{2}$. By substituting any basis vector (say $\vec{e}_N$) into the distance formula, the possible values of a can be found:

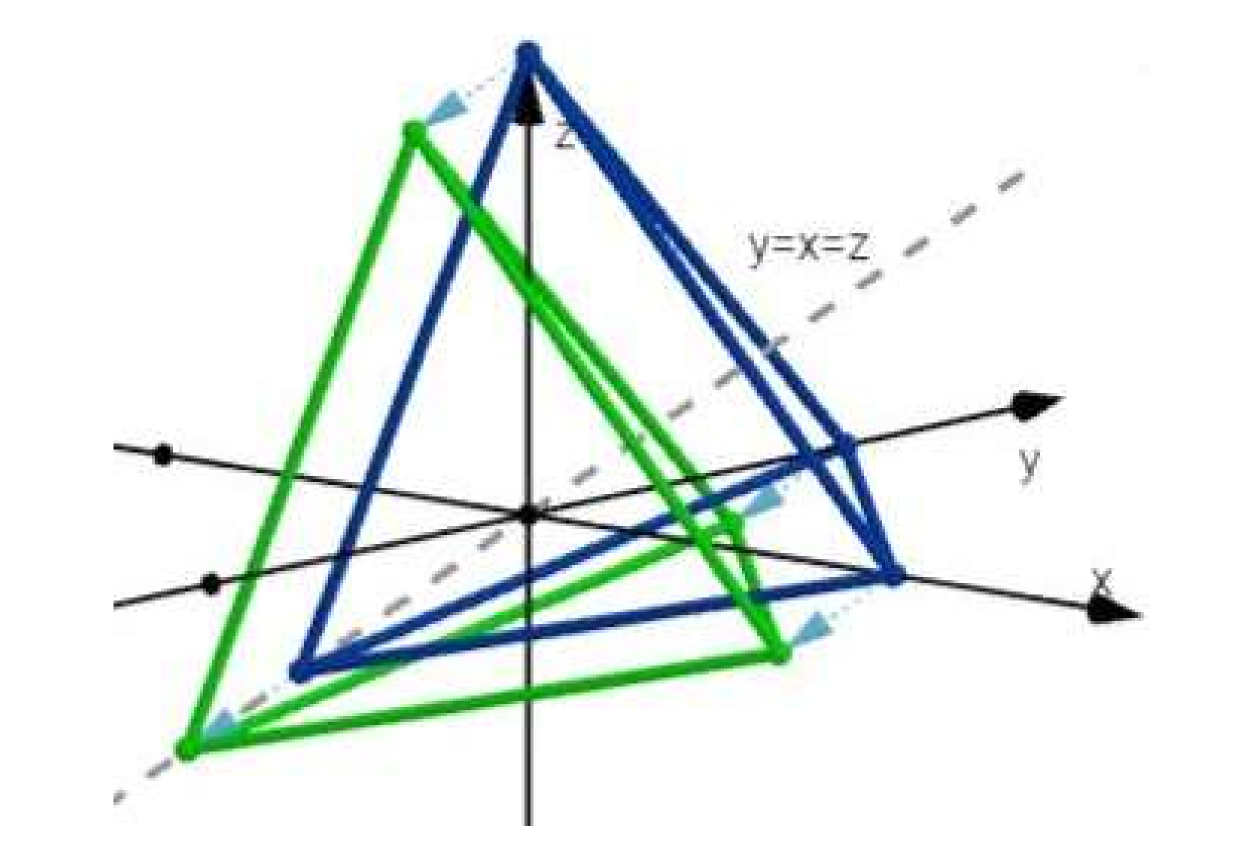

Figure 5: Creation of a Permutation-Symmetric 3-Simplex by Using Translation Method. A Rotatable GeoGebra Construction Can be Found at Anderson (2015)

$$\sqrt{2} = \sqrt{a^2 + \ldots + a^2 + (a-1)^2}$$

$$\Rightarrow a = \frac{1 \pm \sqrt{N+1}}{N} \quad \ldots(25)$$

Either value of a can be chosen: we choose the negative value to bring the simplex closer to the origin (the positive value will yield a unit simplex that is the negative of the one we are finding). The simplex is translated so that the centroid is at $\vec{0}$ by the transformation $\vec{x} \to \vec{x} - \vec{c}$, where

$$\vec{c} := \frac{1}{N+1}\left(\vec{e}_1 + \ldots + \vec{e}_N + a \cdot \vec{1}\right)$$

$$= \frac{1+a}{N+1}\vec{1}$$

$$= \frac{1}{N}\left(1 - \frac{1}{\sqrt{N+1}}\right)\vec{1} \quad \ldots(26)$$

Applying this transformation to the vertices gives the new vertices

$$\vec{u}'_j = \vec{e}_j - \vec{c}, 1 \le j \le N+1 \quad \ldots(27)$$

But this is exactly the same vector we subtracted in (21)! So the vertices $\{\vec{u}_j', \ldots, \vec{u}_N'\}$ are the same as before. Straightforward algebra also verifies that the $N+1$ vertex also agrees with (22). The upshot is that we have recreated the same unit simplex as before. Once again, **Facts B and C** apply to this derivation, so we have yet another proof of permutation invariance.

9. Conclusion

The following formulas give a set of equally spaced points on the unit N-sphere, which can be used for numerical integration.

$$\vec{v}_j = \sqrt{\frac{N+1}{N}}\vec{e}_j - \frac{1}{N\sqrt{N}}\left(\sqrt{N+1}-1\right)\vec{1},\ j=1,\ \ldots,\ N$$

$$\vec{v}_{N+1} = \frac{-1}{\sqrt{N}}\vec{1} \qquad \text{...(28)}$$

The set $\{-\vec{v}_1,\ \ldots,\ \vec{v}_{N+1}\}$ is also coordinate invariant, and gives vertices for a different unit N-simplex.

The length of any edge of a unit N-simplex is $\sqrt{\frac{2(N+1)}{N}}$.

The cosine of the angle α between any two vertex vectors is $\cos(\alpha) = \frac{-1}{N}$.

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Appendix

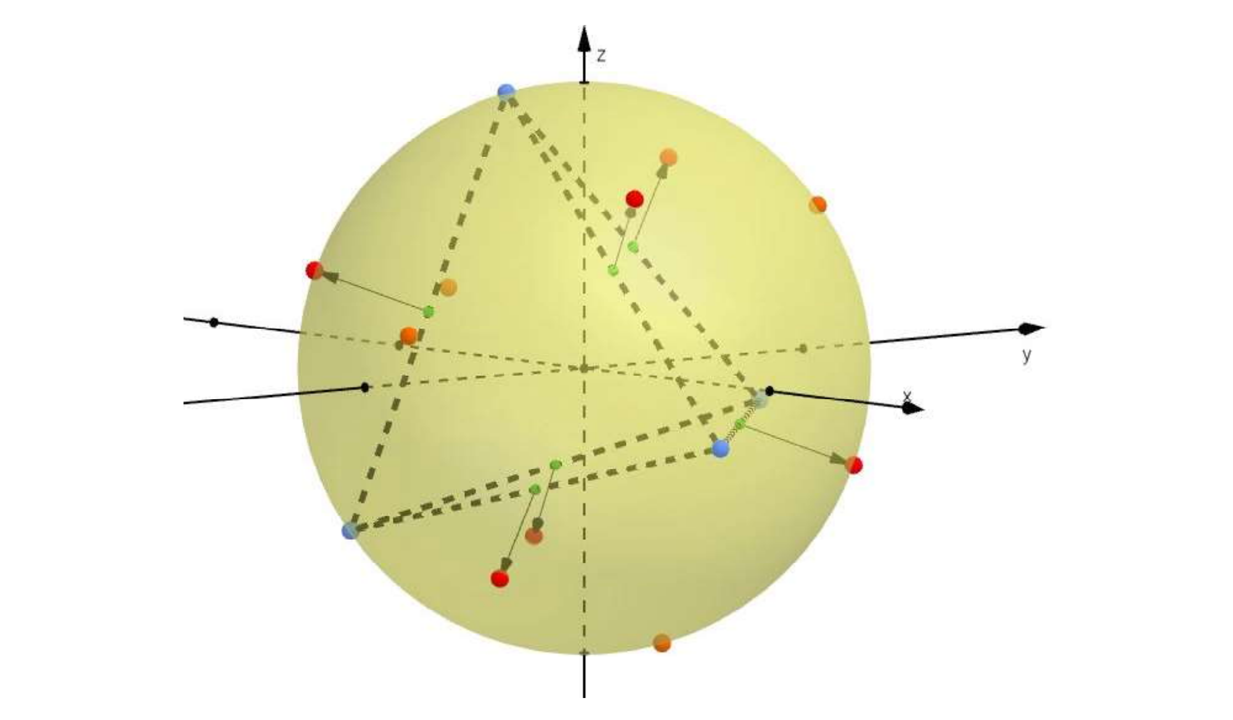

Figure 1: Pointson Unit Sphere

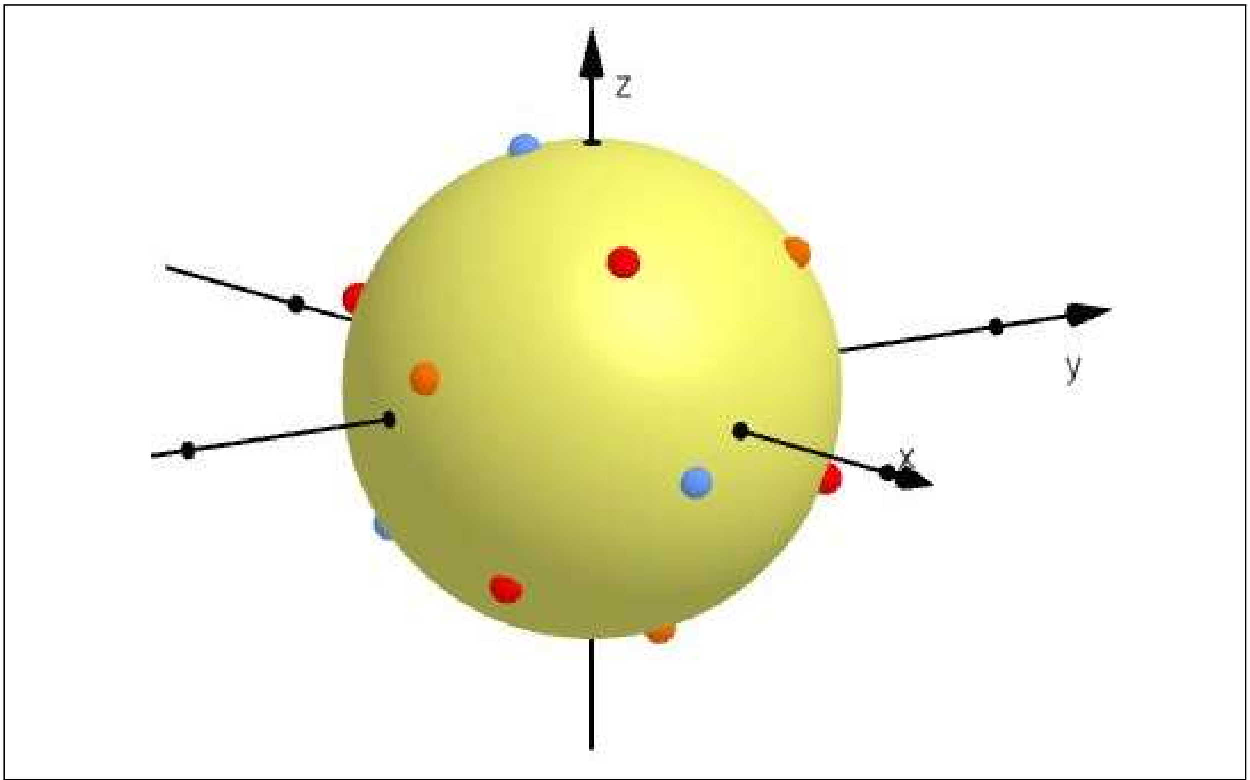

Figure 2: Pointson Unit Sphere 1

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