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Metrics in Three-Dimensional Lattices

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Abstract. In this article we find formulas for metrics on three-dimensional point lattices which count the number of steps required connect a given lattice point to the origin. Such formulas are previously known for the simple cubic lattice and the face-centered cubic lattice. We provide analogous formulas for the simple hexagonal lattice and the body-centered cubic lattice.

Key Words: point lattices, metrics

MSC 2000: 52C07

1. Introduction

A *point lattice* $\mathcal{L}$ is a $\mathbb{Z}$-module of the form

$$\mathcal{L} = \{a_i v_1 + \cdots + a_n v_n \mid a_i \in \mathbb{Z}\}$$

where $v_1, v_2, \ldots, v_n \in \mathbb{R}^n$ are linearly independent. $\mathcal{B} = \{v_1, \ldots, v_n\}$ is a *basis* of the lattice. A given basis $\mathcal{B}$ is *Minkowski-reduced* if v_1 is the shortest vector in $\mathcal{B}$ and for $2 \leq i \leq n$, v_i is the shortest vector in $\mathcal{L}$ such that $\{v_1, \ldots, v_i\}$ may be extended to a basis of $\mathcal{L}$. A *lattice point* $(a_1, \ldots, a_n)$ is defined by $(a_1, \ldots, a_n) = a_1 v_1 + \cdots + a_n v_n$ where $a_i \in \mathbb{Z}$. Given a lattice point $P \in \mathcal{L}$, the *Voronoi cell* containing P is the set

$$V(P) = \{x \in \mathbb{R}^n : \|x - P\| \leq \|x - Q\| \text{ for all } Q \in \mathcal{L}\}$$

where $\|\ \|$ is the usual Euclidean metric on $\mathbb{R}^n$. For a three-dimensional point lattice, we define two lattice points to be *neighbours* if their Voronoi cells share a face (note that this definition is easily extended to any dimension). A *step* in a lattice is a straight line segment adjoining two neighbouring lattice points. Fig. 1 illustrates these definitions for a 2-dimensional lattice.

By a result of Fedorov, there are only five combinatorially distinct convex polyhedra (Fig. 2) that tessellate 3-space by translation [3]. These five polyhedra are called *parallelohedra*. A correspondence between monohedral tilings of space by translation and lattices can be established: Given a monohedral tiling of space by translation, the prototile of this tiling

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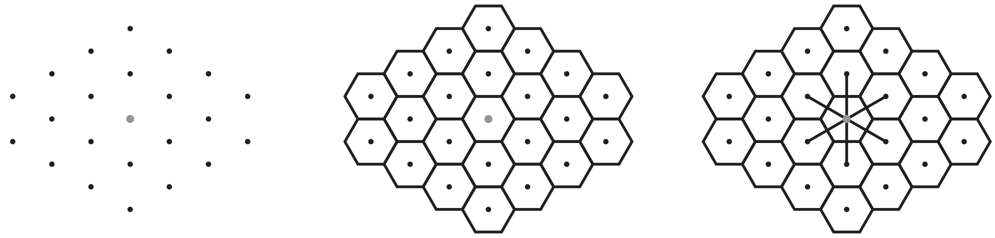

Figure 1: At left is a two-dimensional point lattice. In the middle is the Voronoi tessellation of that lattice. At right, the neighbours of a central lattice point are connected by steps.

is one of FEDOROV's five parallelohedra and the centroids of the tiles in such a tessellation form a lattice. Conversely, given a lattice, the corresponding Voronoi tessellation is a monohedral tiling of space by translation because lattices are known to be translation invariant. This correspondence limits the scope of our discussion to at most five distinct lattices. We note that under our definition of neighbours, the centroids of the tessellations of space by rhombic dodecahedra and by elongated dodecahedra give lattices that are, for our purposes, equivalent in the sense that the points of both of these lattices both have twelve neighbours and the geometry of the lattices are virtually the same; one being a "stretched" copy of the other. For this reason, we do not consider these two cases separately. Under our definition of neighbours, we will consider the following four distinct lattices.

- The simplest of these is the *simple cubic lattice (sc)* which arises as the centroids of the tessellation of space by cubes meeting face-to-face and vertex-to-vertex. Each simple cubic lattice point has six neighbours. A Minkowski-reduced basis for this lattice is the standard basis $\{\langle 1,0,0\rangle,\ \langle 0,1,0\rangle,\ \langle 0,0,1\rangle\}$.
- The *simple hexagonal lattice (sh)* is the lattice formed from the centroids of the tessellation of space by hexagonal prisms. Each simple hexagonal lattice point has eight neighbours. A Minkowski-reduced basis for this lattice is $\left\{\langle 1,\ 0,\ 0\rangle,\ \left\langle 1/2,\ \sqrt{3}/2,\ 0\right\rangle,\ \langle 0,\ 0,\ 1\rangle\right\}$.
- The *face-centered cubic lattice (fcc)* is formed from the centroids of the tessellation of space by rhombic dodecahedra. Each point in this lattice has twelve neighbours. A Minkowski-reduced basis for this lattice is

$$\left\{\langle 1,\ 0,\ 0\rangle,\ \left\langle 1/2,\ \sqrt{3}/2,\ 0\right\rangle,\ \left\langle 1/2,\ 1/(2\sqrt{3}),\ \sqrt{2/3}\right\rangle\right\}.$$

- The *body-centered cubic lattice (bcc)* is the set of centroids of a tessellation of space by truncated octahedra. A Minkowski-reduced basis for this lattice is

$$\{\langle 1,\ 1,\ 1\rangle,\ \langle 2,\ 0,\ 0\rangle,\ \langle 0,\ 2,\ 0\rangle\},$$

  although we choose to work with $\{\langle 2,\ 0,\ 0\rangle,\ \langle 0,\ 2,\ 0\rangle,\ \langle 1,\ 1,\ 1\rangle\}$ instead for convenience. The usual notion of neighbours in bcc (like the one chemists use) puts eight neighbours around each lattice point. We will call this version bcc-8. But, in keeping with the Voronoi cell motivated definition of neighbour given in this paper, we will consider another possibility where there are fourteen neighbours about each point; we call this version bcc-14. We stress that as point lattices, bcc-8 and bcc-14 are identical, the difference between the two being in how neighbours are defined.

The results of this paper concern finding metrics on these lattices which measure the minimum number of steps necessary to connect two given lattice points (or, equivalently, the

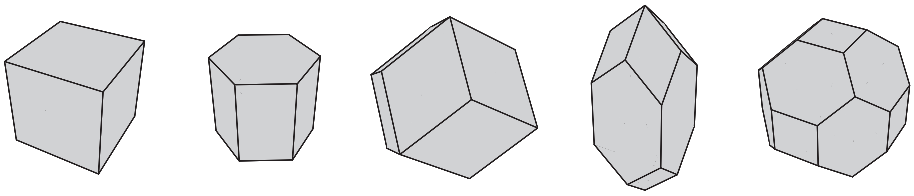

Figure 2: FEDOROV's space-filling parallelohedra: cube, hexagonal prism, rhombic dodecahedron, elongated dodecahedron, and truncated octahedron

minimum number of steps necessary to connect a point to the origin). We point out that any 3-dimensional lattice is simply a stretched version of one of the four given above, so finding metrics for these four lattices give a complete characterization of metrics for 3-dimensional lattices (using our definitions for neighbors and steps).

2. Known results

Metrics which measure the minimum number of steps necessary to connect a given lattice point to the origin are known for sc and fcc [6]. The (well-known) formula for sc is

$$d_{sc}(x,y,z) = |x| + |y| + |z|$$

where the lattice point (x,y,z) is expressed in terms of the standard basis for sc. For fcc, if (x,y,z) is expressed in terms of the Minkowski-reduced basis

$$\mathcal{B} = \left\{ \langle 1,\ 0,\ 0 \rangle\,,\ \langle 1/2,\ \sqrt{3}/2,\ 0 \rangle,\ \langle 1/2,\ 1/(2\sqrt{3}),\ \sqrt{2/3} \rangle \right\},$$

then the desired metric is

$$d_{fcc}(x,y,z) = \max\{|x|,\ |y|,\ |z|,\ |x+y|,\ |x+z|,\ |y+z|,\ |x+y+z|\}\,.$$

As we will see in bcc, simpler expressions for lattice metrics can be obtained if we do not require that lattice points be expressed in terms of a basis. For fcc in particular, if one uses the Conway-Sloan characterization [2] of fcc as the set of point $(x,y,z) \in \mathbb{Z}^3$ such that $x+y+z$ is even, we can derive an even simpler metric for fcc:

$$\hat{d}_{fcc}(x,y,z) = \max\left\{ |x|,\ |y|,\ |z|,\ \frac{1}{2}\left(|x|+|y|+|z|\right) \right\}.$$

The authors are unsure if this formula for $\hat{d}$ is previously known, but point out that formula for $\hat{d}$ follows easily from the formula for d.

3. The simple hexagonal lattice

The basis we will use for this lattice is $\left\{ \langle 1,\ 0,\ 0 \rangle\,,\ \langle 1/2,\ \sqrt{3}/2,\ 0 \rangle\,,\ \langle 0,\ 0,\ 1 \rangle \right\}$ which is clearly Minkowski-reduced. In terms of this basis, the eight neighbours of the origin (corresponding to the faces of the hexagonal prism) are $(\pm 1,0,0)$, $(0,\pm 1,0)$, $(\pm 1,\mp 1,0)$, and $(0,0,\pm 1)$. It is not difficult to show (using the same approach appearing in the next section) that taking the metric given for the hexagonal plane [5] and adding $|z|$ yields a metric for the simple hexagonal lattice:

$$d_{sh}(x,y,z) = \max\{|x|,\ |y|,\ |x+y|\} + |z|$$

4. Body-centered cubic lattice

4.1. bcc-14

A basis for bcc-14 is $\{\langle 2,0,0\rangle, \langle 0,2,0\rangle, \langle 1,1,1\rangle\}$ where the fourteen neighbours of the origin are $(\pm 1,0,0)$, $(0,\pm 1,0)$, $(\pm 1,\pm 1,\pm 1)$, and $(0,0,\pm 2)$. We will give a formula for a metric on bcc-14 in terms of this basis later, but it turns out that we can state a simpler formula for this metric if we use the Conway-Sloan description of fcc [2] to model bcc. As point sets, the only difference between fcc and bcc is that bcc is a slightly vertically stretched copy of fcc. Ignoring the distance between the points in the ambient space, what really differentiates fcc and bcc is how neighbours are distributed around points in these lattices. Our approach will be to use the Conway-Sloan description of the point set fcc to model bcc, but we will use the neighbours corresponding to bcc-14. The Conway-Sloan description of fcc is $\{(x,y,z)\in\mathbb{Z}^3:\ x+y+z \text{ is even}\}$. To turn fcc in to a lattice combinatorially equivalent to bcc-14, we declare that the fourteen adjacent points to $(0,0,0)$ are $(\pm 1,\pm 1,0)$, $(\pm 1,0,\pm 1)$, $(0,\pm 1,\pm 1)$, $(0,0,\pm 2)$.

Define

$$d_{14}(x,y,z) = \max\left\{|x|,\ |y|,\ \frac{1}{2}\left(|x|+|y|+|z|\right)\right\}$$

where $(x,y,z)\in\mathbb{Z}^3$ and $x+y+z$ is even. As we will prove, this function measures the minimum number of edges required to connect (x,y,z) to the origin. We point out that if you remove the $|z|$ from the metric for fcc given in [6], then you get the metric above; this demonstrates the similarity between the two lattices. The absence of the $|z|$ term exhibits the efficiency of using vertical steps $(0,0,\pm 2)$ in the bcc-14. Observe that if $|z|\geq |x|+|y|$, then $\max\left\{|x|,\ |y|,\ \frac{1}{2}\left(|x|+|y|+|z|\right)\right\} = \frac{1}{2}\left(|x|+|y|+|z|\right)$. This observation will be rather useful in the proof the lemma we state below.

For simplicity, the following lemma is proven for nonnegative z. The proof for negative z is similarly proven.

Lemma 1 *Suppose $d_{14}(x,y,z)=n$ with $z\geq 0$ and $n>0$. Then (x,y,z) neighbours a point (a,b,c) for which $d_{14}(a,b,c)=n-1$.*

Proof: We will consider two cases corresponding to the conditionality of d_{14}: $z\geq |x|+|y|$ and $z<|x|+|y|$.

1. Suppose $z\geq |x|+|y|$. We will consider two subcases of this case where $z\geq 2$ and $z\leq 1$.
   (a) Suppose $z\geq 2$.
      i. Suppose $z-2\geq |x|+|y|$. Then

$$\begin{aligned} d_{14}(x,y,z-2) &= \frac{1}{2}\left(|x|+|y|+|z-2|\right) \\ &= \frac{1}{2}\left(|x|+|y|+|z|\right)-1 \\ &= d_{14}(x,y,z)-1. \end{aligned}$$

      ii. Suppose $z-2<|x|+|y|$. Note that since we have $z\geq |x|+|y|$, then either $z=|x|+|y|$ or $z-1=|x|+|y|$. But, since $x+y+z$ is even, then we must have $z=|x|+|y|$. We will find it convenient to consider the further subcases that either x or y is zero or x and y are both nonzero.

A. Suppose x and y are both nonzero. Then

$$\begin{aligned} d_{14}(x,y,z-2) &= \max\left\{|x|,\,|y|,\,\frac{1}{2}\left(|x|+|y|+|z-2|\right)\right\} \\ &= \max\left\{|x|,\,|y|,\,\frac{1}{2}\left(|x|+|y|+|x|+|y|\right)-1\right\} \\ &= \max\left\{|x|,\,|y|,\,|x|+|y|-1\right\} \\ &= |x|+|y|-1. \end{aligned}$$

This last equality is true since neither $|x|$ nor $|y|$ are zero here. Also, observe that

$$\begin{aligned} d_{14}(x,y,z) &= \frac{1}{2}\left(|x|+|y|+|z|\right) \\ &= \frac{1}{2}\left(|x|+|y|+|x|+|y|\right) \\ &= |x|+|y|. \end{aligned}$$

Therefore we see that $d_{14}(x,y,z-2) = d_{14}(x,y,z)-1$.

B. Suppose $x=0$ or $y=0$. Without loss of generality, suppose $y=0$ and $x \neq 0$ (both x and y cannot be zero since $z=|x|+|y|$ and $z>0$.) Then $z=|x|$.
If $z=x$, then $|z-1| \geq |x-1|+|0|$, so

$$\begin{aligned} d_{14}(x-1,0,z-1) &= \frac{1}{2}\left(|x-1|+|0|+|z-1|\right) \\ &= \frac{1}{2}\left(z-1+z-1\right) \\ &= z-1 \\ &= d_{14}(x,0,z)-1. \end{aligned}$$

Similarly, if $z=-x$, we can argue that $d_{14}(x+1,0,z-1) = d_{14}(x,0,z)-1$.

(b) Suppose $z \leq 1$. Since $z=0$ implies that $x=y=0$ which violates our overall assumption that the point (x,y,z) has distance greater than zero, we have $z=1$. The only points that satisfy the inequality $1=z \geq |x|+|y|$ with $x+y+z$ even are $(1,0,1)$, $(-1,0,1)$, $(0,1,1)$, and $(0,-1,1)$. Choose $(a,b,c)=(0,0,0)$.

2. Suppose $z < |x|+|y|$. This case can be broken into three subcases: $z=0$, $z \geq 1$ and $|x|=|y|$, and $z \geq 1$ and $|x| \neq |y|$.

(a) The cases $(z=0)$ and $(z \geq 1$ and $|x|=|y|)$ can be handled simultaneously. Since not both x and y can be zero in either case, we have $|x|,|y| \geq 1$. The point (a,b,c) that will result in a distance of one less than (x,y,z) depends on the signs of x and y. If $x>0$ and $y>0$, then

$$\begin{aligned} d_{14}(x-1,y-1,z) &= \max\left\{|x-1|,\,|y-1|,\,\frac{1}{2}\left(|x-1|+|y-1|+|z|\right)\right\} \\ &= \max\left\{x-1,\,y-1,\,\frac{1}{2}\left(x-1+y-1+|z|\right)\right\} \\ &= \max\left\{|x|-1,\,|y|-1,\,\frac{1}{2}\left(|x|+|y|+|z|\right)-1\right\} \\ &= \max\left\{|x|,\,|y|,\,\frac{1}{2}\left(|x|+|y|+|z|\right)\right\}-1 \\ &= d_{14}(x,y,z)-1. \end{aligned}$$

Similarly, if $x > 0$ and $y < 0$ then $d_{14}(x-1, y+1, z) = d_{14}(x, y, z) - 1$, if $x < 0$ and $y > 0$ then $d_{14}(x+1, y-1, z) = d_{14}(x, y, z) - 1$, and if $x < 0$ and $y < 0$ then $d_{14}(x+1, y+1, z) = d_{14}(x, y, z) - 1$.

(b) Assume $z \geq 1$ and $|x| \neq |y|$. Without loss of generality, assume $|x| > |y|$. We consider the cases $x > 0$ and $x < 0$ separately: If $x > 0$, then

$$\begin{aligned}
d_{14}(x-1, y, z-1) &= \max\left\{|x-1|,\, |y|,\, \frac{1}{2}\left(|x-1| + |y| + |z-1|\right)\right\} \\
&= \max\left\{|x-1|,\, \frac{1}{2}\left(|x-1| + |y| + |z-1|\right)\right\} \\
&= \max\left\{x-1,\, \frac{1}{2}\left(x-1 + |y| + z-1\right)\right\} \\
&= \max\left\{|x|-1,\, \frac{1}{2}\left(|x| + |y| + |z|\right) - 1\right\} \\
&= \max\left\{|x|,\, \frac{1}{2}\left(|x| + |y| + |z|\right)\right\} - 1 \\
&= \max\left\{|x|,\, |y|,\, \frac{1}{2}\left(|x| + |y| + |z|\right)\right\} - 1 \\
&= d_{14}(x, y, z) - 1.
\end{aligned}$$

If $x < 0$ then one similarly shows $d_{14}(x+1, y, z-1) = d_{14}(x, y, z) - 1$. □

Theorem 1 *In bcc-14, the minimum number of steps required to form a path from the point (x, y, z) to the origin is given by d_{14}.*

Proof: Using Lemma 4.1 we are able to induct on $n = d_{14}(x, y, z)$. That is, we show that if $d_{14}(x, y, z) = n$, then (x, y, z) can be reached from the origin in no fewer than n steps.

Suppose $n = 1$. We will argue that the points (x, y, z) that have $d_{14}(x, y, z) = 1$ are exactly the points neighbouring the origin. For this, if $|z| \geq |x| + |y|$, then the metric gives $|x| + |y| + |z| = 2$. Now

$$\begin{aligned}
|z| &\geq |x| + |y| \\
2|z| &\geq |x| + |y| + |z| = 2 \\
|z| &\geq 1.
\end{aligned}$$

The points that satisfy $|z| \geq 1$ and $|x|+|y|+|z| = 2$ are $(0, 0, \pm 2)$, $(0, \pm 1, \pm 1)$, and $(\pm 1, 0, \pm 1)$. On the other hand, if $|z| < |x| + |y|$ and

$$1 = \max\left\{|x|,\, |y|,\, \frac{1}{2}\left(|x| + |y| + |z|\right)\right\},$$

then $|x| \leq 1$ and $|y| \leq 1$. The cases where either $x = 0$ or $y = 0$ yield no solutions. If $|x| = 1$ and $|y| = 1$, then $|z| < 2$. However, $z \neq \pm 1$ as the sum $|x| + |y| + |z|$ is not even. Thus $z = 0$ and we have the solutions $(\pm 1, \pm 1, 0)$.

Let $n \geq 1$ and suppose that for $1 \leq k \leq n-1$, if a lattice point (a, b, c) satisfies $d_{14}(a, b, c) = k$, then (a, b, c) is no fewer than k steps from the origin. Let (x, y, z) be a lattice point for which $d_{14}(x, y, z) = n$. By Lemma 4.1 there is a neighbouring lattice point (a, b, c) for which $d_{14}(a, b, c) = n - 1$. By the inductive hypothesis, (a, b, c) is no fewer than $n - 1$ steps from the origin, and because (a, b, c) neighbours (x, y, z), we have (x, y, z) is at most n steps from the origin.

To see that (x, y, z) is no fewer than n steps from the origin, suppose to the contrary that (x, y, z) is $n-1$ or less steps from the origin. Then by inductive hypothesis, $d_{14}(x, y, z) \neq n$, contrary to our choice of (x, y, z). □

The metric found above using the Conway-Sloane description can be converted to yield a metric for bcc-14 relevant to the basis given at the opening of the section. The formula in terms of that basis is

$$\overline{d}_{14}(x, y, z) = \max\left\{|x+y+z|,\, |x-y|,\, \frac{1}{2}\left(|x+y+z| + |x-y| + |z|\right)\right\}.$$

4.2. bcc-8

In a manner similar to the way in which we used the Conway-Sloan description of fcc to model bcc-14, we model bcc-8 as the set of points in $\mathbb{Z}^3$ where the coordinates are all odd or they are all even and the neighbours of the origin include the eight points $(\pm 1, \pm 1, \pm 1)$. We proceed to show that

$$d_8(x, y, z) = \max\{|x|,\, |y|,\, |z|\}$$

is a metric on bcc-8 which measures the minimum number of steps necessary to connect (x, y, z) to $(0, 0, 0)$.

Theorem 2 *In bcc-8, the minimum number of steps required to form a path from the point (x, y, z) to the origin is given by d_8.*

Proof: We induct on $n = d_8(x, y, z)$. If $n = 0$, then (x, y, z) is the origin. If $n = 1$, then all coordinates of (x, y, z) must be odd yielding all eight points neighbouring the origin. The minimum number of steps required to connect these points to the origin is indeed 1.

Now suppose that $d_8(x, y, z) = n > 2$. We will first show that (x, y, z) can be connected to the origin using n steps by finding a neighbour of (x, y, z) a distance of $n-1$ from the origin and then we will establish that n is the minimum number of steps required to connect (x, y, z) to the origin. To find a point that is one step closer to the origin than (x, y, z), if $x > 0$, then let the x-coordinate of the new point be $x-1$ so that $|x-1| = |x| - 1$. If $x < 0$, then let the x-coordinate of the new point be $x+1$ so that $|x+1| = |x| - 1$. Similarly make choices for all nonzero coordinates. If (x, y, z) has all nonzero coordinates, then upon appropriate choice of signs we have

$$\begin{aligned} d_8(x \pm 1,\, y \pm 1,\, z \pm 1) &= \max\{|x \pm 1|,\, |y \pm 1|,\, |z \pm 1|\} \\ &= \max\{|x| - 1,\, |y| - 1,\, |z| - 1\} \\ &= \max\{|x|,\, |y|,\, |z|\} - 1 \\ &= n - 1. \end{aligned}$$

For points (x, y, z) that have zero coordinates, not all coordinates will be zero since $n > 2$. In fact, one coordinate's absolute value will be greater than or equal to 2. Without loss of generality, say $x = 0$ and $|z| \geq 2$. Then consider

$$\begin{aligned} d_8(x + 1,\, y \pm 1,\, z \pm 1) &= \max\{|x + 1|,\, |y \pm 1|,\, |z \pm 1|\} \\ &= \max\{1,\, |y \pm 1|,\, |z| - 1\} \\ &= n - 1. \end{aligned}$$

To see that no fewer than $\max\{|x|, |y|, |z|\}$ steps can connect (x, y, z) to the origin, notice that making one step in bcc-8 changes all coordinates by ± 1. Thus any point (x, y, z) that is n steps from the origin satisfies $|x| \leq n$, $|y| \leq n$, and $|z| \leq n$ so that $\max\{|x|, |y|, |z|\} \leq n$. □

5. Final remarks

In our definition of neighbours, we required that neighbouring points have Voronoi cells that share a face. This definition fits with the common notion of neighbours for $\mathbb{Z}^3$; six neighbours corresponding to the centers of cubes placed face-to-face around a centrally placed cube. We could, however, define points to be neighbours if their Voronoi cells intersect. For example, under this proposed definition, every point in $\mathbb{Z}^3$ would have 26 neighbours (think of a Rubik's Cube).

Open Question 1 *What are the metrics of the three-dimensional lattices if we adjust our notion of neighbours to mean that Voronoi cells simply intersect?*

The answer for fcc is given in [6]. Under the new formulation of adjacency there are eighteen neighbours at every point. The metric for the McAndrew-Osborne characterization is

$$d_{18}(x, y, z) = \max\{|x|,\ |y|,\ |z|,\ |x + y + z|\}$$

and the metric for the Conway-Sloane characterization is

$$\hat{d}_{18}(x, y, z) = \max\left\{\frac{1}{2}|-x + y + z|,\ \frac{1}{2}|x - y + z|,\ \frac{1}{2}|x + y - z|,\ \frac{1}{2}|x + y + z|\right\}.$$

We point out that this last metric can be simplified to the much nicer form

$$\hat{d}_{18}(x, y, z) = \frac{1}{2}\left(|x| + |y| + |z|\right).$$

Open Question 2 *Using our definition of neighbours, classify the distinct four-dimensional point lattices and find metrics which measure the minimum number of steps required to connect a lattice point to the origin.*

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