Distances based on neighbourhood sequences in non-standard three-dimensional grids

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Abstract

Properties for distances based on neighbourhood sequences on the face-centred cubic (fcc) and the body-centred cubic (bcc) grids are presented. Formulas to both compute the distances and assure that the distances satisfy the conditions for being metrics are presented and proved to be correct. The formulas are used to calculate the neighbourhood sequences that generates distances with lowest deviation from the Euclidean distance.

Keywords: Distance functions; 3D image processing; Non-standard grids; Distances based on neighbourhood sequences

1. Introduction

When acquiring three-dimensional images using projections with techniques such as X-ray CT scans, magnetic resonance imaging (MRI), and positron emission tomography (PET), the image is obtained by two-dimensional projections of a three-dimensional object. Traditionally, the intensity values are computed for grid points in the cubic grid. There are, however, reasons for considering other grids such as the face-centred cubic (fcc) and body-centred cubic (bcc) grids. First of all, there are many similarities with the cubic grid; all three grids are lattices and have integer grid point coordinates. Also, it is very easy to construct efficient data-structures for the fcc and bcc grids. An important difference is that less samples are needed on the fcc and bcc grids to obtain the same image representation/reconstruction quality compared to the cubic grid \cite{16,10}. An image processing package for electron microscopy with support for the fcc and bcc grids has recently been developed \cite{26}. The literature is, however, still lacking in image analysis and image processing algorithms developed for the fcc and bcc grids.

There are several reasons for using the fcc and bcc grids. For example, since these grids are reciprocal and both have higher packing density than the cubic grid (the fcc grid is a densest packing lattice in 3D), less samples can be used without affecting the image representation/reconstruction quality \cite{16}. The high number of neighbours at approximately
the same distance on these grids (12 neighbours at distance \(\sqrt{2}\) for the fcc grid and 14 neighbours at distance \(\sqrt{3}\) and 2 for the bcc grid) implies that the rotational dependency for these grids is lower than for the cubic grid. In [17], this difference is quantified using surface area estimates and it is shown that the fcc and bcc grids produce more accurate surface area estimates for random planes than the cubic grid.

Each grid is equipped with some neighbourhood relations. For example, the usual two-dimensional square grid is equipped with the 4- and 8-neighbourhoods. A more flexible distance is obtained by alternating these neighbourhoods using a sequence of neighbourhood relations, a neighbourhood sequence. Distances based on neighbourhood sequences approximate the Euclidean distance better. This was first noted in [25]; the authors state that the approximation obtained when the ratio between the number of steps using the different neighbourhood relations in \(\mathbb{Z}^2\) is equal to 1 : \(\sqrt{2}\) is optimal. The literature on distances based on neighbourhood sequences is rich; a theory for periodic neighbourhood sequences not connected to any specific neighbourhood relations in \(\mathbb{Z}^n\) is presented in [29,30] and further developed for the natural neighbourhood structure, by the so-called octagonal neighbourhood sequences in [7,6]. Results for general (not necessarily periodic) neighbourhood sequences are presented in [9,21].

There is another very common way of modifying the city block and chessboard distances in order to obtain a less rotational dependent distance, the weighted distances, [1]. With these distances, each local step is given a weight, which is considered when computing the distance, i.e., when finding the shortest path. The calculation of optimal local weights have been the subject of many papers, see for example [1,28]. For optimal weights on the fcc and bcc grids, see [27]. Note that the computation of the Euclidean distance as in e.g. [3] is not included here, since we consider only rational values in the discrete spaces in this paper.

Many approaches where the deviation from the Euclidean distance is minimized in order to find the optimal neighbourhood sequence have been proposed for \(\mathbb{Z}^2\) and \(\mathbb{Z}^3\). Several error functions minimizing the asymptotic maximum difference of two balls of equal radius using a distance based on periodic neighbourhood sequences and a Euclidean sphere, respectively, is presented in [5,8,30] (\(\mathbb{Z}^2\), [18] (\(\mathbb{Z}^3\)). An investigation of optimal non-periodic neighbourhood sequences in \(\mathbb{Z}^2\) with optimal sequences also for finite distances is found in [12]. In [4], an optimization for \(\mathbb{Z}^3\) is carried out using a geometric approach. All the above approaches are based on the difference between a Euclidean ball and a ball generated by distances based on neighbourhood sequences of the same radius. Such error functions are natural to use in \(\mathbb{Z}^n\), because a ball generated by a distance obtained by only considering first-order/\(n\)th order neighbours will always be an underestimation/overestimation of the Euclidean ball of the same radius. Using non-standard grids as in this paper, there is in general no order of neighbours generating a distance that is an overestimation of the Euclidean one. Instead, an error function that is independent of the radius of the Euclidean ball is used in the optimization. It should be mentioned that such error function has been applied on \(\mathbb{Z}^3\) in [11].

Distances based on neighbourhood sequences have been applied, e.g., for shading of three-dimensional objects [19] using a medial axis representation for distances based on neighbourhood sequences [15]. Also, distances based on neighbourhood sequences have been used for indexing and segmenting colour images [13].

In this paper, the theory of distances based on neighbourhood sequences is developed for the fcc and bcc grids. Formulas for computing the distance generated by given neighbourhood sequences are presented and proved to be correct in Section 3. Note the difference between such formulas, which are very important for theoretical considerations, and the more application-oriented chamfer algorithm presented for weighted distances in e.g. [1,27] and for distances based on neighbourhood sequences in [3,4]. In applications, it is often desirable that the resulting distances are metrics. Necessary and sufficient conditions for a distance generated by a neighbourhood sequence to be a metric are presented in Section 4. Also, a computationally efficient formula for deciding whether a neighbourhood sequence generates a metric or not is presented. Using these results, neighbourhood sequences generating distances with minimal deviation from the Euclidean distance is presented in Section 5.

2. Notation and definitions

The following definitions of the fcc and bcc grids from [14] are used:

\[
F = \{(c_1, c_2, c_3) : c_1, c_2, c_3 \in \mathbb{Z} \text{ and } c_1 + c_2 + c_3 \equiv 0 \text{ (mod 2)}\}. \quad (1)
\]

\[
B = \{(c_1, c_2, c_3) : c_1, c_2, c_3 \in \mathbb{Z} \text{ and } c_1 \equiv c_2 \equiv c_3 \text{ (mod 2)}\}. \quad (2)
\]

Observe that, using these definitions, each grid point has integer coordinates.
Two grid points $p, q \in \mathbb{F}$ or $\mathbb{B}$ are $r$-neighbours, $1 \leq r \leq 2$ if

\begin{align}
& (1) \sum_{i=1}^{3} |p(i) - q(i)| \leq 3 \text{ and} \\
& (2) \max_{i \in \{1, 2, 3\}} |p(i) - q(i)| \leq r.
\end{align}

The neighbourhood relations are visualized in Fig. 1 by showing the Voronoi regions (the voxels) corresponding to some grid points.

From now on we refer to the $r$-neighbours which are not $(r - 1)$-neighbours as strict $r$-neighbours. In addition, we will use path-generated distances therefore the terms 1- and (strict) 2-steps will also be used instead of step to a 1-neighbour and step to a (strict) 2-neighbour, respectively.

Observe that in both the fcc and bcc grids, in analogy with the cubic grid, the strict 2-neighbours can be connected by two 1-steps.

When the two grids are handled in parallel, $\mathbb{G}$ is used to denote either $\mathbb{F}$ or $\mathbb{B}$. The points $p, q \in \mathbb{G}$ are adjacent if $p$ and $q$ are $r$-neighbours for some $r$.

The grids considered here are lattices, [2]. This means that the grids can be defined by a basis and thus have the following properties: if $p, q \in \mathbb{G}$, then $p + q \in \mathbb{G}$. Also, if $p, p' \in \mathbb{G}$ are $r$-neighbours, then so are $p + q, p' + q$ and $p - q, p' - q$ for any $q \in \mathbb{G}$. Observe that, e.g., the two-dimensional triangular grid is not a lattice, but the theory of neighbourhood sequences is developed for this grid as well [20,22,24].

A neighbourhood sequence is a sequence $B = (b(i))_{i=1}^{\infty}$. If $B$ is periodic, i.e., if for some (positive) fixed $l \in \mathbb{N}$, $b(i) = b(i + l)$ is valid for all $i \in \mathbb{N}$, then $B$ is written $B = (b(1), b(2), \ldots, b(l))$.

A path in a grid is a sequence $(p = p_0, p_1, \ldots, p_m = q)$ of adjacent grid points. A path is a $B$-path of length $m$ if, for all $i \in \{1, 2, \ldots, m\}$, $p_{i-1}$ and $p_i$ are $b(i)$-neighbours. The $B$-distance $d(p, q; B)$ is defined as the length of the shortest $B$-path(s) between them. Usually in digital geometry the shortest path is not unique. The distance function generated by $B$ is denoted $d(B)$.

**Remark 1.** Opposed to the fcc grid, the bcc grid has the following property: If a grid point $(x, y, z)$ is such that a path from $(0, 0, 0)$ can consist of either only 1-steps or only strict 2-steps, the path with 1-steps can be shorter than the path with strict 2-steps. (For example $(x, y, z) = (2, 2, 2)$.)

Let

\begin{align}
1^k_B &= |\{i : b(i) = 1, 1 \leq i \leq k\}| \text{ and} \\
2^k_B &= |\{i : b(i) = 2, 1 \leq i \leq k\}|.
\end{align}

When $B$ is clear from the context, we will exclude the subscript and write $1^k$ and $2^k$ for short. Observe that, for any $B$ and any $k$, $1^k_B + 2^k_B = k$. 

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**Fig. 1.** The grid points corresponding to the dark and the light grey voxels are 1-neighbours. The grid points corresponding to the dark grey and white voxels are (strict) 2-neighbours. Left: fcc, right: bcc.
3. Formulas for computing the distance

In the previous section the $B$-distances are defined for the fcc and bcc grids. Both in theory and in applications it is very useful to have formulas to compute the actual values of the distances. For $\mathbb{Z}^n$ the computation is given in [7] and in [23, 24], for the periodic and not necessarily periodic cases, respectively. To know more about the $B$-distances in fcc and bcc grids, in this section, formulae are given to compute them.

For the sake of simplicity we use the values $(x, y, z)$ as the absolute-difference of the coordinate values of the points in a sorted way, such that $x \geq y \geq z \geq 0$. We will compute the length of a shortest path from the point $(x, y, z)$ to the point $(0, 0, 0)$. Since the distance is translation invariant and the coordinate values are freely chosen in each step, one can have the $B$-distance for all point-pairs.

**Theorem 2 (B-distance in $\mathbb{F}$).** Let a neighbourhood sequence $B$ be given. Let $d$ be the distance of the two points (having sorted absolute difference vector $(x, y, z)$). Then

$$d = \min \left\{ k \left| k \geq \max \left\{ \frac{x + y + z}{2}, x - 2^k \right\} \right. \right\}.$$  

**Proof.** First, the vectors that can be used in a path from $(x, y, z)$ to $(0, 0, 0)$ are listed. At a 1-step the vectors $(-1, -1, 0), (-1, 0, -1)$ and $(0, -1, -1)$ can be used. In addition to these, the vectors $(-2, 0, 0), (0, -2, 0)$ and $(0, 0, -2)$ are allowed in a 2-step. So in each step the sum of the coordinate values is modified by 2. If one can decrease the sum of the coordinate values by 2 in each step then there is a shortest path from $(x, y, z)$ to $(0, 0, 0).$ The fcc grid is a lattice, therefore any two steps can be interchanged, every permutation of the two steps can be 1-steps to reach the point $(0, 0, 0)$. The first $z$ steps can be 1-steps to reach the point $(x - z, y, 0)$ (the sum of the coordinate values decreased by 2 in each step). Then the next $y$ steps can be 1-steps as well, reaching the point $(x - (y + z), 0, 0)$ having a non-zero coordinate. (There were together $y + z$ 1-steps.) Then to build a shortest path (decreasing the sum of the coordinates by 2 in each step) $\frac{x - y - z}{2}$ strict 2-steps are needed to reach the point $(0, 0, 0)$. The fcc grid is a lattice, therefore any two steps can be interchanged, every permutation of the steps of a (shortest) path gives a (shortest) path. So, if there are $\frac{x - y - z}{2}$ value 2 among the first $y + z + \frac{x - y - z}{2}$ elements of $B$ then there is a shortest path from $(x, y, z)$ to $(0, 0, 0)$ with length $y + z + \frac{x - y - z}{2} = \frac{x + y + z}{2}$. If there are not so many values 2 among the first elements of $B$, i.e., $2^k < \frac{x - y - z}{2}$ for $k = \frac{x + y + z}{2}$, then a 2-step can be substituted by two 1-steps. That increases the length of the path by 1, so in this way the distance will be larger. At least $\frac{x + y + z}{2}$ steps are
needed plus one more for each missing value 2. So,
\[
d = \min \left\{ k \left| k \geq \frac{x + y + z}{2} + \max \left\{ 0, \frac{x - y - z}{2} - 2^k \right\} \right. \right\} \\
= \min \left\{ k \left| k \geq \max \left\{ \frac{x + y + z}{2}, x - 2^k \right\} \right. \right\}.
\]

\textbf{Corollary 3.} Let \( p = (x, y, z) \) be any point in \( \mathbb{F} \) with \( x \geq y \geq z \geq 0 \) and \( B \) be any neighborhood sequence. Then \( \frac{x + y + z}{2} \leq d(p, 0; B) \leq x + y + z \), where the equalities are attained when

- (minimum) \( x \leq y + z \) or there is at least \( \frac{x - y - z}{2} \) values 2 in the initial part of \( B \) up to the \( \frac{x + y + z}{2} \)th element;
- (maximum) \( y = z = 0 \) and there is no value 2 in \( B \) up to the first \( x - 1 \) elements.

\textbf{Corollary 4.} Given a neighborhood sequence \( B \) and a positive integer \( k \), the maximal value of \( (x^2 + y^2 + z^2 : d((x, y, z), (0, 0, 0), B) = k) \) in \( \mathbb{F} \) is given by
\[
(1_B^k + 2 \cdot 2^k_B, 1_B^k, 0).
\]

\textbf{Proof.} By using as many strict 2-steps as possible, the distance will be maximal. This is the case when \( 2^k = \frac{x - y - z}{2} \) which implies \( k = \frac{x + y + z}{2} \). Using \( 1^k + 2^k = k \), we get
\[
2^k = \frac{x - y - z}{2},
\]
\[
k = \frac{x + y + z}{2}
\]
and
\[
1^k + 2^k = k.
\]
This results in \( x = 1^k + 2 \cdot 2^k \) and \( y + z = 1^k \). Finding the \( y \) that maximizes \( (1^k + 2 \cdot 2^k)^2 + y^2 + (1^k - y)^2 \) under the condition \( x \geq y \geq z \geq 0 \) gives \( y = 1^k, z = 0 \).

\textbf{Theorem 5 (B-distance in \( \mathbb{B} \)).} Let a neighborhood sequence \( B \) be given. Let \( d \) be the distance of the two points (having sorted absolute difference vector \((x, y, z)\)). Then
\[
d = \min \left\{ k \left| k \geq \max \left\{ \frac{x + y}{2}, x - 2^k \right\} \right. \right\}.
\]

\textbf{Proof.} In the bcc grid one can modify all the three coordinate values with a 1-step and only one value by 2 with a strict 2-step. Let us build a shortest path from \((x, y, z)\) to \((0, 0, 0)\) (using arbitrary steps). In the first \( z \) steps the 1-steps are the best choice to reach the point \((x - z, y - z, 0)\) by decreasing each value in each step (i.e. decreasing the sum of the coordinate values by three, which is more efficient than the usage of the strict 2-steps). According to the definition of the bcc grid, both \( x - z \) and \( y - z \) are even. Now, we can reach the point \((x - y, 0, 0)\) by alternating use of 1-steps: \((-1, -1, -1)\) and \((-1, -1, +1)\) (using a minimum number of steps). So there were \( y \) 1-steps together until this point. Now, \( \frac{x+y}{2} \) strict 2-steps are needed to have a shortest path (together with the \( y \) 1-steps there are \( \frac{x+y}{2} \) steps in the shortest path). If there are enough values 2 in the first part of \( B \), then we can use them, otherwise each missing 2-step can be replaced by two 1-steps which increases the distance by one. Therefore, the distance is
\[
d = \min \left\{ k \left| k \geq \frac{x + y}{2} + \max \left\{ 0, \frac{x - y}{2} - 2^k \right\} \right. \right\} \\
= \min \left\{ k \left| k \geq \max \left\{ \frac{x + y}{2}, x - 2^k \right\} \right. \right\}.
\]
Corollary 6. Let \( p = (x, y, z) \) be any point in \( \mathbb{B} \) with \( x \geq y \geq z \geq 0 \) and \( B \) be any neighborhood sequence. Then 
\[
\frac{x+y+z}{3} \leq d(p, 0; B) \leq x + y + z,
\]
where the equalities are attained when 
- (minimum) \( x = y = z \); 
- (maximum) \( y = z = 0 \) and there is no value 2 in \( B \) up to the first \( x - 1 \) elements.

Corollary 7. Given a neighborhood sequence \( B \) and a positive integer \( k \), the maximal value of \( (x^2 + y^2 + z^2 : d((x, y, z), (0, 0, 0); B) = k) \) in \( \mathbb{B} \) is given by 
\[
(1_B^k + 2 \cdot 2_B^k, 1_B^k, 1_B^k) \quad \text{if} \quad 2 \cdot 1_B^k \leq 2_B^k,
\]
\[
(1_B^k + 2_B^k, 1_B^k + 2_B^k, 1_B^k + 2_B^k) \quad \text{otherwise}.
\]

Proof. By Remark 1, we know that the Euclidean distance can be maximal if we use as many strict 2-steps or as many 1-steps as possible, depending on \( B \). 
If \( B \) is such that the Euclidean distance is maximized by using as many strict 2-steps as possible, then, by the previous proof, it is optimal to use \( x \) and \( y \) such that \( 2^k = \frac{x-y}{2} \), which implies \( k = \frac{x+y}{2} \). Using \( 1^k + 2^k = k \), we get 
\[
2^k = \frac{x-y}{2},
\]
\[
k = \frac{x+y}{2}
\]
and 
\[
1^k + 2^k = k.
\]
The system of equations is solved by \( x = 1^k + 2 \cdot 2^k \) and \( y = 1^k \). Finding the \( z \) that maximizes \( (1^k + 2 \cdot 2^k)^2 + (1^k)^2 + z^2 \) under the condition \( x \geq y \geq z \geq 0 \) gives \( z = 1^k \).
But it might be the case that \( B \) is such that the Euclidean distance is maximal when using as many 1-steps as possible. Then, obviously the Euclidean distance is maximized for \( (x, y, z) = (1_B^k + 2_B^k)(1, 1, 1) \).
Finally, we note that 
\[
3(1_B^k + 2_B^k)^2 \leq (1_B^k + 2 \cdot 2_B^k)^2 + 2(1_B^k)^2 \iff 2 \cdot 1_B^k \leq 2_B^k,
\]
which completes the proof. \( \square \)

Remark 8. In contrast to the fcc grid, the distance in the bcc grid does not depend on the value of the coordinate with the lowest value in the absolute difference of the points.

4. Conditions for a distance to be a metric

Definition 9. A function \( f : \mathbb{G} \times \mathbb{G} \rightarrow \mathbb{R} \) is a metric on \( \mathbb{G} \) if it satisfies the following conditions:

1. \( \forall p, q \in \mathbb{G} : f(p, q) \geq 0 \) and \( f(p, q) = 0 \) if and only if \( p = q \)
2. \( \forall p, q \in \mathbb{G} : f(p, q) = f(q, p) \)
3. \( \forall p, q, r \in \mathbb{G} : f(p, q) + f(q, r) \geq f(p, r) \)

For the distance function generated by a neighborhood sequence \( B \), \( d(B) \) to be a metric, some conditions on \( B \) must be fulfilled. Necessary and sufficient conditions for periodic neighborhood sequences on \( \mathbb{Z}^n \) for \( d(B) \) to be a metric is presented in [7] and for non-periodic neighborhood sequences in \( \mathbb{Z}^n \) in [21]. In this section, conditions for metricity for distances based on neighborhood sequences on the fcc and bcc grids are derived.

Definition 10. Let \( A \) and \( B \) be two neighborhood sequences in \( \mathbb{G} \). The relation \( A \equiv^* B \) (\( A \) is faster than \( B \)) is defined as 
\[
d(p, q; A) \leq d(p, q; B) \quad \forall p, q \in \mathbb{G}.
\]
Observe that the distance function is used in the definition of the relation. There is a natural question: how one can decide whether a neighbourhood sequence $A$ is faster than $B$ without calculating the actual distances of all possible point-pairs. It is easy to check, that the relation does not depend on the distances of points, but only on the compared neighbourhood sequences.

**Theorem 11.** For the fcc and bcc grids, a neighbourhood sequence $A$ is faster than a neighbourhood sequence $B$ if and only if

$$
\sum_{i=1}^{j} a(i) \geq \sum_{i=1}^{j} b(i) \quad \text{for all } j \in \mathbb{N}.
$$

It can be written in the following equivalent condition:

$$
2^j_A \geq 2^j_B \quad \text{for all } j \in \mathbb{N}.
$$

**Proof.** This theorem is a consequence of the Theorems 2 and 5, respectively, for the fcc and bcc grids. □

**Definition 12.** For any neighbourhood sequence $B=(b(i))_{i=1}^{\infty}$, the sequence $B(j)=(b(i))_{i=j}^{\infty}$ is the $j$-shifted sequence of $B$.

**Theorem 13.** The distance function based on a neighbourhood sequence $B$ is a metric on $\mathbb{G}$ if and only if $B(i) \sqsupseteq B$ for all $i \in \mathbb{N}$.

**Proof.** Property (1) in Definition 9 is trivially fulfilled.

Property (2): Let $p, p' \in \mathbb{G}$, $B$ be a neighbourhood sequence, and $(p = p + q_0), p + q_1, p + q_2, \ldots, (p + q_n = p')$ be a shortest $B$-path between $p$ and $p'$. By the lattice-structure of the grids, if $p + q_i, p + q_{i+1}$ are $r$-neighbours, then so are $p - q_i, p - q_{i+1}$. It follows that $(p = p - q_0), p - q_1, p - q_2, \ldots, p - q_n$ is a shortest $B$-path between $p$ and $p - q_n$. Obviously, for any $p, q \in \mathbb{G}$: $d(p, p - q; B) = d(p, p + q; B)$. The distance functions are also translation-invariant, so $d(p + q, p; B) = d(p, p - q; B)$. The result follows.

The triangular inequality (property (3)) is now considered. Assume, for some fixed $j \in \mathbb{Z}$, $B(j)$ is not faster than $B$. Let $p, q, r \in \mathbb{G}$ such that $(p = p_0), p_1, \ldots, p_j, (r = r_0), r_1, r_2, \ldots, (r_k = q)$ is a shortest $B$-path between $p$ and $q$ and such that (by assumption) $d(r, q; B) < d(r, q; B(j))$. Now, $d(p, q; B) = d(p, r; B) + d(r, q; B(j)) > d(p, r; B) + d(r, q; B)$.

Assume now that $B(i) \sqsupseteq B$ for all $i \in \mathbb{N}$. Again, let $p, q, r \in \mathbb{G}$ such that $(p = p_0), p_1, \ldots, p_i, (r = r_0), r_1, r_2, \ldots, (r_k = q)$ is a shortest $B$-path between $p$ and $q$. By Definition 3, $d(r, q; B) \geq d(r, q; B(i))$. Now, $d(p, q; B) = d(p, r; B) + d(r, q; B(i)) = d(p, r; B) + d(r, q; B(i)) \leq d(p, r; B) + d(r, q; B)$. □

As seen in the following example, the order of the $b(i)$: $s$ in $B$ is of importance for the metricity of the distance.

**Example 14.** Let $B_1 = (1, 2)$ and $B_2 = (2, 1)$. Now, $d(B_1)$ is a metric but $d(B_2)$ is not. We use the bcc grid as an example:

$$
3 = d((0, 0, 0), (2, 2, 0); B_2) > d((0, 0, 0), (2, 0, 0); B_2) + d((2, 0, 0), (2, 2, 0), B_2) = 2,
$$

so the triangular inequality is not fulfilled for $B_2$. We use Theorem 13 to show that $d(B_1)$ is a metric. We see that $B_1 = B_1(2k + 1)$ and $B_1(2) = B_1(2k)$, so we only need to check that $B_1(2) \sqsupseteq B_1$, which is trivially fulfilled.

5. **Best approximating neighbourhood sequences**

In this section, the sequence $B$ that gives the best approximation of the Euclidean distance will be computed. Let

$$
\mathcal{B}_G(B, k) = \{ q \in \mathbb{G} : d(0, q; B) \leq k \}.
$$
Fig. 2. The shape of $\mathcal{H}_G(B, k)$, where $1_B^k = 2_B^k = k/2$. Left: fcc, right: bcc.

These balls are digital polyhedra represented by the grid points in the respective grids. The convex hull of $B_G(B, k)$ in $\mathbb{R}^3$ is denoted as $\mathcal{H}_G(B, k)$. The polyhedra obtained can easily be compared to a Euclidean ball using area and volume measures. The shape of $\mathcal{H}_G(B, k)$ for $B$ and $k$ satisfying $1_B^k = 2_B^k = k/2$ is shown in Fig. 2.

Lemma 15. The vertices of $\mathcal{H}_G(B, k)$ are:

- $\mathbb{F}$: $\pm(1^k + 2 \cdot 2^k), \pm(1^k), 0$,

- $\mathbb{B}$: $\pm(1^k + 2 \cdot 2^k), \pm(1^k), \pm(1^k)$ and $\pm(1^k + 2^k), \pm(1^k + 2^k), \pm(1^k + 2^k)$,

and all possible permutations of the coordinates.

Proof. It is obvious that among the points having the same $B$-distance the points having maximal Euclidean distances from the origin are vertices of the polyhedron. The coordinates of these points are given by Corollaries 4 and 7 for fcc and bcc, respectively. It is easy to check that the number of these points gives exactly the number of possible vertices, therefore the statement is fulfilled. □

Using the vertices of the polyhedra, the surface area and the volume of the polyhedra are computed.

Lemma 16. Given a neighbourhood sequence $B$ and a positive integer $k$, the surface area and the volume of $\mathcal{H}_G(B, k)$ are

$$
A_F = 16(1^k + 2^k)^2\sqrt{3} - 12(1^k)^2\sqrt{3} + 12(1^k)^2,
$$

$$
A_B = 24(1^k)^2 + 24(2^k)^2\sqrt{2} + 48 \cdot 2^k 1^k \sqrt{2},
$$

$$
V_F = \frac{32}{3}(2^k)^3 + 32(2^k)^3 1^k + 32 \cdot 2^k (1^k)^2 + \frac{20}{3}(1^k)^3,
$$

$$
V_B = 16(2^k)^3 + 48(2^k)^3 1^k + 48 \cdot 2^k (1^k)^2 + 8(1^k)^3.
$$

The proof of Lemma 16 consists entirely of geometric calculations (volume integrals) and is omitted. The following compactness measure is used:

$$
E_G = \frac{A_B^3}{V_F^2} - \frac{36\pi}{36\pi},
$$

which is equal to zero if and only if $A$ is the surface area and $V$ is the volume of a Euclidean ball. First, the asymptotic optima are found. We substitute $1^k$ in the formulas in Lemma 16 with the real variable $\alpha$. With a fixed integer $k$, $2^k = k - \alpha$. The equation $\frac{dE_G}{d\alpha} = 0$ is now solved. The solutions in the interval $0 \leq \alpha \leq k$ are

$$
\alpha = \left(\frac{2}{3}(\sqrt{3} - 1)\sqrt{3}\right) k \approx 0.8453k
$$

for the fcc grid and

$$
\alpha = ((\sqrt{2} - 1)\sqrt{2})k \approx 0.5858k
$$

(6) (7)
Table 1
The optimal values of $1^k$ and $2^k$ for different $k$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$1^k$</th>
<th>$2^k$</th>
<th>$E_F$</th>
<th>$1^k$</th>
<th>$2^k$</th>
<th>$E_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0.3491</td>
<td>0</td>
<td>1</td>
<td>0.3505</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0.3491</td>
<td>1</td>
<td>1</td>
<td>0.2231</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>1</td>
<td>0.3274</td>
<td>2</td>
<td>1</td>
<td>0.2248</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>1</td>
<td>0.2949</td>
<td>2</td>
<td>2</td>
<td>0.2231</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>1</td>
<td>0.2832</td>
<td>3</td>
<td>2</td>
<td>0.2150</td>
</tr>
<tr>
<td>10</td>
<td>8</td>
<td>2</td>
<td>0.2832</td>
<td>6</td>
<td>4</td>
<td>0.2150</td>
</tr>
<tr>
<td>100</td>
<td>85</td>
<td>15</td>
<td>0.2794</td>
<td>59</td>
<td>41</td>
<td>0.2148</td>
</tr>
<tr>
<td>1000</td>
<td>845</td>
<td>155</td>
<td>0.2794</td>
<td>586</td>
<td>414</td>
<td>0.2147</td>
</tr>
</tbody>
</table>

for the bcc grid. These values give $E_F = 0.2794$ and $E_B = 0.2147$ independently of $k$. Optimally, the ratio $1^k : 2^k$ should equal $x : (k - x)$ with $x$ as in (6) and (7) for the fcc and bcc grids, respectively. This cannot be achieved in reality, since the values are irrational numbers and it would require neighbourhood sequences of infinite length. By using a sufficiently long initial part of the neighbourhood sequence, the ratio can be approximated as close as needed. Among the neighbourhood sequences of length $k$, the ones with closest approximations of the above ratios results in the distances with the least deviation from the Euclidean distance.

For $k = 1, 2, 3, 4, 5, 10, 100, 1000$, the values of $1^k$ and $2^k$ that give the lowest values of $E_G$ are listed in Table 1. Observe that, by Theorem 11 and 13, it is very easy to construct periodic neighbourhood sequences that generates metric distances. For example, the neighbourhood sequences with period 5 on the bcc grid with $1^k = 3$ and $2^k = 2$ generating metric distances are $(1, 1, 1, 2, 2)$ and $(1, 1, 2, 1, 2)$.

6. Conclusions

Several important contributions concerning distances based on neighbourhood sequences on the fcc and bcc grids have been presented. Since there are only two direct neighbours to each grid point in these grids, the theory becomes somewhat easier to handle compared to the cubic grid. For example, the condition for a distance being a metric presented in Theorem 11 is less complicated than in the cubic grid.

Furthermore formulas for computing the distances have been presented. These formulas have been used to define a compactness measure which then was used to calculate the theoretical optimal ratio between the number of 2-steps and 1-steps in a neighbourhood sequence. The compactness measure has also been used to evaluate which periodic neighbourhood sequences give the best results. Since the performance of the periodic neighbourhood sequences approaches the optimal limit resonably fast, a periodic neighbourhood sequence of length five seems to be a good choice if it is preferable to have a short neighbourhood sequence.

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