# Path-Based Distance Functions in $n$-Dimensional Generalizations of the Face- and Body-Centered Cubic Grids 

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#### Abstract

Path-based distance functions are defined on $n$-dimensional generalizations of the face-centered cubic and body-centered cubic grids. The distance functions use both weights and neighborhood sequences. These distances share many properties with traditional path-based distance functions, such as the city-block distance, but are less rotational dependent. For the three-dimensional case, we introduce four different error functions which are used to find the optimal weights and neighborhood sequences that can be used to define the distance functions with low rotational dependency.


## 1 Introduction

By adding a grid point in the center of each cube with vertices on grid points in a cubic grid, a body-centered cubic (bcc) grid is obtained. The face-centered cubic (fcc) is obtained by instead adding a grid point at the center of each face of the cubes. When using non-standard grids such as the fcc and bcc grids for 3D images, less samples are needed to obtain the same representation/reconstruction quality compared to the cubic grid [1]. This is one reason for the increasing interest in using these grids in, e.g., image acquisition [1], image processing [2-4], and visualization [5,6]. See also [7].

[^0]Optimal sampling in the sense of the Shannon sampling theorem is obtained when the reciprocal of a dense grid is used for representing the image. In this way, a sparse as possible grid is used for image representation [7]. The fcc grid is the densest three-dimensional point-lattice [8] and its reciprocal is the bcc grid. In number theory [8], the fcc grid is usually denoted $D_{3}$ and is a special case of the point-lattice $D_{n}$, here refered to as the $n$-dimensional fcc grid. The reciprocal of this point-lattice is $D_{n}^{*}$, here called the $n$-dimensional bcc grid. The $n$-dimensional fcc grid is the densest point-lattice in three, four, and five dimensions [8]. Thus, the $n$-dimensional fcc and bcc grids are potentially important for high-dimensional image processing. The 3-dimensional fcc and bcc grids can, e.g., be used when reconstructing, e.g., images from computed tomography with increased accuracy, see [1,7]. The results in this paper can be used to find appropriate distance functions for processing such images.

Measuring distances on digital grids is of great importance both in theory and in many applications. Because of its low rotational dependency, the Euclidean distance is often used as distance function. Even though the rotational dependency is higher, there are many reasons to use distances defined as minimal cost-paths instead. In some aspects, distance functions defined by minimal cost-paths fits the digital geometry-approach better, [9]. For example, the set of the points of the digital plane (square grid) having Euclidean distance, e.g., 9 from a point consists of four points far from each other. Instead, digital circles using some path-based distances (for instance, distances based on neighborhood sequences) are sets of consecutive neighbor points. Another aspect is that when minimal cost-paths are computed, a distance function defined as the minimal cost path between any two points is better suited, see, e.g., [10], where the constrained distance transform is computed using the Euclidean distance. The resulting algorithm is complex since distances can be propagated only to "visible points". The computational complexity (w.r.t. both time and space) of this algorithm is larger than the corresponding algorithm using a path-based approach which is simple, fast, and easy to generalize to higher dimensions $[11,12]$. We conclude that path-based digital distances are important both from a theoretical point of view and for several applications.

Examples of path-based distances are weighted distances, where weights define the cost (distance) between neighboring grid points [2,3,13], and distances based on neighborhood sequences, where the cost is fixed but the adjacency relation is allowed to vary along the path [4,14]. These path-based distance functions are generalizations of the well-known city-block and chessboard distance function defined for the square grid in [15]. We will abbreviate neighborhood sequence with $n s$, distance based on neighborhood sequences with $n s$-distances, and weighted distances based on neighborhood sequences with weighted ns-distances or just wns-distances.

Many approaches where the deviation from the Euclidean distance is mini-
mized in order to find the optimal ns (ns-distances) or weights (weighted distances) have been proposed for $\mathbb{Z}^{2}$. In most papers, error functions minimizing the asymptotic maximum difference of a Euclidean ball and a ball obtained by using ns-distances [16-19] or weighted distances [3,13,20] are minimized. Other approaches have also been considered for ns-distances. In [21], optimal ns for the 2D hexagonal and triangular grids are found using a compactness ratio - the ratio between the squared perimeter and the area of the convex hull of the disks obtained by using ns. In [22], the symmetric difference is used for ns in $\mathbb{Z}^{2}$ and in [23], the following error functions are considered for ns on the fcc and the bcc grids: absolute error, relative error, compactness ratio, maximal inscribed ball, and minimal covering ball.

In [16], a general definition allowing both weights and ns was presented. The full potential of using both weights and ns was discovered in [24], where ns and weights were together used in the sense of [16], but with the well-known natural neighborhood structure of $\mathbb{Z}^{2}$. In [24], the basic theory for weighted ns-distances on the square grid is presented including a formula for the distance between two points, conditions for metricity, optimal parameter calculation, and an algorithm to compute the distance transform. In [25], some basic theoretical results for weighted ns-distances on the fcc and bcc grids were presented. The theory for weighted ns-distances on the fcc and bcc grids was further developed in [26] by presenting sufficient conditions for metricity and algorithms that can be used to compute the distance transform and a minimal cost-path between two points. In [27] the theory for weighted distances based on neighborhood sequences with two neighborhood relations for the general case of point-lattices is considered.

The asymptotic error using the compactness ratio was used to find the optimal weights and ns for weighted ns-distances on the fcc and bcc grids in [25]. The basic analysis presented in [25] is extended in [28] by considering the relative error, the compactness ratio, the maximal inscribed ball, and the minimal covering ball. As in, e.g., $[3,13,16-18,20]$, the digital ball is compared with the Euclidean ball to get a measure of rotational dependency of a digital distance. Also, we analyze the behavior when ns of finite length, i.e., periodic ns is used. Note that the results presented here also applies to weighted distances and ns-distances, since they are both special cases of the proposed distance function. The distance function proposed here is used to find optimal weights for the weighted distance and optimal ns for ns-distances. It follows that the rotational dependency for the weighted ns-distance is less than or equal to both the weighted distance and the ns-distance.

When the paper [28] was presented at the 12 th international workshop on combinatorial image analysis (IWCIA 2008), there were several questions and comments about $n$-dimensional generalizations of the fcc and bcc grids. Therefore, in this paper, some results are extended to higher dimensions.

This paper consists of two parts. First, we define weighted ns-distances in the $n$-dimensional fcc and bcc grids by applying the theoretical framework presented in [27] to these grids. Formulas for point-to-point distance and conditions for metricity are presented. We also present the optimal parameter computations for the 3D fcc and bcc grids from [28].

## 2 Distance Functions and Grids

We will now give definitions of $n$-dimensional generalizations of the fcc and bcc grids. Using some previous results, we will also define the ns-distance and the weighted ns-distance for these grids. Let the set $\mathcal{N}_{1}=\left\{\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{M}\right\}$ define the 1-neighbors of the point $\mathbf{0}$ in a point-lattice $\mathbb{G}$. Let also $\mathcal{N}_{2}=$ $\left\{\mathbf{u}_{1}, \mathbf{u}_{2}, \ldots, \mathbf{u}_{N}\right\}$ define the strict 2-neighbors. We denote the set of 2-neighbors by $\mathcal{N}_{1,2}=\mathcal{N}_{1} \cup \mathcal{N}_{2}$.

A ns $B$ is a sequence $B=(b(i))_{i=1}^{\infty}$, where each $b(i)$ denotes a neighborhood relation in $\mathbb{G}$. If $B$ is periodic, i.e., if for some fixed strictly positive $l \in \mathbb{Z}_{+}$, $b(i)=b(i+l)$ is valid for all $i \in \mathbb{Z}_{+}$, then we write $B=(b(1), b(2), \ldots, b(l))$. A path, denoted $\mathcal{P}$, in a grid is a sequence $\mathbf{p}_{0}, \mathbf{p}_{1}, \ldots, \mathbf{p}_{n}$ of adjacent grid points. A path is a $B$-path of length $n$ if, for all $i \in\{1,2, \ldots, n\}, \mathbf{p}_{i-1}$ and $\mathbf{p}_{i}$ are $b(i)$-neighbors. The notation 1- and (strict) 2-steps will be used for a step to a 1-neighbor and step to a (strict) 2-neighbor, respectively.

Definition 1 Given the ns $B$, the ns-distance $d\left(\mathbf{p}_{0}, \mathbf{p}_{n} ; B\right)$ between the points $\mathbf{p}_{0}$ and $\mathbf{p}_{n}$ is the length of (one of) the shortest $B$-path(s) between the points.

Let the real numbers $\alpha$ and $\beta$ (the weights) and a path $\mathcal{P}$ of length $n$, where exactly $l(l \leq n)$ adjacent grid points in the path are strict 2 -neighbors, be given. The length of the $(\alpha, \beta)$-weighted $B$-path $\mathcal{P}$ is $(n-l) \alpha+l \beta$. The $B$ path $\mathcal{P}$ between the points $\mathbf{p}_{0}$ and $\mathbf{p}_{n}$ is a minimal $\operatorname{cost}(\alpha, \beta)$-weighted $B$-path between the points $\mathbf{p}_{0}$ and $\mathbf{p}_{n}$ if no other $(\alpha, \beta)$-weighted $B$-path between the points is shorter than the length of the $(\alpha, \beta)$-weighted $B$-path $\mathcal{P}$.

Definition 2 Given the ns $B$ and the weights $\alpha, \beta$, the weighted ns-distance $d_{\alpha, \beta}\left(\mathbf{p}_{0}, \mathbf{p}_{n} ; B\right)$ is the length of (one of) the minimal cost $(\alpha, \beta)$-weighted $B$ path(s) between the points.

The following notation is used:

$$
\mathbf{1}_{B}^{k}=|\{i: b(i)=1,1 \leq i \leq k\}| \text { and } \mathbf{2}_{B}^{k}=|\{i: b(i)=2,1 \leq i \leq k\}|
$$

We associate with the sets $\mathcal{N}_{1}$ and $\mathcal{N}_{1,2}$ the chamfer masks $\mathbf{C}_{1}=\left\{\left(\mathbf{v}_{i}, 1\right)\right\}_{i=1}^{M}$ and $\mathbf{C}_{2}=\mathbf{C}_{1} \cup\left\{\left(\mathbf{u}_{i}, 1\right)\right\}_{i=1}^{N}$. The vectors in $\mathcal{N}_{1}$ and $\mathcal{N}_{1,2}$ are associated with
weight 1 , and the chamfer masks are thus nothing but unit weighted vectors. A $\mathbb{G}$-basis wedge of any chamfer mask $\mathbf{C}\left(\mathbf{C}\right.$ could be, e.g., either $\mathbf{C}_{1}$ or $\left.\mathbf{C}_{2}\right)$ is a set of $n$ linearly independent vectors $\mathbf{v}_{i_{1}}, \mathbf{v}_{i_{1}}, \ldots, \mathbf{v}_{i_{n}}$ from $\mathbf{C}$ such that

- $\mathbf{v}_{i_{1}}, \mathbf{v}_{i_{1}}, \ldots, \mathbf{v}_{i_{n}}$ is a basis of $\mathbb{G}$ and
- no vector of $\mathbf{C}$ except $\mathbf{v}_{i_{1}}, \mathbf{v}_{i_{1}}, \ldots, \mathbf{v}_{i_{n}}$ can be written as a linear combination with positive (not necesarily integer-valued) coefficients of these vectors.

See [3] for details. Each wedge defines a polytope by the convex hull of $\mathbf{0}$ and the points $\mathbf{0}+\mathbf{v}_{i_{j}}$. With unit weights, the polytope $\mathcal{B}_{\mathbf{C}}$ of a chamfer mask $\mathbf{C}$, [3], is the union of the polytopes of the wedges.

Definition 3 A chamfer mask with unit weights is restricted (see [3]) if

$$
\begin{align*}
& \text { (symmetry) }(\mathbf{v}, \omega) \in \mathbf{C} \Longrightarrow(-\mathbf{v}, \omega) \in \mathbf{C}  \tag{1}\\
& \forall \mathbf{p} \in \mathbb{G}, \exists \mathcal{W} \text { of } \mathbf{C} \text { such that } \\
& \text { (Organized in } \mathbb{G} \text {-basis-wedges) }  \tag{2}\\
& \mathbf{p} \in \mathcal{W} \text { and } \mathcal{W} \text { is a } \mathbb{G} \text {-basis-wedge. } \\
& \text { (Convex normalized polytope) } \mathcal{B}_{\mathbf{C}}=\operatorname{conv}\left(\mathcal{B}_{\mathrm{C}}\right) \text {. } \tag{3}
\end{align*}
$$

Definition 4 A grid $\mathbb{G}$ is wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ if $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ are such that

- $\mathbf{C}_{1}=\left\{\left(\mathbf{v}_{i}, 1\right)\right\}_{i=1}^{M}$ and $\mathbf{C}_{2}=\mathbf{C}_{1} \cup\left\{\left(\mathbf{w}_{i}, 1\right)\right\}_{i=1}^{N}$ are restricted Chamfer masks, - $\forall i, \exists j, k: \mathbf{w}_{i}=\mathbf{v}_{j}+\mathbf{v}_{k}$, and
- each $\mathbb{G}$-basis-wedge of $\mathcal{N}_{1}$ is the union of some $\mathbb{G}$-basis-wedges of $\mathcal{N}_{1,2}$.

In [27], the ns-distance and the weighted ns-distance were presented for an arbitrary point-lattice $\mathbb{G}$ wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$. Let $d_{\mathbf{C}_{1}}$ be the distance function obtained by using the Chamfer mask $\mathbf{C}_{1}$ and $d_{\mathbf{C}_{2}}$ be the distance function obtained by using the Chamfer mask $\mathbf{C}_{2}$. In other words, for any points $\mathbf{p}, \mathbf{q} \in \mathbb{G}, d_{\mathbf{C}_{1}}(\mathbf{p}, \mathbf{q})$ is the length of the shortest path between $\mathbf{p}$ and $\mathbf{q}$ using only local steps from $\mathcal{N}_{1}$ and $d_{\mathbf{C}_{2}}(\mathbf{p}, \mathbf{q})$ is the length of the shortest path between $\mathbf{p}$ and $\mathbf{q}$ using local steps from $\mathcal{N}_{1,2}$. The following theorems are proved in [27].

Theorem 5 (ns-distance in $\mathbb{G}$ wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ ) Let $\mathbb{G}$ wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$, the neighborhood sequence $B$ and the points $\mathbf{p}, \mathbf{q} \in \mathbb{G}$ be given. Then

$$
d(\mathbf{p}, \mathbf{q} ; B)=\min \left\{k \mid k \geq \max \left\{d_{\mathbf{C}_{2}}(\mathbf{p}, \mathbf{q}), d_{\mathbf{C}_{1}}(\mathbf{p}, \mathbf{q})-\mathbf{2}_{B}^{k}\right\}\right\} .
$$

When the square grid is considered and $d_{\mathbf{C}_{2}}$ is the chessboard distance and $d_{\mathbf{C}_{1}}$ is the city-block distance, the ns-distance is less than (or equal to) the city-block distance and greater than (or equal to) the chessboard distance.

Theorem 5 says that by replacing pairs of 1 -steps from $d_{\mathbf{C}_{1}}$ with as many 2 -steps as the sequence allows, the ns-distance is obtained.

Remark 6 We will consider weights $\alpha$ and $\beta$ as real numbers $\alpha$ and $\beta$ such that $0<\alpha \leq \beta \leq 2 \alpha$. This is natural since

- a 2-step should be more expensive than a 1-step since strict 2-neighbors are intuitively at a larger distance than 1-neighbors (projection property) and
- two 1-steps should be more expensive than a 2-step - otherwise no 2-steps would be used in a minimal cost-path.

In the following theorem, the 1 -steps are weighted with $\alpha$ and the 2 -steps are weighted with $\beta$. A formal proof is found in [27].

Theorem 7 (Weighted ns-distance in $\mathbb{G}$ wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ ) Let $\mathbb{G}$ wedge-D-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$, the ns $B$, the weights $\alpha$, $\beta$ such that $0<\alpha \leq \beta \leq 2 \alpha$, and the points $\mathbf{p}, \mathbf{q} \in \mathbb{G}$ be given. Then

$$
d_{\alpha, \beta}(\mathbf{p}, \mathbf{q} ; B)=\left(2 d(\mathbf{p}, \mathbf{q} ; B)-d_{\mathbf{C}_{1}}(\mathbf{p}, \mathbf{q})\right) \alpha+\left(d_{\mathbf{C}_{1}}(\mathbf{p}, \mathbf{q})-d(\mathbf{p}, \mathbf{q} ; B)\right) \beta
$$

We will now define $n$-dimensional generalizations of the fcc and bcc grids and apply Theorem 5 and 7 to these grids.

### 2.1 The $n$-dimensional fcc grid

We use the following definition of the $n$-dimensional fcc grid for $n \geq 3$ :

$$
\mathbb{F}^{n}=\left\{\mathbf{p} \in \mathbb{Z}^{n}: x_{1}+x_{2}+\ldots+x_{n} \equiv 0 \quad(\bmod 2)\right\}
$$

together with the straight-forward generalization of the neighborhoods in the three-dimensional grid $\mathbb{F}$ used in, e.g., $[4,25,26,28]$, to get the natural neighborhoods $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ for $\mathbb{F}^{n}$ :

$$
\begin{aligned}
& \mathcal{N}_{1}=\left\{\mathbf{v}=\left(v_{1}, v_{2}, \ldots, v_{n}\right) \in \mathbb{F}^{n}: \max \left\{\left|v_{i}\right|\right\}=1 \text { and } \sum\left|v_{i}\right|=2\right\} \\
& \mathcal{N}_{2}=\left\{\mathbf{v}=\left(v_{1}, v_{2}, \ldots, v_{n}\right) \in \mathbb{F}^{n}: \max \left\{\left|v_{i}\right|\right\}=2 \text { and } \sum\left|v_{i}\right|=2\right\} .
\end{aligned}
$$

The following lemma gives a sufficient and necessary condition for a set of vectors in $\mathbb{F}^{n}$ to be a basis of $\mathbb{F}^{n}$.

Lemma $8 A$ set $\mathcal{F}=\left\{\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}\right\}$ of vectors in $\mathbb{F}^{n}$ is a basis of $\mathbb{F}^{n}$ iff

$$
\operatorname{det}\left(\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}\right)= \pm 2
$$

The proof of Lemma 8 is technical and is therefore omitted. The lemma can be proved analogously to Lemma 4.2 in [3]. To do so, we need to prove that any determinant of the vectors $\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}$ of $\mathbb{F}^{n}$ is a multiple of 2 . Indeed, given any vector $\mathbf{v}=\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{F}^{n}, x_{1}=\sum_{i=2}^{n} x_{i}+2 a$ for some integer $a$. Then

$$
\mathbf{v}=\left(2 a, x_{2}-\sum_{i=2}^{n} x_{i}, x_{3}-\sum_{i=2}^{n} x_{i}, \ldots, x_{n}-\sum_{i=2}^{n} x_{i}\right)
$$

It follows that both $\left|\operatorname{det}\left(\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}\right)\right|$ and that $\left|\operatorname{det}\left(\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{w}, \ldots, \mathbf{v}_{n}\right)\right|$, where $\mathbf{w} \in \mathbb{F}^{n}$, are divisible by 2 .

The following remark is used to find the wedges used to define the weighted ns-distance for $\mathbb{F}^{n}$.

Remark 9 The systems of equations

$$
\left(\begin{array}{ccccccc}
1 & 1 & 1 & \cdots & 1 & 1 & 1 \\
1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
0 & 0 & 0 & \cdots & 1 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 & -1
\end{array}\right)\left(\begin{array}{c}
a_{1} \\
a_{2} \\
a_{3} \\
\vdots \\
a_{n-1} \\
a_{n}
\end{array}\right)=\left(\begin{array}{c}
x_{1} \\
x_{2} \\
x_{3} \\
\vdots \\
x_{n-1} \\
x_{n}
\end{array}\right)
$$

and

$$
\left(\begin{array}{ccccccc}
1 & 1 & 1 & \cdots & 1 & 1 & 2 \\
1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
0 & 0 & 0 & \cdots & 1 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 & 0
\end{array}\right)\left(\begin{array}{c}
b_{1} \\
b_{2} \\
b_{3} \\
\vdots \\
b_{n-1} \\
b_{n}
\end{array}\right)=\left(\begin{array}{c}
x_{1} \\
x_{2} \\
x_{3} \\
\vdots \\
x_{n-1} \\
x_{n}
\end{array}\right) .
$$

have solutions

$$
\begin{aligned}
a_{1} & =x_{2} \\
a_{2} & =x_{3} \\
& \vdots \\
a_{n-2} & =x_{n-1} \\
a_{n-1} & =\frac{x_{1}+x_{n}-\left(x_{2}+\ldots+x_{n-1}\right)}{2} \\
a_{n} & =\frac{x_{1}-\left(x_{2}+x_{3}+\ldots+x_{n}\right)}{2} \text { and }
\end{aligned}
$$

$$
\begin{aligned}
b_{1} & =x_{2} \\
b_{2} & =x_{3} \\
& \vdots \\
b_{n-1} & =x_{n} \\
b_{n} & =\frac{x_{1}-\left(x_{2}+x_{3}+\ldots+x_{n}\right)}{2}
\end{aligned}
$$

which are all non-negative when $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$ and $x_{1} \geq x_{2}+x_{3}+\ldots+x_{n}$.
The following lemma says that to find a shortest path between $\mathbf{0}$ and any point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{F}^{n}$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n} \geq 0$ and $x_{1} \leq \sum_{i=2}^{n} x_{i}$, it is enough to use only 1 -steps.

Lemma 10 For any point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{F}^{n}$ such that $x_{1} \geq x_{2} \geq$ $\ldots \geq x_{n} \geq 0$ and $x_{1} \leq \sum_{i=2}^{n} x_{i}$, the following algorithm terminates in $\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$ steps.

Initially, let $j=1$ and $\mathbf{q}_{j}=\mathbf{p}$.
$\star$ Decrease the two largest coordinate values in $\mathbf{q}_{j}$ by 1, increase $j$ by 1 and let the result be $\mathbf{q}_{j}$.
Repeat $\star$ until $\mathbf{q}_{j}=\mathbf{0}$.

PROOF. Since the sum of coordinates is even by definition, $\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$ is an integer. It follows from $x_{1} \leq \sum_{i=2}^{n} x_{i}$ that, if $\mathbf{q}_{i} \neq \mathbf{0}$, there will always be at least two coordinates with positive values: Assume that this is not the case, then at some step $\mathbf{q}_{i}=(b, 0,0, \ldots, 0)$, where $b>0$. Since the coordinate with the largest value is decreased in each step, $x_{1}=b+\sum_{i=2}^{n} x_{i}$. But this contradicts that $x_{1} \leq \sum_{i=2}^{n} x_{i}$.

Now we give a formula that gives the ns-distance in the $n$-dimensional facecentered cubic grid.

Theorem 11 (ns-distance in $\mathbb{F}^{n}$ ) Let $\mathbb{F}^{n}$ be wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ and let the neighborhood sequence $B$ and the point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n} \geq 0$ be given. Then

$$
d(\mathbf{0}, \mathbf{p} ; B)=\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}, x_{1}-\mathbf{2}_{B}^{l}\right\}\right.\right\} .
$$

PROOF. First the case $x_{1} \geq x_{2}+x_{3}+\ldots+x_{n}$ is considered. With the neighborhoods $\mathcal{N}_{1}$ and $\mathcal{N}_{1,2}$, we use

$$
\left.\mathcal{F}_{1}=\left\{\begin{array}{c}
(1,1,0, \cdots, 0,0, \\
(1,0,1, \cdots, 0,0, \\
\vdots
\end{array}\right)\right\}
$$

and

$$
\mathcal{F}_{2}=\left\{\begin{array}{c}
(1,1,0, \cdots, 0,0,0) \\
(1,0,1, \cdots, 0,0,0) \\
\vdots \\
(1,0,0, \cdots, 0,0,1) \\
(2,0,0, \cdots, 0,0,0)
\end{array}\right\}
$$

By Lemma 8 , the sets $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ are bases of $\mathbb{F}^{n}$ and by Remark 9 , any point $\mathbf{p}$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$ and $x_{1} \geq x_{2}+x_{3}+\ldots+x_{n}$ can be written as a linear combination of vectors from $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ with positive coefficients. Therefore, $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ define the 1 -wedge and 2 -wedge for any point $\mathbf{p}$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$ and $x_{1} \geq x_{2}+x_{3}+\ldots+x_{n}$. Remark 9 gives the number of local steps needed to reach the point $\mathbf{p}$, i.e., $d_{\mathbf{C}_{1}}(\mathbf{0}, \mathbf{p} ; B)=\sum a_{i}=x_{1}$ and $d_{\mathbf{C}_{2}}(\mathbf{0}, \mathbf{p} ; B)=\sum b_{i}=\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$. Using Theorem 5, we get the formula in Theorem 11.

For the case $x_{1} \leq x_{2}+x_{3}+\ldots+x_{n}$, we have not found the wedges in the general $n$-dimensional case. It is, however, clear that the ns-distance is $\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$ independent of the neighborhood sequence $B$ (using only local steps from $\mathcal{N}_{1}$ ) as Lemma 10 shows.

Since $x_{1} \leq x_{2}+x_{3}+\ldots+x_{n}$, the path $\left\langle\mathbf{q}_{j}, \mathbf{q}_{j-1}, \ldots, \mathbf{q}_{1}\right\rangle$ obtained from the algorithm in Lemma 10 is a path of length $\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$ using only local steps from $\mathcal{N}_{1}$. Also, $\frac{x_{1}+x_{2}+\ldots+x_{n}}{2} \geq x_{1} \geq x_{1}-2_{B}^{k}$ for any $B$ and $k$, so the formula in Theorem 11 is valid.

As one can see there are two cases. In the first case a shortest path is obtained by only 1-steps; while in the second case $\left(x_{1}>x_{2}+\ldots+x_{n}\right) 2$-steps should be considered to find the shortest path. Now we give the cost of a minimal cost path when the weights $\alpha$ and $\beta$ are used.

Theorem 12 (weighted ns-distance in $\mathbb{F}^{n}$ ) Let $\mathbb{F}^{n}$ be wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ and let the ns $B$, the weights $\alpha$, $\beta$ s.t. $0<\alpha \leq \beta \leq 2 \alpha$,
and the point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{F}^{n}$, where $x_{1} \geq x_{2} \geq \ldots \geq x_{n} \geq 0$, be given. The weighted $n s$-distance between $\mathbf{0}$ and $\mathbf{p}$ is given by

$$
\begin{aligned}
d_{\alpha, \beta}(\mathbf{0}, \mathbf{p} ; B) & =\left\{\begin{array}{cc}
k \cdot \alpha & \text { if } x_{1} \leq \sum_{i=2}^{n} x_{i} \\
\left(2 k-x_{1}\right) \cdot \alpha+\left(x_{1}-k\right) \cdot \beta & \text { otherwise }
\end{array}\right. \\
\text { where } k & =\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}, x_{1}-\mathbf{2}_{B}^{l}\right\}\right.\right\} .
\end{aligned}
$$

PROOF. We use Theorem 7. By the proof of Theorem 11, we know that $d(\mathbf{0}, \mathbf{p} ; B)=d_{\mathbf{C}_{1}}(\mathbf{0}, \mathbf{p})=\frac{x_{1}+x_{2}+\ldots+x_{n}}{2}$ when $x_{1} \leq \sum_{i=2}^{n} x_{i}$. For the case $x_{1} \geq$ $\sum_{i=2}^{n} x_{i}$, both $d(\mathbf{0}, \mathbf{p} ; B)$ and $d_{\mathbf{C}_{1}}(\mathbf{0}, \mathbf{p})$ are given in the proof of Theorem 11.

### 2.2 The $n$-dimensional bcc grid

An $n$-dimensional generalization of the bcc grid for $n \geq 3$ is:

$$
\mathbb{B}^{n}=\left\{\mathbf{p} \in \mathbb{Z}^{n}: x_{1} \equiv x_{2} \equiv \ldots \equiv x_{n} \quad(\bmod 2)\right\}
$$

We use the straight-forward generalizations of the neighborhoods in the threedimensional grid $\mathbb{B}$ used in, e.g., $[4,25,26,28]$, to get the natural neighborhoods $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ for $\mathbb{B}^{n}$ :

$$
\begin{aligned}
& \mathcal{N}_{1}=\left\{\mathbf{v}=\left(v_{1}, v_{2}, \ldots, v_{n}\right) \in \mathbb{B}^{n}:\left|v_{i}\right|=1 \text { for all } 1 \leq i \leq n\right\} \\
& \mathcal{N}_{2}=\left\{\mathbf{v}=\left(v_{1}, v_{2}, \ldots, v_{n}\right) \in \mathbb{B}^{n}: \sum\left|v_{i}\right|=2\right\} .
\end{aligned}
$$

Now a technical lemma follows for $\mathbb{B}^{n}$ analogously to the role of Lemma 8 in $\mathbb{F}^{n}$.

Lemma $13 A$ set $\mathcal{F}=\left\{\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}\right\}$ of vectors in $\mathbb{F}^{n}$ is a basis of $\mathbb{B}^{n}$ iff

$$
\operatorname{det}\left(\mathbf{v}_{1}, \mathbf{v}_{2}, \ldots, \mathbf{v}_{n}\right)= \pm 2^{n-1}
$$

The lemma can be proven using the same technique as in the proof of Lemma 8 by noting that for any point $\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{B}^{n}$, there are integers $a_{j}$ such that $x_{j}=x_{1}+2 a_{j}$ for all $j>1$.

We now find the wedges used to define the weighted ns-distance on $\mathbb{B}^{n}$.

Remark 14 The systems of equations

$$
\left(\begin{array}{ccccccc}
1 & 1 & 1 & \cdots & 1 & 1 & -1 \\
1 & 1 & 1 & \cdots & 1 & -1 & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
1 & 1 & -1 & \cdots & -1 & -1 & -1 \\
1 & -1 & -1 & \cdots & -1 & -1 & -1
\end{array}\right)\left(\begin{array}{c}
a_{1} \\
a_{2} \\
\vdots \\
a_{n-1} \\
a_{n}
\end{array}\right)=\left(\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{n-1} \\
x_{n}
\end{array}\right)
$$

and

$$
\left(\begin{array}{ccccccc}
1 & 1 & 1 & \cdots & 1 & 1 & 2 \\
1 & 1 & 1 & \cdots & 1 & 1 & 0 \\
1 & 1 & 1 & \cdots & 1 & -1 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \\
1 & 1 & -1 & \cdots & -1 & -1 & 0 \\
1 & -1 & -1 & \cdots & -1 & -1 & 0
\end{array}\right)\left(\begin{array}{c}
b_{1} \\
b_{2} \\
\vdots \\
b_{n-1} \\
b_{n}
\end{array}\right)=\left(\begin{array}{c}
x_{1} \\
x_{2} \\
\vdots \\
x_{n-1} \\
x_{n}
\end{array}\right)
$$

have solutions

$$
\begin{aligned}
& a_{1}=\frac{x_{1}+x_{n}}{2}, a_{2}=\frac{x_{n-1}-x_{n}}{2}, a_{3}=\frac{x_{n-2}-x_{n-1}}{2}, \ldots, a_{n}=\frac{x_{1}-x_{2}}{2} \text { and } \\
& b_{1}=\frac{x_{2}+x_{n}}{2}, b_{2}=\frac{x_{n-1}-x_{n}}{2}, b_{3}=\frac{x_{n-2}-x_{n-1}}{2}, \ldots, b_{n}=\frac{x_{1}-x_{2}}{2}
\end{aligned}
$$

which are all non-negative when $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$.

The ns-distance is given for the $n$-dimensional bcc grid in the following corollary.

Theorem 15 (ns-distance in $\mathbb{B}^{n}$ ) Let $\mathbb{B}^{n}$ be wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ and let the neighborhood sequence $B$ and the point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right)$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n} \geq 0$ be given. Then

$$
d(\mathbf{0}, \mathbf{p} ; B)=\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x_{1}+x_{2}}{2}, x_{1}-\mathbf{2}_{B}^{l}\right\}\right.\right\} .
$$

PROOF. With the neighborhoods $\mathcal{N}_{1}$ and $\mathcal{N}_{1,2}$, we use

$$
\left.\left.\mathcal{F}_{1}=\left\{\begin{array}{cccc}
(1, & 1, & 1, \cdots, & 1, \\
(1, & 1, & 1, \cdots, & 1,-1,-1
\end{array}\right)\right\} \begin{array}{c}
\vdots \\
(1, \\
1,
\end{array}\right)
$$

and

$$
\mathcal{F}_{2}=\left\{\begin{array}{cccc}
(1,1, & 1, \cdots, & 1, & 1,-1
\end{array}\right)
$$

By Lemma 13 , the sets $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ are bases of $\mathbb{B}^{n}$ and by Remark 14 , any point $\mathbf{p}$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$ can be written as a linear combination of vectors from $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ with positive coefficients. Therefore, $\mathcal{F}_{1}$ and $\mathcal{F}_{2}$ define the 1-wedge and 2-wedge for any point $\mathbf{p}$ such that $x_{1} \geq x_{2} \geq \ldots \geq x_{n}$. Remark 14 gives $d_{\mathbf{C}_{1}}(\mathbf{0}, \mathbf{p} ; B)=\sum a_{i}=x_{1}$ and $d_{\mathbf{C}_{2}}(\mathbf{0}, \mathbf{p} ; B)=\sum b_{i}=\frac{x_{1}+x_{2}}{2}$. Using Theorem 5, we get the formula in Theorem 15.

As the following corollary states, by adding weights to the shortest paths, the weighted ns-distance is given.

Theorem 16 (weighted ns-distance in $\mathbb{B}^{n}$ ) Let $\mathbb{B}^{n}$ be wedge-2-generated by $\mathcal{N}_{1}$ and $\mathcal{N}_{2}$ and let the ns $B$, the weights $\alpha$, $\beta$ s.t. $0<\alpha \leq \beta \leq 2 \alpha$, and the point $\mathbf{p}=\left(x_{1}, x_{2}, \ldots, x_{n}\right) \in \mathbb{B}^{n}$, where $x_{1} \geq x_{2} \geq \ldots \geq x_{n} \geq 0$, be given. The weighted ns-distance between $\mathbf{0}$ and $\mathbf{p}$ is given by

$$
\begin{aligned}
d_{\alpha, \beta}(\mathbf{0}, \mathbf{p} ; B) & =\left(2 k-x_{1}\right) \cdot \alpha+\left(x_{1}-k\right) \cdot \beta \\
\text { where } k & =\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x_{1}+x_{2}}{2}, x_{1}-\mathbf{2}_{B}^{l}\right\}\right.\right\} .
\end{aligned}
$$

PROOF. Both $d(\mathbf{0}, \mathbf{p} ; B)$ and $d_{\mathbf{C}_{1}}(\mathbf{0}, \mathbf{p})$ are given in Theorem 15 and its proof. Applying the formula in Theorem 7 gives the result.

Not all weights and ns give metric distance functions. The following sufficient conditions for metricity valid for the distance functions presented here were derived in [27] for a general case that contains these special subcases.

Theorem 17 If

$$
\begin{aligned}
& \sum_{i=1}^{N} b(i) \leq \sum_{i=j}^{j+N-1} b(i) \forall j, N \geq 1 \text { and } \\
& \quad 0<\alpha \leq \beta \leq 2 \alpha
\end{aligned}
$$

then $d_{\alpha, \beta}(\cdot, \cdot ; B)$ is a metric on $\mathbb{F}^{n}$ and $\mathbb{B}^{n}$.

## 3 Optimization of Weights and Neighborhood Sequences for 3D

In three dimensions, we have the following special-case of $\mathbb{F}^{n}$ and $\mathbb{B}^{n}$ for $n=3$ :

$$
\begin{align*}
& \mathbb{F}=\{(x, y, z): x, y, z \in \mathbb{Z} \text { and } x+y+z \equiv 0 \quad(\bmod 2)\}  \tag{4}\\
& \mathbb{B}=\{(x, y, z): x, y, z \in \mathbb{Z} \text { and } x \equiv y \equiv z \quad(\bmod 2)\} \tag{5}
\end{align*}
$$

The neighborhood relations are visualized in Figure 1 by showing the Voronoi regions, i.e. the voxels, corresponding to some adjacent grid points.

When $n=3$ in Theorem 11 and 15, we get the following two formulas.
Corollary 18 Let the ns $B$, the weights $\alpha, \beta$ and the point $(x, y, z) \in \mathbb{F}$, where $x \geq y \geq z \geq 0$, be given. The weighted ns-distance between $\mathbf{0}$ and $(x, y, z)$ is given by


Fig. 1. The grid points corresponding to the dark and the light grey voxels are 1-neighbors. The grid points corresponding to the dark grey and white voxels are (strict) 2-neighbors. Left: fcc, $\mathbb{F}^{3}$, right: bcc, $\mathbb{B}^{3}$.

$$
\begin{aligned}
& d_{\alpha, \beta}(\mathbf{0},(x, y, z) ; B)=\left\{\begin{array}{cc}
\frac{x+y+z}{2} \cdot \alpha & \text { if } x \leq y+z \\
(2 k-x) \cdot \alpha+(x-k) \cdot \beta & \text { otherwise }
\end{array}\right. \\
& \text { where } k=\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x+y+z}{2}, x-\mathbf{2}_{B}^{l}\right\}\right.\right\}
\end{aligned}
$$

The value of $k$ is the smallest integer, not less than $\frac{x+y+z}{2}$, such that $\mathbf{2}_{B}^{k}+k \geq x$.
Corollary 19 Let the ns $B$, the weights $\alpha$, $\beta$, and the point $(x, y, z) \in \mathbb{B}$, where $x \geq y \geq z \geq 0$, be given. The weighted ns-distance between $\mathbf{0}$ and $(x, y, z)$ is given by

$$
\begin{aligned}
d_{\alpha, \beta}(\mathbf{0},(x, y, z) ; B) & =(2 k-x) \cdot \alpha+(x-k) \cdot \beta \text {, where } \\
k & =\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x+y}{2}, x-\mathbf{2}_{B}^{l}\right\}\right.\right\} .
\end{aligned}
$$

Here $k$ is the smallest integer, not less than $\frac{x+y}{2}$, such that $\mathbf{2}_{B}^{k}+k \geq x$.
The optimization is carried out in $\mathbb{R}^{3}$ by finding the best shape of polyhedra corresponding to balls of constant radii using the proposed distance functions. To do this, the distance functions presented for the fcc and bcc grids in the previous section are stated in a form that is valid for all points $(x, y, z) \in \mathbb{R}^{3}$, where $x \geq y \geq z \geq 0$. Note that this gives the asymptotic shape of the balls. The following distance functions are considered:

$$
\begin{aligned}
& d_{\alpha, \beta}^{f c c}(\mathbf{0},(x, y, z) ; \gamma)=\left\{\begin{array}{cc}
\frac{x+y+z}{2} \cdot \alpha & \text { if } x \leq y+z \\
(2 k-x) \cdot \alpha+(x-k) \cdot \beta & \text { otherwise }
\end{array}\right. \\
& \text { where } k=\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x+y+z}{2},\right.\right.\right. \\
&\left.\left.\frac{x}{2-\gamma}\right\}\right\}
\end{aligned}
$$

and

$$
\begin{aligned}
d_{\alpha, \beta}^{b c c}(\mathbf{0},(x, y, z) ; \gamma) & =(2 k-x) \cdot \alpha+(x-k) \cdot \beta, \text { where } \\
k & =\min \left\{l \left\lvert\, l \geq \max \left\{\frac{x+y}{2}, \frac{x}{2-\gamma}\right\}\right.\right\},
\end{aligned}
$$

where $k \in \mathbb{R}$ and $\gamma \in \mathbb{R}, 0 \leq \gamma \leq 1$ is the fraction of the steps where 2-steps are not allowed (so $\mathbf{1}_{B}^{k}$ and $\mathbf{2}_{B}^{k}$ corresponds to $\gamma k$ and $(1-\gamma) k$, respectively). Note that $k \geq x /(2-\gamma)$ if and only if $(1-\gamma) k+k \geq x$, which is analogous to the condition $2_{B}^{k}+k \geq x$ of Corollary 18 and 19. In this way we obtain a distance function defined on $\mathbb{R}^{3}$ (for points $(x, y, z)$ such that $x \geq y \geq z \geq 0$ ) that
behaves like the distance function in discrete space $\mathbb{G}$ does asymptotically. By considering

$$
\begin{equation*}
d_{\alpha, \boldsymbol{\beta}}^{f c c}(\mathbf{0},(x, y, z) ; \gamma)=r \text { and } d_{\alpha, \boldsymbol{\beta}}^{b c c}(\mathbf{0},(x, y, z) ; \gamma)=r, \tag{6}
\end{equation*}
$$

for some radius $r$, the points on a sphere of constant radius $r$ are found. When $\gamma \in \mathbb{R}(0<\gamma<1)$ the functions $d^{f c c}$ and $d^{b c c}$ can be understood as asymptotic approximations to the distance functions of Corollary 18 and 19 for large values of $x$.

For any triplet $\alpha, \beta, \gamma(\alpha, \beta>0$ and $0 \leq \gamma \leq 1)$, (6) defines polyhedra $P$ in $\mathbb{R}^{3}$. The vertices of the polyhedra are derived in [25]. Based on this, up to permutation of the coordinates and change of signs, the vertices of polyhedra with radius $r$ are


Fig. 2. Shapes of balls for $d_{\alpha, \beta}^{f c c}(\cdot, \cdot ; \gamma)$ for a fixed radius $r, \alpha=1$, and (left to right) $\gamma=0,0.25,0.5,0.75,1$ and (top to bottom) $\beta=1,1.25,1.5,1.75,2$.

$$
\begin{array}{r}
r\left(\frac{2-\gamma}{\gamma \alpha+\beta-\beta \gamma}, \frac{\gamma}{\gamma \alpha+\beta-\beta \gamma}, 0\right) \text { and } r\left(\frac{1}{\alpha}, \frac{1}{\alpha}, 0\right) \text { for } d^{f c c} \text { and } \\
r\left(\frac{2-\gamma}{\gamma \alpha+\beta-\beta \gamma}, \frac{\gamma}{\gamma \alpha+\beta-\beta \gamma}, \frac{\gamma}{\gamma \alpha+\beta-\beta \gamma}\right) \text { and } r\left(\frac{1}{\alpha}, \frac{1}{\alpha}, \frac{1}{\alpha}\right) \text { for } d^{b c c} .
\end{array}
$$

The shape of the polyhedra obtained for some values of $\alpha, \beta, \gamma$ are shown in Figure 2 and 3 for the fcc and bcc grids, respectively. In approximations the ratio of $\alpha$ and $\beta$ matters.

Let $A_{P}$ be the surface area and $V_{P}$ the volume of the (region enclosed by the) polyhedron $P$. The values of $A_{P}$ and $V_{P}$ are determined by the vertices of the polyhedra.

Let $B_{r}$ be a Euclidean ball of radius $r$. The following error functions are considered


Fig. 3. Shapes of balls for $d_{\alpha, \beta}^{b c c}(\cdot, \cdot ; \gamma)$ for a fixed radius $r, \alpha=1$, and (left to right) $\gamma=0,0.25,0.5,0.75,1$ and (top to bottom) $\beta=1,1.25,1.5,1.75,2$.

$$
\begin{align*}
& E_{1}=\max _{p, q \in \partial P}\left(\frac{|p|}{|q|}\right)-1 \quad \text { (relative error) }  \tag{7}\\
& E_{2}=\frac{\frac{A_{P}^{3}}{V_{P}^{2}}}{36 \pi}-1 \quad \text { (compactness ratio) }  \tag{8}\\
& E_{3}=\min _{r: B_{r} \subset P}\left(V_{P} / V_{B_{r}}\right)-1 \text { (maximal inscribed ball) }  \tag{9}\\
& E_{4}=\min _{r: P \subset B_{r}}\left(V_{B_{r}} / V_{P}\right)-1 \text { (minimal covering ball) } \tag{10}
\end{align*}
$$

These error functions attain their minimum value 0 when $A$ is the surface area and $V$ is the volume of a Euclidean ball. The values of $\alpha, \beta$, and $\gamma$ that minimize the error functions are computed numerically. The polyhedra are given by their vertices, given above. All error functions attain a minimum value within the domain $0<\alpha \leq \beta \leq 2 \alpha, 0 \leq \gamma \leq 1$, so the computation is straight-forward (when an analytic solution could not be found, the NelderMead simplex method was used). The error function $E_{1}$ gets optimal value not only in a point when weights are used on the fcc grid. In these cases the parameters $C_{1}, C_{2}$ and $C_{3}$ are used in Table 1. $C_{1}$ can be any value such that

$$
\begin{equation*}
\sqrt{2} \leq C_{1} \leq 5 / 3 \tag{11}
\end{equation*}
$$

Moreover, $C_{3}$ can be any value in the range $0 \leq C_{3} \leq 2(\sqrt{2}-1)$ and $C_{2}$ any value satisfying the following inequalities (see also Figure 7):

$$
\begin{equation*}
\frac{\sqrt{C_{3}^{2}+2-2 C_{3}}-C_{3}}{1-C_{3}} \leq C_{2} \leq \min \left(\frac{\sqrt{3}-C_{3}\left(\frac{1}{2} \sqrt{3}+1\right)}{1-C_{3}}, \frac{5}{3}\right) \tag{12}
\end{equation*}
$$

For the relative error on the fcc grid, the optimum is obtained on a region as shown in Figure 7. The optimal values are found in Table 1 and visualized by the shape of the corresponding polyhedra in Figure 6.

In Figure 4 and 5 , the asymptotic behavior is shown by letting $\alpha=1$ and $\beta$ be constant and for each $k, 1 \leq k \leq 1000$ using a ns $B$ of length $k$ that approximates the optimal fraction $\gamma$. The values of the error functions and $k$ are plotted in the figures. The plots in Figure 4 and 5 show how the error functions perform for ns of finite lengths (periodic ns). Neighborhood sequences obtained by the following recursive formula are used

$$
b(k+1)=\left\{\begin{array}{lc}
1 & \text { if } \mathbf{1}_{B}^{k}<\gamma k \\
2 & \text { otherwise }
\end{array}\right.
$$

The value of $\gamma$ is shown in Table 1. When $\gamma$ is not uniquely defined, we use constant values within the allowed interval. The same thing applies to $\beta$.

Table 1
Performance of wns-, weighted- (w), and ns-distances using the error functions $E_{1}-$ $E_{4}$ defined in the text. The optima of the error functions are attained whenever $t$ is a strictly positive real number. The values shown in bold are fixed in the optimization. The parameters $C_{1}, C_{2}$, and $C_{3}$ are related as is shown in inequalities (11) and (12).

Relative error, $E_{1}$

|  | fcc |  |  |  |  | bcc |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Name | $\alpha$ | $\beta$ | $\gamma$ | $E_{1}$ | $\alpha$ | $\beta$ | $\gamma$ | $E_{1}$ |  |
| w | $t$ | $C_{1} t$ | $\mathbf{0}$ | 0.2247 | $t$ | $1.1547 t$ | $\mathbf{0}$ | 0.2393 |  |
| ns | $\mathbf{1}$ | $\mathbf{1}$ | 0.8453 | 0.2393 | $\mathbf{1}$ | $\mathbf{1}$ | $[1 / 3,2-\sqrt{2}]$ | 0.2247 |  |
| wns | $t$ | $C_{2} t$ | $C_{3}$ | 0.2247 | $t$ | $t$ | $[1 / 3,2-\sqrt{2}]$ | 0.2247 |  |

Compactness ratio, $E_{2}$

|  | fcc |  |  |  |  | bcc |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Name | $\alpha$ | $\beta$ | $\gamma$ | $E_{2}$ | $\alpha$ | $\beta$ | $\gamma$ | $E_{2}$ |  |
| w | $t$ | $1.5302 t$ | $\mathbf{0}$ | 0.1367 | $t$ | $1.2808 t$ | $\mathbf{0}$ | 0.1815 |  |
| ns | $\mathbf{1}$ | $\mathbf{1}$ | 0.8453 | 0.2794 | $\mathbf{1}$ | $\mathbf{1}$ | $2-\sqrt{2}$ | 0.2147 |  |
| wns | $t$ | $1.4862 t$ | 0.4868 | 0.1267 | $t$ | $1.2199 t$ | 0.4525 | 0.1578 |  |

Maximal inscribed ball, $E_{3}$

|  | fcc |  |  |  |  | bcc |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Name | $\alpha$ | $\beta$ | $\gamma$ | $E_{3}$ | $\alpha$ | $\beta$ | $\gamma$ | $E_{3}$ |  |
| w | $t$ | $(5 / 3) t$ | $\mathbf{0}$ | 0.1578 | $t$ | $1.2808 t$ | $\mathbf{0}$ | 0.1815 |  |
| ns | $\mathbf{1}$ | $\mathbf{1}$ | 0.8453 | 0.2794 | $\mathbf{1}$ | $\mathbf{1}$ | $2-\sqrt{2}$ | 0.2147 |  |
| wns | $t$ | $(5 / 3) t$ | 0.3280 | 0.1563 | $t$ | $1.2199 t$ | 0.4525 | 0.1578 |  |

Minimal covering ball, $E_{4}$

|  | fcc |  |  |  |  | bcc |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Name | $\alpha$ | $\beta$ | $\gamma$ | $E_{4}$ | $\alpha$ | $\beta$ | $\gamma$ | $E_{4}$ |  |
| w | $t$ | $\sqrt{2} t$ | $\mathbf{0}$ | 0.4234 | $t$ | $1.1547 t$ | $\mathbf{0}$ | 0.5708 |  |
| ns | $\mathbf{1}$ | $\mathbf{1}$ | 0.7408 | 0.4448 | $\mathbf{1}$ | $\mathbf{1}$ | $1 / 3$ | 0.3860 |  |
| wns | $t$ | $1.2179 t$ | 0.5425 | 0.3272 | $t$ | $t$ | $1 / 3$ | 0.3860 |  |



Fig. 4. Optimal values of $E_{1}-E_{4}$ (vertical axis) on the fcc grid for neighborhood sequences of length $k\left(0<k \leq 1000\right.$, horizontal axis showing $\left.\log _{10} k\right)$ with $\alpha=1$. See Table 1 for asymptotic optima.


Fig. 5. Optimal values of $E_{1}-E_{4}$ (vertical axis) on the bcc grid for neighborhood sequences of length $k\left(0<k \leq 1000\right.$, horizontal axis showing $\left.\log _{10} k\right)$ with $\alpha=1$. See Table 1 for asymptotic optima.

| fcc |  |  | bcc |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $E_{1}$ |  |  |  |  |  |
| $\begin{gathered} \beta=1.414 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.845 \end{gathered}$ | $\begin{aligned} & \beta=1.5 \\ & \gamma=0.3 \end{aligned}$ | $\begin{gathered} \beta=1.154 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.586 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.586 \end{gathered}$ |
| $E_{2}$ |  |  |  |  |  |
| $\begin{gathered} \beta=1.530 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.845 \end{gathered}$ | $\begin{aligned} & \beta=1.486 \\ & \gamma=0.487 \end{aligned}$ | $\begin{gathered} \beta=1.281 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.586 \end{gathered}$ | $\begin{aligned} & \beta=1.220 \\ & \gamma=0.453 \end{aligned}$ |
| $E_{3}$ |  |  |  |  |  |
| $\begin{gathered} \beta=1.667 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.845 \end{gathered}$ | $\begin{aligned} & \beta=1.667 \\ & \gamma=0.328 \end{aligned}$ | $\begin{gathered} \beta=1.281 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.586 \end{gathered}$ | $\begin{aligned} & \beta=1.220 \\ & \gamma=0.453 \end{aligned}$ |
| $E_{4}$ |  |  |  |  |  |
| $\begin{gathered} \beta=1.414 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.741 \end{gathered}$ | $\begin{aligned} & \beta=1.218 \\ & \gamma=0.543 \end{aligned}$ | $\begin{gathered} \beta=1.155 \\ \gamma=0 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.333 \end{gathered}$ | $\begin{gathered} \beta=1 \\ \gamma=0.333 \end{gathered}$ |

Fig. 6. Shapes of balls using $\alpha=1$ and values of $\beta$ and $\gamma$ that minimize $E_{1}-E_{4}$, see Table 1.


Fig. 7. The domain for $C_{2}$ and $C_{3}$ in Table 1

## 4 Conclusions

We have given generalizations of the fcc and bcc grids to any dimension. For these grids, formulas for the ns-distance and weighted ns-distance were presented. We note that the weighted ns-distance in $\mathbb{B}^{n}$ between $\mathbf{0}$ and a point p only depends on the two coordinates of $\mathbf{p}$ with highest absolute value. For $\mathbb{F}^{n}$, all coordinates are needed to calculate the distance values.

In 4D bcc the Euclidean distance of the 1-neighbors are the same as the 2neighbors. In higher dimensions the 2-neighbors have less Euclidean distance, therefore it seems to be fruitful to consider weights $\beta<\alpha$ for future research.

By introducing a number of error functions that all favor "round" balls (in the Euclidean sense), the weighted ns-distance is analyzed for the fcc and bcc grids. It turns out that the optimal parameters for the special cases of weighted distances $(\gamma=0$ or $B=(2))$ and ns-distances $(\alpha=\beta=1)$ are also found from this procedure by keeping one of the parameters fixed in the optimization. The same weights and neighborhood sequences as were derived for weighted distances $[2,3]$ and ns-distances [4] are found in this paper. Figure 2 and 3 gives an overview of this fact - weighted distances are shown in the left columns $(\gamma=0)$ and ns-distances are shown in the top rows $(\beta=1)$. We also note that, as expected, the value of the error functions for the wns distance function are lower than (or, in some cases, equal to) the weighted distance and ns-distance.

We use the coordinates of the vertices of polyhedra corresponding to the asymptotic shape of the balls in the fcc and bcc grids. Note that the ver-
tices can be found also for higher-dimensional generalizations of the fcc and bcc grids. Since the optimization methods use geometric features, such as area and volume, their extensions to higher dimension should be used. The parameter optimization in higher dimensions is left for future research.

In the optimization, we let $\gamma$ represent the fraction of $1:$ s in the ns. We note that when $\gamma$ is fixed to 0 (for weighted distances), this corresponds to a ns with only 2:s. This can be attained for a neighborhood sequence of any length. Therefore, in this case the optimum is not asymptotic and thus, the error is valid also for short distances (between e.g. neighboring grid points). When $\gamma$ is also subject to optimization (i.e. when the neighborhood sequence is used to define the distance function), the error functions have an asymptotic behavior. However, some of the optima for the relative error $\left(E_{1}\right)$ are located on regions where $E_{1}$ is constant. For example, $E_{1}$ for the weighted ns is optimal when $\gamma=0$, i.e. for the weighted distance, and therefore the optimum is attained for any neighborhood sequence consisting of only 2 :s. See Figure 4 and 5 and Figure 7. This indicates that this error function, which has been widely used in the literature, is not well-suited for finding the optimal weights and ns here. The reason that $E_{1}$ is minimal on a region (and not a point) is that there are two vertices and two surfaces that have points that can be at minimal distance (up to symmetry). Thus, there are more degrees of freedom than the restrictions in the optimization process. For the other error functions $\left(E_{2}-E_{4}\right)$, differentiable functions are defined and they have all a single minimum, see Table 1.

We note that the error functions $E_{2}$ (compactness ratio) and $E_{3}$ (maximal inscribed ball) give the same asymptotic optimal result for the bcc grid and the same for ns-distances on the fcc grid, see Table 1. However, as is seen in Figure 4 and 5, the error functions perform differently for finite, i.e., periodic, neighborhood sequences. This illustrates that the different error functions are different, even though they all are used to approximate the Euclidean distance. Different applications require different aspects of the "roundness" of the balls and different types of rotational (in)dependency.

Analyzing the plots in Table 1, we see that the error converges quite fast and that a ns of length (period) 10 is sufficient in general.

The application in which the distance function will be applied should be used to select which error function that should be considered. Also, by using Theorem 17, it is easy to find neighborhood sequences such that the resulting distance function is a metric, which is preferable in many applications. Intuitively, the polyhedra that best approximate the Euclidean ball are given by a distance function where both $\gamma$ and $\beta$ are non-trivial, see Figure 2 and 3. From the "optimal shapes" in Figure 6, we see that this is what, e.g., the compactness ratio $E_{2}$ favors. Thus, without any specific application in mind, we suggest
the parameters $B=(1,2), \beta=1.4862 \alpha$ for the fcc grid and $\beta=1.2199 \alpha$ for the bcc grid. This gives $E_{2}=0.1276$ for the fcc grid (the optimum is 0.12757 and the approximated value is 0.12760 ) and $E_{2}=0.1591$ (the optimum is 0.1578 ) for the bcc grid. We conclude that we get a good approximation of the optimal values also with a short neighborhood sequence.

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