A practical algorithm for degree-k Voronoi domains of three-dimensional periodic point sets

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Abstract. Degree-k Voronoi domains of a periodic point set are concentric regions around a fixed centre consisting of all points in Euclidean space that have the centre as their k-th nearest neighbour. Periodic point sets generalise the concept of a lattice by allowing multiple points to appear within a unit cell of the lattice. Thus, periodic point sets model all solid crystalline materials (periodic crystals), and degree-k Voronoi domains of periodic point sets can be used to characterise the relative positions of atoms in a crystal from a fixed centre. The paper describes the first algorithm to compute all degree-k Voronoi domains up to any degree $k \geq 1$ for any two or three-dimensional periodic point set.

Keywords: Degree-k Voronoi Domains · Periodic Point Sets · Crystals

1 Introduction: motivations and key contributions

A *discrete set* $C \subset \mathbb{R}^n$ consists of (possibly, infinitely many) points whose pairwise distances have a positive lower bound. The *Voronoi domain* $Z_1(C;p)$ or Wigner-Seitz cell or Brillouin zone of a point $p \in C$ consits of all ambient points in $\mathbb{R}^n$ that are (non-strictly) closer to p than to all other points of C. Fig. 1 shows Voronoi domains in yellow when C is a lattice and p is the origin.

For any $k \geq 1$, the *degree-k Voronoi domain* $Z_k(C;p)$ consists of all points in $\mathbb{R}^n$ that have p as its k-th nearest neighbour in C, thus covering relative positions of distant points beyond the closest neighbours, see Fig. 1. Our key example of C is a periodic point set that generalises the concept of a lattice by allowing multiple points to lie within a unit cell of the lattice. Such periodic point sets geometrically model any solid crystalline material (briefly, a *crystal*) whose atoms are represented by points, possibly with added chemical types.

Key physical properties of a crystal depend on atomic interactions beyond immediate neighbours within larger degree-k Voronoi domains. These domains were called k-th Brillouin zones in [13] for lattices and later helped compute density functions [12, Theorem 6.1], which distinguish all periodic point sets in general position up to isometry in $\mathbb{R}^3$. Section 7 in [12] described how density functions detected a previously missing crystal in the Cambridge Structural Database. This paper complements [12] by describing structural results and a practical algorithm for degree-k Voronoi domains for three-dimensional periodic point sets.

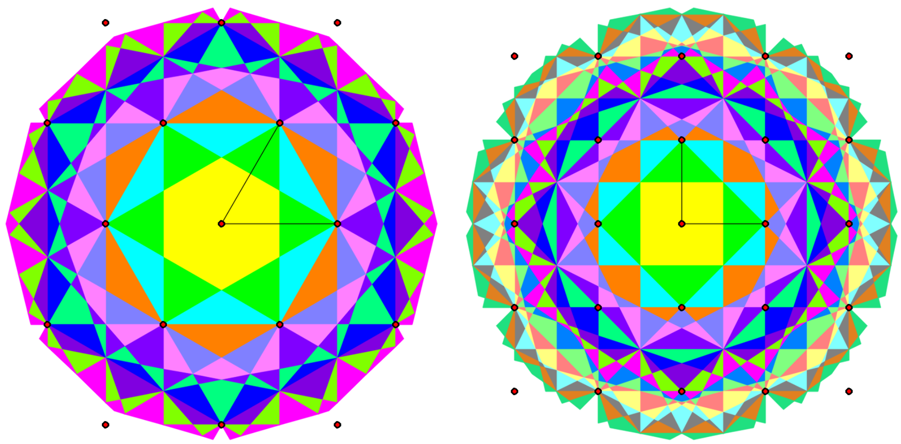

Fig. 1. The degree-k Voronoi domain is the union of polygons of the same colour, and has the origin as its k-th nearest neighbour among all lattice points. **Left**: the hexagonal lattice, degrees $1 \leq k \leq 12$. **Right**: the square lattice, degrees $1 \leq k \leq 20$.

The first algorithm to compute Voronoi domains for periodic point sets appeared in [10], but did not consider degree-k Voronoi domains for $k \geq 2$. The algorithm for dual periodic Delaunay triangulations or mosaics was recently improved in [23]. Previously, degree-k Voronoi domains were studied and computed only for lattices whose motif is a single point [13].

In the more restrictive case of lattices, the Teaching and Learning Package of Cambridge University [25] visualises the degree-k Voronoi domains only for:

- the square and hexagonal lattices up to $k = 10$ and $k = 6$ respectively;
- the cubic, body centred cubic and face centred cubic lattices up to $k = 5$.

Again restricted to lattices, Andrew et al. [1] described an algorithm which approximates the domains simply by assigning each point of a fixed square/cubical grid at a given resolution to the appropriate degree-k Voronoi domain.

Degree-k Voronoi domains relate to the more widely known order-k Voronoi domains, which have been studied for a long time. Only recently degree-k Voronoi domains have begun to be properly investigated [11].

One could extend algorithms that compute order-k Voronoi domains to construct the desired degree-k Voronoi domains. Though there are many algorithms that for order-k Voronoi domains in dimension 2 [9], to the best of the authors' knowledge, there is no publicly available algorithm for order-k Voronoi domains in dimension 3, which has motivated us to propose the algorithm in this paper.

We substantially improve on the past work in two ways: by generalising to any periodic point set, and by computing exactly the polytopes that comprise each domain, which can be used for visualisations and precise computations.

• Theorem 6 will describe the structure of the degree-k Voronoi domain $Z_k(C;p)$ from Definition 4 for any point p in a periodic point set $C \subset \mathbb{R}^n$.

• The total volume of the degree-k Voronoi domains $Z_k(C;p)$ over all points p in a motif M of a periodic set $C \subset \mathbb{R}^n$ is *independent of* k, see Theorem 7.

• The algorithm in Section 4 computes any degree-k Voronoi domain $Z_k(C;p)$ of a periodic point set in polynomial time in the motif size of C, see Theorem 17. The actual runtime takes only milliseconds on a modest laptop, see Section 5.

Section 2 defines necessary concepts. Section 3 states Theorems 6 and 7. Section 4 describes the practical algorithm for computing degree-k Voronoi domains of periodic point sets in dimensions two and three. Section 5 contains experimental analysis whose polynomial complexity is justified in Theorem 17.

2 Background definitions from computational geometry

Any point $p \in \mathbb{R}^n$ can be represented by the vector $\vec{p}$ from the origin $0 \in \mathbb{R}^n$ to p. The symbol $\vec{p}$ also denotes all equal vectors with the same length and direction. We use only the Euclidean distance $|\vec{p} - \vec{q}|$ between points $p, q \in \mathbb{R}^n$. The *perpendicular bisector* between p and q is an $\mathbb{R}^{n-1}$-dimensional subspace composed of all points that are equidistant from p and q, and has the property that $\vec{p} - \vec{q}$ is perpendicular to this subspace. For a standard orthonormal basis $\vec{e}_1, \dots, \vec{e}_n$ of $\mathbb{R}^n$, the lattice $\mathbb{Z}^n \subset \mathbb{R}^n$ consists of all points with integer coordinates.

Definition 1 (*lattice Λ, periodic point set C*)**.** For n linearly independent vectors $\vec{v}_1, \dots, \vec{v}_n$ in $\mathbb{R}^n$, the set of integer combinations $\Lambda = \{\sum_{i=1}^n c_i \vec{v}_i \,|\, c_i \in \mathbb{Z}\}$ is called a *lattice*. The *unit cell* spanned by this basis is the parallelepiped $U = \{\sum_{i=1}^n t_i \vec{v}_i \,|\, t_i \in [0,1)\}$. The lattice generated by this basis or unit cell is denoted by $\Lambda(U)$. A *motif* $M \subset U$ is a finite subset of U, and the *periodic point set* C for M and Λ is the *Minkowski* sum $M + \Lambda = \{p + \vec{v} \,|\, p \in M, v \in \Lambda\}$. ■

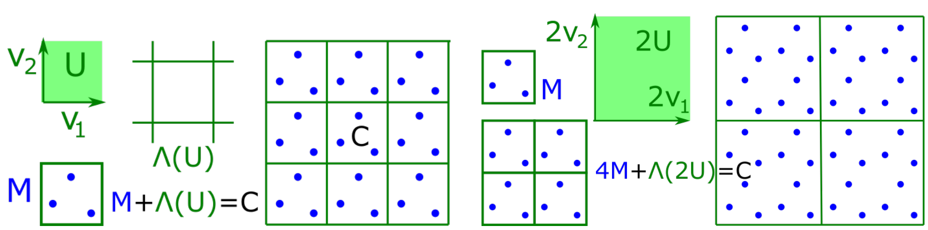

Fig. 2. Left: the green lattice Λ is generated by the orthonormal basis $\vec{v}_1, \vec{v}_2$. The blue motif M consists of three points in the square unit cell U. The periodic set $C = \Lambda + M$ is the Minkowski sum of the lattice and the finite motif M of points. **Right**: if a unit cell $U \subset \mathbb{R}^n$ has m motif points, then the 2-extended unit cell has $2^n m$ motif points.

The periodic point set C can be thought of as the union of translates of M by all vectors of Λ, and hence is invariant under translations by all vectors of Λ.

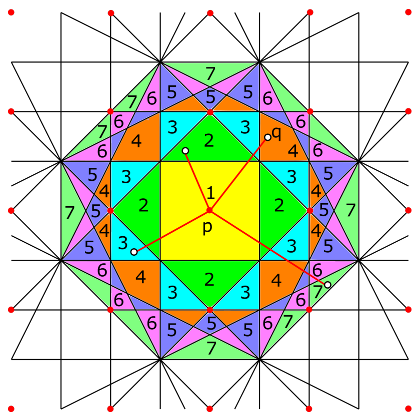

Fig. 3. Four red line segments $[p, q)$ go from the centre p to points q in polygons with indices $k = \text{ind}(q)$ from Definition 5 and intersect $k-1$ bisectors.

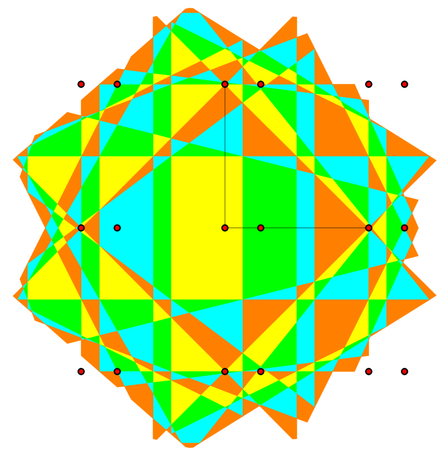

Fig. 4. Degree-k Voronoi domains of a periodic set (not a lattice) with a 2-point motif.

If a periodic point set C is invariant *only* under translations by vectors $\vec{v} \in \Lambda$, then the lattice Λ and its unit cell U are called *primitive* for C.

One can consider any lattice Λ as a periodic point set on the lattice 2Λ with a motif of 2^n points inside the 2-extended unit cell more formally as follows.

Definition 2 (k-extended unit cell kU)**.** Let a unit cell $U \subset \mathbb{R}^n$ have a basis $\vec{v}_1, \dots, \vec{v}_n \in \mathbb{R}^n$ and a finite motif $M \subset U$ of m points. For any integer $k > 1$, the *k-extended unit cell kU* has motif $M + \sum\limits_{i=1}^{n} c_i \vec{v}_i$ of $k^n m$ points obtained from M by k^n translations along the vectors $\sum\limits_{i=1}^{n} c_i \vec{v}_i$ with $c_i \in \{0, \dots, k-1\}$. ■

Degree-k Voronoi domains of periodic point sets are introduced in Definition 4 as the relative complement between sequential index-k Voronoi domains below.

Definition 3 (Index-k Voronoi domains $V_k(C; p)$)**.** For a finite or periodic set $C \subset \mathbb{R}^n$ and a point $p \in C$, the *index-k Voronoi domain* $V_k(C; p)$ is the (closure of the) set of all points $q \in \mathbb{R}^n$ such that p is among the k nearest points of C to q. In particular, $V_1(C; p)$ is the classical Voronoi domain $V(C; p)$. ■

The index-k Voronoi domain $V_k(C; p) \subset \mathbb{R}^n$ is defined as a closed set above to cover all cases where p has equal distances to several neighbours, so a k-th neighbour of p may not be unique. Unlike order-k Voronoi domains which tile $\mathbb{R}^n$ [15], index-k Voronoi domains form a nested sequence. Any $V_k(C; p)$ is *star-convex*, which means it contains all line segments connecting $\partial V_k(C; p)$ to p. Indeed, if $p \in C$ is among the k nearest to $q \in \partial V_k(C; p)$, then any intermediate point in the line segment $[p, q]$ has p among its k nearest neighbours of C.

An order-k Voronoi domain [14] is defined for a k-point subset $Q \subset A \subset \mathbb{R}^n$ and consists of all points for whom the points in Q are the closest k points in A.

Definition 4 (Degree-k Voronoi domains $Z_k(C;p)$)**.** For any periodic point set $C \subset \mathbb{R}^n$ and $p \in C$, the ***degree-k Voronoi domain*** is the difference between successive closed index-k Voronoi domains: $Z_k(C;p) = V_k(C;p) - V_{k-1}(C;p)$ for $k \geq 1$, $V_0(C;p) = \emptyset$, which differs from order-k Voronoi domains in [14]. ■

Fig. 4 shows degree-k Voronoi domains for a point in the periodic point set C that has a 2-point motif. For a point $p \in C \subset \mathbb{R}^n$, any $q \in \mathbb{R}^n$ belongs to exactly one degree-k Voronoi domain $Z_k(C;p)$ for some $k \geq 1$, hence $\cup_{k=1}^{+\infty} Z_k(C;p)$ covers $\mathbb{R}^n$ without overlaps. Unlike index-k Voronoi domains which are closed, $Z_k(C;p)$ are neither open nor closed for $k > 1$. The closure of the domain $Z_k(C;p)$ includes all points q for whom p is a non-unique k-th nearest neighbour within C.

3 The geometric structure of degree-k Voronoi domains

The main results of this section are Theorem 6 describing the structure of degree-k Voronoi domains and Theorem 7 saying that the total volume of the degree-k Voronoi domains for all motif points is independent of k for a fixed set. So all coloured regions in Fig. 3 have the same area, which might seem surprising.

Definition 5 (Zone index $\text{ind}(q;C;p)$)**.** For a periodic set $C \subset \mathbb{R}^n$ and $p \in C$, let $b(C;p)$ be the set of perpendicular bisectors between p and all other points of C. For any $q \in \mathbb{R}^n$, consider the half-open line segment $[p,q)$ joining p to q, but not including q, see Fig. 3. Let i be the number of bisectors from $b(C;p)$ that intersect $[p,q)$. The *zone index* of q relative to $b(C;p)$ is $\text{ind}(q;C;p) = i + 1$. ■

For any point q in the closed Voronoi domain $V_1(C;p)$, the half-open segment $[p,q)$ belongs to the interior of $V_1(C;p)$, and hence doesn't intersect any bisectors from $b(C;p)$. Consider other polytopes obtained from $\mathbb{R}^n$ by cutting out all bisectoral hyperplanes between p and other points $q \in C$. The zone indices of these polytopes can be computed in gradual increments as we travel radially outwards from p and count intersecting bisectors, see Fig. 3.

The following structural description of a degree-k Voronoi domain $Z_k(C;p)$ justifies its spherical shape consisting of polytopes of the same degree k.

Theorem 6 (Structure of Voronoi domains)**.** For any point p in a periodic point set $C \subset \mathbb{R}^n$, the closure of the degree-k Voronoi domain $Z_k(C;p)$ is a union of convex polytopes whose interior points have zone index k. Moreover, the closure of the degree-k Voronoi domain is spherical in the sense that its image under the radial projection $Z_k(C;p) \to S^{n-1}$ covers the whole unit sphere $S^{n-1} \subset \mathbb{R}^n$. ■

Proof. First we prove that any point $q \in \mathbb{R}^n$ that has the central point p as its exact k-th nearest neighbour in C should have zone index $\text{ind}(q;C;p) = k$, see Definition 5. Let us slide a point s along the half-open line segment $[p,q)$ starting from the central point p as in Fig. 3. While s is in the interior of $V_1(C;p)$, our point s has p as exactly its 1st nearest neighbour in C and $\text{ind}(s;C;p) = 1$.

When we slide the point s further along the half-closed line segment $[p,q)$, the zone index $\text{ind}(s;C;p)$ jumps up only when we intersect a bisector separating

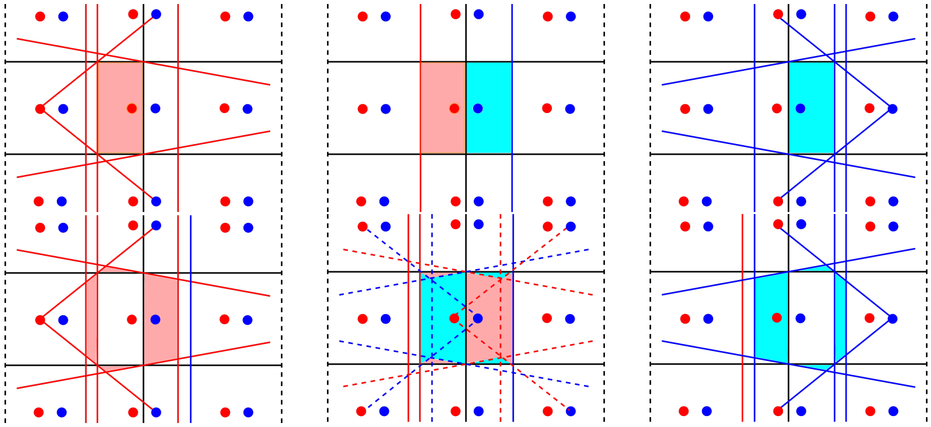

Fig. 5. Top left: the Voronoi domain of the red point is bounded by red and black bisectors. **Top middle:** both Voronoi domains of the red and blue points form the Voronoi domain $V(\Lambda;0)$ of the lattice Λ of C. **Top right:** the Voronoi domain of the blue point is bounded by blue and black bisectors. **Bottom left:** the degree-2 Voronoi domain of the red point in C. **Bottom middle:** both degree-2 Voronoi domains form $V(\Lambda;0)$ after applying translations of the polygons that form the degree-2 Voronoi domains. **Bottom right:** the degree-2 Voronoi domain of the blue point.

p from another point of C. If we intersect $i \geq 1$ bisectors, then $\text{ind}(s;C;p)$ jumps by i. As the final point $s = q$ has p as its exact k-th nearest neighbour in C, s will intersect $k-1$ bisectors as it travels along $[p,q)$, and so the zone index becomes k. Then $Z_k(C;p)$ is a finite union of convex polytopes (obtained from $\mathbb{R}^n$ by cutting out bisectors) that includes all index k points. The boundary of any such polytope includes points of index at most $k-1$ ('internal' faces closer to p) and points of index k ('external' faces further away from p).

So the closure of $Z_k(C;p)$ is the union of all convex polytopes whose internal points have zone index k. Then any straight ray R emanating from p either contains points of index k, hence intersects the interior of $Z_k(C;p)$, or R passes through an intersection point a of several bisectors. In the latter case, when a point s moves along R via the intersection a, the index of s can change from $k' < k$ to $k'' > k$. Then any small neighbourhood of a contains points of all intermediate indices from k' to k'' (including k). So the closure of $Z_k(C;p)$ contains a and its image under the radial projection covers the sphere S^{n-1}. □

Fig. 5 illustrates the key idea for the periodic point set $C \subset \mathbb{R}^2$, which has the primitive square unit cell $[-1,1] \times [-1,1]$ containing the red point at $(-0.25,0)$ and the blue point at $(0.25,0)$. The bottom row in Fig. 5 shows how the polygons of the degree-2 Voronoi domain can be rearranged to form the classical degree-1 Voronoi domain in the first row, see the proof of Theorem 7 below.

Theorem 7 (volumes of a degree-k Voronoi domain, extending [13, Section 2.2])**.** For a periodic point set $C = \Lambda + M$, the sum of the volumes of the degree-k Voronoi domains $Z_k(C;p)$ over all motif points $p \in M$ is independent of k. ■

Definition 8 (open subdomains $V^{(k)}(C;0)$)**.** A lattice Λ of a periodic set $C = \Lambda + M$ is *primitive* if C is not a Minkowski sum $\Lambda' + M'$ whose motif M' has a smaller number of points than M. Then the *subdomain* $V^{(k)}(C;0)$ in the interior of the Voronoi domain $V(\Lambda;0)$ consists of all points that have a unique k-th nearest neighbour in the set C. So this subdomain $V^{(k)}(C;0)$ is obtained from the classical Voronoi domain $V(\Lambda;0)$ around the origin 0 by removing the measure 0 subset of points that have several k-th nearest neighbours in C. ■

Definition 9 (subzone Z_k°)**.** Let Λ be a primitive lattice of a periodic set C. The open *subzone* $Z_k^\circ(C;p)$ in the interior of the degree-k Voronoi domain $Z_k(C;p)$ consists of all points that have a unique closest node in Λ. ■

Since $V^{(k)}(C;0)$ is in the interior of $V(\Lambda;0)$, the origin 0 is a unique closest point of Λ to every point of $V^{(k)}(C;0)$. Since $Z_k^\circ(C;p)$ is in the interior of $Z_k(C;p)$, every point of $Z_k^\circ(C;p)$ has a unique k-th nearest neighbour in C.

Definition 10 (half-open Voronoi domain $\tilde{V}(\Lambda;0)$)**.** For a lattice $\Lambda \subset \mathbb{R}^n$, the closed Voronoi domains $V(\Lambda;q)$ of the lattice points $q \in \Lambda$ tile $\mathbb{R}^n$, overlapping only at their boundaries. We define a *half-open Voronoi domain* $\tilde{V}(\Lambda;0) \subset V(\Lambda;0)$ to be such that all translational copies tile $\mathbb{R}^n$ without overlaps. ■

A half-open Voronoi domain $\tilde{V}(\Lambda;0)$ differs from $V(\Lambda;0)$ only by a measure 0 subset and can be obtained by removing boundary points of $V(\Lambda;0)$ until there remains exactly one representative of each class of boundary points that are related via lattice translations. Definition 11 adapts the piecewise shifts f_i from the case of lattices in [13, p. 754] to any periodic point set $C \subset \mathbb{R}^n$.

Definition 11 (piecewise shift f_k)**.** For any periodic set $C \subset \mathbb{R}^n$ with lattice Λ, any point $p \in V^{(k)}(C;0)$ has a unique k-th nearest neighbour $p_k \in C$. Since all translates of $\tilde{V}(\Lambda;0)$ cover $\mathbb{R}^n$ without overlaps, p_k is contained in a translate $\tilde{V}(\Lambda;0) + q_k$ for a unique lattice node $q_k \in \Lambda$. Then we set $f_k(p) = \vec{p} - \vec{q}_k$. ■

Lemma 12. The map $f_k : V^{(k)}(C;0) \to \bigcup\limits_{p \in C \cap \tilde{V}(\Lambda;0)} Z_k^\circ(C;p)$ is a bijection. ■

Proof. We first show that the image of f_k is in $\bigcup\limits_{p \in C \cap \tilde{V}(\Lambda;0)} Z_k^\circ(C;p)$. Any $p \in V^{(k)}(C;0)$ has a unique k-th nearest neighbour $p_k \in C$, which is covered by a unique translate $\tilde{V}(\Lambda;0) + q_k$ for some $q_k \in \Lambda$. Shifting these neighbouring relations by $-\vec{q}_k$, we conclude that $f_k(p) = p - q_k$ has the unique k-th neighbour $p' = p_k - q_k \in C$, which is covered by $\tilde{V}(\Lambda;0)$. Then $f_k(p) = p - q_k \in Z_k^\circ(C;p') \subset \bigcup\limits_{p \in C \cap \tilde{V}(\Lambda;0)} Z_k^\circ(C;p)$. To prove that f_k is injective, let $p, p' \in V^{(k)}(C;0)$ have unique k-th neighbours $p_k, p'_k \in C$, which are covered by unique translates of $\tilde{V}(\Lambda;0)$ along $\vec{q}_k, \vec{q}'_k \in \Lambda$, respectively. If $q_k = q'_k$, then $f_k(p) - f_k(p') = p - p'$, so that $p \neq p'$ implies $f_k(p) \neq f_k(p')$. Otherwise, if $q_k \neq q'_k$, then $f_k(p) \neq f_k(p')$ since they lie in the interiors of two different translates of $\tilde{V}(\Lambda; 0)$. To prove that f_k is surjective, any point q in the target set belongs to a $Z^{\circ}_k(C; p_k)$ for $p_k \in C \cap \tilde{V}(\Lambda; 0)$. Then q has p_k as its unique k-th neighbour in C and a unique closest lattice node $q_k \in \Lambda$ such that $V(\Lambda, 0) + q_k$ covers q. Subtracting q_k, we conclude that $p = q - q_k$ has $p_k - q_k$ as its unique k-th neighbour in C and 0 as its unique closest lattice node in Λ. So $p \in V^{(k)}(C; 0)$ and $f_k(p) = q$. □

Proof of Theorem 7. By Lemma 12 the shifts f_k from Definition 11 translate different pieces of the Voronoi domain $V(\Lambda; 0)$ to the union of degree-k Voronoi domains over all motif points (modulo measure 0), so the volumes are equal. □

4 Computing degree-k Voronoi domains of a periodic set

Let the dimension $n = 2$ or 3. The **algorithm input** consists of:

- a unit cell U given by a basis $\vec{v}_1, \dots, \vec{v}_n$ with rational coordinates in practice;
- a finite motif $M \subset U$ of points given by their coefficients in the basis of U;
- a degree $k \geq 1$ and a point $p \in M$ that will be the centre of the degree-k Voronoi domains $Z_k(C; p)$ of the periodic point set $C = \Lambda + M \subset \mathbb{R}^n$.

Up to rigid motions, we can assume that the point $p \in M$ is at the origin.

The output is the degree-k Voronoi domains $Z_i(C; 0)$, $i = 1, \dots, k$. Each domain is a union of polygons ($n = 2$) or polytopes ($n = 3$) defined by:

- vertices: arbitrarily ordered points in $\mathbb{R}^n$;
- edges: unordered pairs of vertices indexed above;
- 2-dimensional faces: cyclically ordered lists of edges indexed above for $n = 3$.

We introduce the algorithm for $n = 2$ in the plane $\mathbb{R}^2$ for simplicity, while the natural extension to $\mathbb{R}^3$ will be described in an extended version.

Stage 1: cell reduction. A given basis of a unit cell U is reduced to a Minkowski basis [22], see Lemma 15. A basis reduction is needed due to Lemma 13 below.

Lemma 13 (insufficiency of cell extensions)**.** For any $k > 1$, any lattice $\Lambda \subset \mathbb{R}^n$ has a unit cell U whose k-extension doesn't cover the domain $V(\Lambda; 0)$. ■

Proof. The example in Fig. 6 can be generalised for any lattice $\Lambda \subset \mathbb{R}^n$ as follows. One can choose a basis $\vec{v}_1, \dots, \vec{v}_n$ of Λ in such a way that the nearest neighbour of the origin $0 \in \mathbb{R}^n$ is the vertex v_2 of the unit cell spanned by this basis. If we add the multiple $(k+1)\vec{v}_1$ to $\vec{v}_2$, then the vertex v_2 of the initial unit cell U will not be covered by the k-extended cell U_k based on $\vec{v}_1, \vec{v}_2 + (k+1)\vec{v}_1, \dots, \vec{v}_n$, see Fig. 6. Indeed, to reach the vertex $\vec{v}_2$, we need $k + 1$ subtractions from $\vec{v}_2 + (k+1)\vec{v}_1$. Hence at least the $(k+1)$-extension of the cell U_k is needed. □

The degree-1 Voronoi domain is covered by the 2-extension of a Minkowski-reduced cell for $n = 2, 3$ as proved in [16, Appendix A.1]. For degrees $k > 1$, we need the stronger Lemma 14 covering any degree-k Voronoi domain.

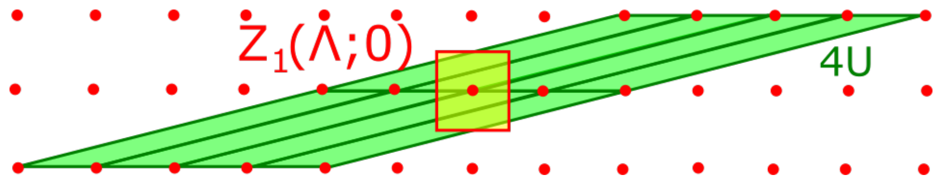

Fig. 6. If a unit cell U is not reduced, the extension by any fixed factor k may not cover even the degree-1 Voronoi domain $Z_1(\Lambda; 0)$, see Lemma 13.

Lemma 14. Let $n = 2$ or 3. For any unit cell U with a Minkowski-reduced basis, the unit cell $2kU \subset \mathbb{R}^n$ (symmetrically extended around $0 \in \mathbb{R}^n$) covers the degree-k Voronoi domain $Z_k(C; 0) \subset \mathbb{R}^n$ for any periodic set $C = \Lambda + M$. ■

Lemma 14 states that $Z_k(C; 0)$ is covered by $2kU$ (if U is Minkowski-reduced). Since the boundary of $Z_k(C; 0)$ is defined by bisectors between 0 and other points in C, we need to consider points that lie in the $4k$-extended unit cell.

Lemma 15 (*Minkowski-reduced* basis, Lemma 2.2.1 in [22])**.** A basis $\vec{v}_1, \dots, \vec{v}_n$ of a lattice $\Lambda \subset \mathbb{R}^n$ is *Minkowski-reduced* if and only if for any $i = 1, \dots, n$ and integers $c_1, \dots, c_n \in \mathbb{Z}$ such that $c_i, \dots, c_n$ have no common integer factor $c > 1$, the inequality $|\sum_{i=j}^{n} c_j \vec{v}_j| \geq |\vec{v}_j|$ holds. ■

Lemma 16 (sufficiency of Minkowski-reduced cell extensions)**.** For a unit cell U of a lattice $\Lambda \subset \mathbb{R}^n$, $n \leq 3$, with a Minkowski-reduced basis $\vec{v}_1, \dots, \vec{v}_n$, let Λ_i, $i \geq 1$, be the set of all points of Λ on the boundary of the $2i$-extended unit cell $2iU$ whose centre of symmetry is the origin 0. Then any point $p \in \mathbb{R}^n \setminus 2iU$ is closer to at least one point of Λ_i than to $0 \in \mathbb{R}^n$. ■

Proof. Set $i = 1$. By Appendix A.1 in [16], the Voronoi cell $V(\Lambda; 0)$ is strictly within $2U$. Any point p on the boundary of $2U$ belongs to the Voronoi domain $V(\Lambda; v)$ of a lattice point $v \in \Lambda \setminus 0$. $2U + v$ must strictly contain $V(\Lambda; v)$, and as p is on the boundary of $2U$, we must have $v \in \Lambda_1$. Therefore, any point on the boundary of $2U$ is closer to a point of Λ_1 than to 0, which implies that any point $p \in \mathbb{R}^n \setminus 2U$ is closer to at least one point of Λ_1 than to 0. For $i \geq 1$, consider the lattice $i\Lambda$ with Minkowski-reduced basis vectors $i\vec{v}_1, \dots, i\vec{v}_n$ and unit cell iU. The above result holds for this new lattice, meaning that any $p \in \mathbb{R}^n \setminus 2iU$ is closer to at least one point of $i\Lambda_1$ than to 0. It remains to note that $i\Lambda_1 \subset \Lambda_i$. □

Proof of Lemma 14. It suffices to prove that $V_k(\Lambda; 0) \subset 2kU$ only for a lattice Λ, i.e. for a periodic set with a single point in a motif M. Indeed, adding any extra points to M can only make the Voronoi domain $V_k(\Lambda + M; 0)$ smaller than $V_k(\Lambda; 0)$. Let U be the unit cell with a Minkowski-reduced basis $\vec{v}_1, \dots, \vec{v}_n$. Take any point $p \in \mathbb{R}^n - 2kU$. Applying Lemma 16 for $i = 1, \dots, k$, we conclude that p has k neighbours in $\cup_{i=1}^{k} \Lambda_i$ that are closer to p than 0. Hence p can not have 0 among its k nearest neighbours in Λ. Then p is outside the k-th Voronoi domain $V_k(\Lambda; 0)$. So $p \in \mathbb{R}^n - V_k(\Lambda; 0)$, $\mathbb{R}^n - 2kU \subset \mathbb{R}^n - V_k(\Lambda; 0)$, $V_k(\Lambda; 0) \subset 2kU$. □

Stage 2: sorting points from the extended motif. If the original motif $M \subset \mathbb{R}^n$ had m points including the origin $0 \in \mathbb{R}^n$, the $4k$-extended motif M_k has $(4k)^n m$ points for any dimension n. All these points are inserted into a balanced binary tree whose keys for comparison are distances to the origin.

Stage 3: a loop over motif points. The loop processes all motif points from the $2k$-extended cell (except 0) in increasing order of their distance to $0 \in \mathbb{R}^n$.

For any point $p \neq 0$ in the extended motif M_k, the vector $0.5\vec{p}$ represents the mid-point of the line segment $[0, p] \subset \mathbb{R}^2$. The bisector line $L(p) \subset \mathbb{R}^2$ between 0 and p has the parametric equation $0.5\vec{p} + t\vec{p}_\perp$, where $t \in \mathbb{R}$ and the unit vector $\vec{p}_\perp$ is orthogonal to $\vec{p}$ and anti-clockwisely oriented relative to $0 \in \mathbb{R}^2$.

In the loop of Stage 3, for each point $p \in M_k \setminus \{0\}$, the bisector $L(p)$ is intersected with all previous bisectors. The resulting intersection points can be ordered according to the direction of $L(p)$. We keep these intersection points in a balanced binary tree $T(p)$ whose key for comparison is the parameter t in the equation of $L(p)$. So a tree $T(q)$ of ordered intersections of $L(q)$ will be maintained for every point q in the extended motif M_k. This tree is implemented using the multimap structure in C++ for fast searching and insertions. Every oriented edge $e \subset L(q)$ between successive intersection points has an ordered pair of polygons attached to this edge. This pair is kept as extra information in the tree $T(q)$, for example assigned to the initial vertex a of e in Fig. 7.

To avoid unbounded regions, we restrict all polygons to a large square S containing the extended motif M_k. Every polygon Q in the current splitting of S by previous bisectors has the index $\text{ind}(Q)$ defined similarly to Definition 5 as the number of intersections of all previous bisectors with a line segment $[0, q]$ for any internal point $q \in Q$, see Fig. 3. After finding a new intersection point a of the bisector $L(p)$ with a previous bisector $L(q)$, we follow the steps below.

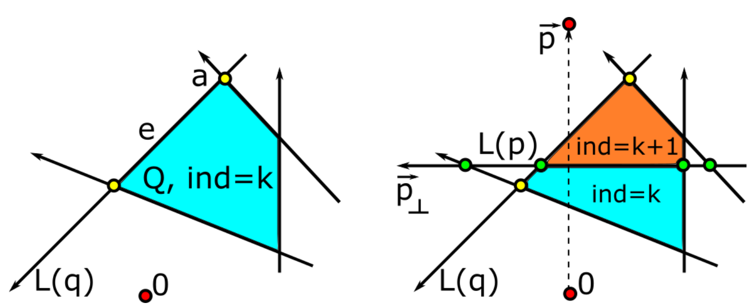

Fig. 7. Left: the blue convex polygon Q after cutting out all bisectors and before inserting the bisector of a more distant point p of the set C. **Right:** the new bisector $L(p)$ meets the previous four bisectors, creates four intersection points, then splits Q.

Step 3a: insert the intersection point a into the binary trees $T(p), T(q)$ according to its positions relative to other intersections of $L(p)$, $L(q)$, respectively.

Step 3b: the appearance of the new intersection point a in the previous bisector $T(q)$ subdivides an edge $e \subset L(q)$ and we mark the two polygons that are attached to the edge e and should be later split by $L(p)$.

Step 3c: splitting the polygons marked in Step 3b. After finding all intersections of $L(p)$ with previous bisectors, we split each marked polygon Q into two smaller polygons and update their zone indices: the polygon closer to 0 keeps its current index, while we increment by 1 the index of the more distant polygon.

Theorem 17 says that degree-k Voronoi domains can be computed in polynomial time in the number m of motif points. The polynomial dependence on m and k seems inevitable, because in general position $m(4k)^n$ bisectors between a fixed centre p and its neighbours in a k-extended motif can intersect each other.

Theorem 17 (Algorithm complexity)**.** Let the dimension be $n \leq 3$, and let a periodic point set $C \subset \mathbb{R}^n$ have a motif of m points in a Minkowski-reduced basis. Then the complexity to compute the first k degree-i Voronoi domains, $Z_i(C;p)$, $i = 1, \ldots, k$, is $O(m^n (4k)^{n^2} (n \log(4k) + \log m))$ for any point $p \in C$. ■

Proof. Starting from a reduced basis in Stage 1, the $4k$-extended motif M_k consists of $m(4k)^n$ points. Sorting these points according to their distance from the origin at Stage 2 takes $O(m(4k)^n(n \log(4k) + \log m))$ time. Stage 3 loops over $m(4k)^n$ points and computes all n-fold intersections of $m(4k)^n$ bisectors, which explains the extra n-th power in the factor $m^n(4k)^{n^2}$. Inserting intersection points into binary trees and marking polyhedra at Stage 3 requires only a logarithmic time in the number of intersection points between $O(m^{n-1}(4k)^{n(n-1)})$ 1-dimensional lines (intersections of $n-1 \geq 2$ bisectors in any dimension $n \geq 3$) and up to $m(4k)^n$ bisectors. Step 3c similarly needs to split only $O(m^n(4k)^{n^2})$ polyhedra linearly depending on the number of intersection points. □

The complexity to compute a Minkowski-reduced basis is quadratic in logarithms of the lengths of initial basis vectors for dimensions $n \leq 3$, see the exact bounds in [22, Theorems 4.2.1 and 5.0.4]. Though the dependence of the time estimate on the dimension n is exponential, the experiments in the next section for $n = 2$ and $n = 3$ show that the algorithm is very fast in practice.

5 Experiments on degree-k Voronoi domains for $n = 2, 3$

The complexity bound from Theorem 17 has been experimentally illustrated as follows. In $\mathbb{R}^2$ we chose 6 different lattices: the square, hexagonal and rectangular lattices, plus 3 more generic ones, as shown in Fig. 8. Given one of these lattices and a fixed number $m \in [1, 50]$, we randomly generated m motif points to get a periodic point set. Repeating the random generation of motif points 100 times for each of the 6 lattices, we get 600 periodic point sets in total for each $m \in [1, 50]$, see Fig. 9 for two periodic point sets with $m = 2$. In Figs. 10-13, each cross represents the mean result, such as runtime in milliseconds, over the 600 periodic point sets of every value of the number m of motif points considered. All experiments were performed on a MacBook Pro with 2.3 GHz, 8GB RAM.

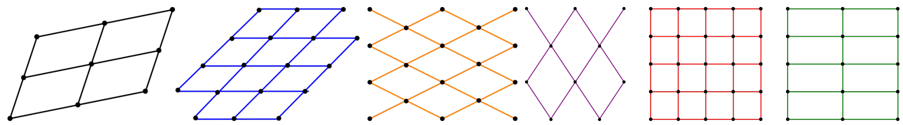

Fig. 8. The 2D lattices in the experiments in Section 5. **1st:** a (black) generic lattice with basis $(1.25, 0.25)$, $(0.25, 0.75)$. **2nd:** a (blue) hexagonal lattice with basis $(1, 0)$, $(0.5, \sqrt{3}/2)$. **3rd:** an (orange) rhombic lattice with basis $(1, 0.5)$, $(1, -0.5)$. **4th:** a (purple) rhombic lattice with basis $(1, 1.5)$, $(1, -1.5)$. **5th:** a (red) square lattice with standard basis $(1, 0)$, $(0, 1)$. **6th:** a (green) rectangular lattice with basis $(2, 0)$, $(0, 1)$.

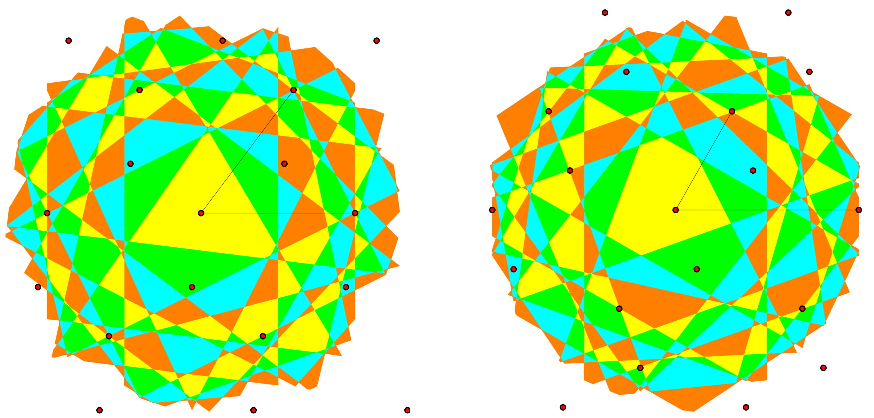

Fig. 9. The first 12 degree-k Voronoi domains of $0 \in \mathbb{R}^2$ for: **Left:** A periodic point set with basis $(1, 0.5)$, $(1, -0.5)$; **Right:** A periodic point set with basis $(1.25, 0.25)$, $(0.25, 0.75)$. In each image, the basis vectors are shown by thin black lines.

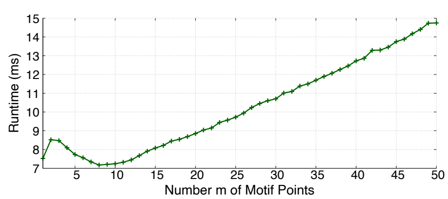

Fig. 10. Runtime for 8 degree-k Voronoi domains for $m = 1, \ldots, 50$ motif points, averaged over 600 2D periodic sets.

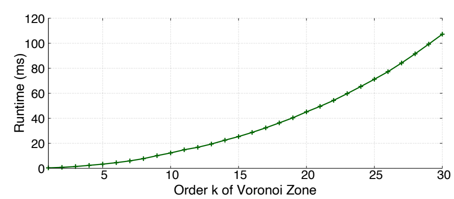

Fig. 11. Runtime for degree-k Voronoi domains for $k = 1, \ldots, 30$, averaged over 600 2D periodic sets for $m = 1, \ldots, 5$.

Fig. 10 indicates that starting from about $m = 10$, the runtime increases almost linearly with respect to the number m of motif points as expected by Theorem 17. Fig. 11 indicates that the runtime for $n = 2$ follows a slow quadratic increase with respect to the degree k of Voronoi domains, see Theorem 17.

The 3D experiments were for periodic sets with m motif points randomly generated for the cubic lattice. Fig. 15 shows degree-5 Voronoi domains for the FCC (face-centred cubic) and BCC (body-centred cubic) lattices, and HCP (hexagonal close packing). Figs. 12-13 illustrate the time in Theorem 17 for $n = 3$.

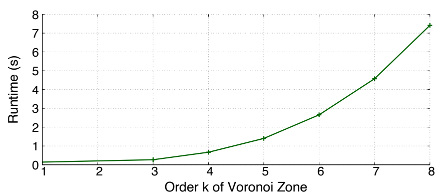

Fig. 12. Runtime to compute the degree-k Voronoi domains for $k = 1, \ldots, 8$, averaged over 10 3D periodic point sets for each value of $m = 1, \ldots, 5$.

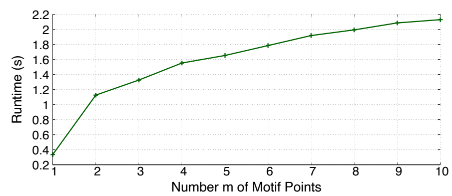

Fig. 13. Runtime to compute the first 5 degree-k Voronoi domains as the number of motif points takes values $m = 1, \ldots, 10$, averaged over 10 3D periodic point sets.

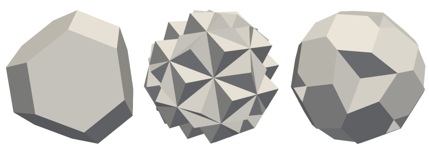

Fig. 14. Degree-k Voronoi domains $Z_k(\Lambda; 0)$ in the cubic lattice, $k = 4, 5, 6$.

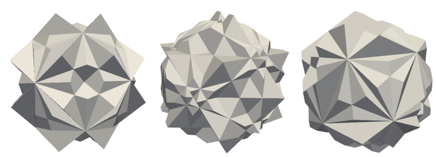

Fig. 15. Degree-5 Voronoi domains for FCC, BCC and HCP respectively.

The algorithm from Section 4 helped compute the density functions in [12] without covering the new results in this paper. These functions were explicitly described for any periodic 1D sequence in [5,6]. The C++ code for the algorithm in Section 4 is available by request. This research opened the wider area of Geometric Data Science studying point sets up to isometry. Persistent homology turned out to be a weaker isometry invariant than previously anticipated [24], but complete isometry invariants with continuous and computable metrics were recently constructed in [17]. Isometry invariants and continuous metrics of periodic sets were initiated in [21,2], see the recent progress in [3,29,4,28,19,20,8,18,7,30,27,26].

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