Recognition of near-duplicate periodic patterns by continuous metrics with approximation guarantees

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Abstract

This paper proposes a rigorous solution to the challenging classification problem of periodic patterns under Euclidean isometry and rigid motion. The 3-dimensional case is practically important for solid crystalline materials (periodic crystals) including all medical drugs that are produced in a rigid tablet form.

Many past invariants based on finite subsets fail when a unit cell of a periodic pattern discontinuously changes under almost any perturbation of atoms, which is inevitable due to noise and atomic vibrations. The major problem is not only to find complete invariants (descriptors with \textit{no false negatives} and \textit{no false positives} for all periodic patterns) but to design efficient algorithms for distance metrics on these invariants that should continuously behave under noise.

The proposed continuous metrics solve this problem in any Euclidean dimension and are algorithmically approximated with small error factors in times that are explicitly bounded in the input size and complexity of a given crystal.

The proved Lipschitz continuity allows us to confirm all near-duplicates filtered by simpler invariants in major databases of experimental and simulated crystals. This practical detection of near-duplicates will stop the artificial generation of ‘new’ materials from slight perturbations of known crystals. Several such duplicates are under investigation by five journals for data integrity.

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1. Continuous metric problem for periodic point sets and crystals

Periodic point sets include lattices and model all periodic crystals since any atom has a physically meaningful nucleus and is represented by its center [1]. This approach is more fundamental than the one with chemical bonds, which are not physical sticks or strings, hence abstractly representing inter-atomic interactions depending on various thresholds for distances and angles [2].

A lattice $\Lambda \subset \mathbb{R}^n$ is the infinite set of all integer linear combinations $\sum_{i=1}^{n} c_i v_i$ of a basis $v_1, \ldots, v_n$ of Euclidean space $\mathbb{R}^n$. Any basis defines a parallelepiped $U$ called a primitive unit cell of $\Lambda$. The first picture in Fig. 1 shows different unit cells in red, green, and blue, which generate the same hexagonal lattice.

A periodic point set $S \subset \mathbb{R}^n$ is a finite union of lattice translates $\Lambda + p$ obtained from $\Lambda$ by shifting the origin to a point $p$ from a finite motif $M \subset U$.

![Diagram of periodic cells and transformations](image)

**Figure 1:** Left: three (of infinitely many) primitive cells $U, U', U''$ of the same minimal area for the hexagonal lattice $\Lambda$. Other images show periodic sets $\Lambda + M$ with different cells and motifs, which are all isometric to $\Lambda$ whose hexagonal Voronoi domain is highlighted in yellow.

This paper is motivated by the growing crisis of ‘fake’ data in crystallography [3] because a slight modification of a known material can be claimed as ‘new’. Indeed, the fundamental question “same or different” [4] was not rigorously answered for periodic crystals. In the mathematical language, what periodic crystals can we consider equivalent, i.e. in the same class under an equivalence relation? One classical equivalence between crystals is by symmetry, e.g. crystallographic space groups were classified into 230 types (if mirror images are distinguished) already in the 19th century by Fedorov [5] and Schonflies [6].

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In 2024, experimental databases, e.g. the Cambridge Structural Database (CSD) of 1.25+ million real materials [7], need much stronger classifications than by 230 space groups or by chemical compositions. Indeed, many crystals such as diamond and graphite consist of the same elements but have vastly different properties due to essential differences in their geometric structures.

Structures of periodic crystals are experimentally determined in a rigid form. Hence the most practical equivalence between crystals is rigid motion, which is a composition of translations and rotations in $\mathbb{R}^n$. The slightly weaker equivalence is isometry (any distance-preserving transformation), which also includes reflections. This paper mainly studies isometry because a classification under rigid motion requires only a minor restriction in Definition 3.9. Periodic crystals form a continuously infinite space of isometry classes, e.g. almost any perturbation of points such as atomic displacement caused by noise in data produces a slightly different isometry class, which might have an arbitrarily scaled-up primitive cell, an enlarged motif, and a different symmetry group as in Fig. 2.

Figure 2: Past descriptors based on a primitive cell cannot continuously quantify a distance between near-duplicates. For example, under almost any perturbation, symmetry groups break down and a primitive cell volume discontinuously changes up to any integer factor.

Perturbations in Fig. 2 work for all periodic crystals and can be used for easily disguising old crystals as ‘new’ by additionally replacing atomic types with similar ones [8]. Such disguises of geometric near-duplicates were exposed first in the CSD, see [9 section 7], [10 section 6], and on a much larger scale in Google’s GNoME database [11], which was reviewed in [12, 13 Tables 1-2].

A pseudo-symmetry approach calls crystals equivalent if their cell parameters or atomic coordinates differ up to some $\varepsilon > 0$ [14]. Then any sets can be joined by a long enough chain of $\varepsilon$-perturbations [15 Prop 2.1]. If we allow any
threshold $\varepsilon > 0$, the transitivity axiom (if $A \sim B$ and $B \sim C$, then $A \sim C$) implies that all periodic sets in $\mathbb{R}^n$ become equivalent to each other. Even for a finite set in $\mathbb{R}^2$, the symmetry detection up to $\varepsilon$-perturbations is NP-hard \[16\].

A mathematical approach to noisy data is to quantify perturbations by a distance metric satisfying all axioms in Definition 1.1 below and taking small positive values on pairs of sets in Fig.2 which is formalized in Problem 1.2(a).

**Definition 1.1 (metric).** A metric on isometry classes of periodic sets of unordered points in $\mathbb{R}^n$ is a real-valued function $d(S,Q)$ satisfying the following axioms:

1.1a) $d(S,Q) = 0$ if and only if sets $S, Q$ are isometric (denoted by $S \simeq Q$);
1.1b) symmetry: $d(S,Q) = d(Q,S)$ for any periodic point sets $S, Q$ in $\mathbb{R}^n$;
1.1c) triangle inequality: $d(S,Q) + d(Q,T) \geq d(S,T)$ for any $S, Q, T$.

Without the first axiom in 1.1a), even the zero function $d(S,Q) = 0$ satisfies Definition 1.1. The atomic vibrations [1, chapter 1] motivate a metric whose continuity is quantified via a maximum displacement of atoms in (1.2a) below.

**Problem 1.2 (continuous metric on periodic sets).** Find a metric $d$ on periodic point sets in $\mathbb{R}^n$ such that all the axioms of Definition 1.1 hold and

1.2a) $d$ is Lipschitz continuous: there is a constant $\lambda > 0$ such that, for any sufficiently small $\varepsilon > 0$, if $Q$ is obtained from any periodic set $S \subset \mathbb{R}^n$ by perturbing each point of $S$ within its $\varepsilon$-neighborhood, then $d(S,Q) \leq \lambda \varepsilon$;
1.2b) $d(S,Q)$ is computed or approximated (up to an explicit error factor) in a time that has a polynomially upper bound in the sizes of motifs of $S, Q$.

Problem 1.2 can be widened to any real data (instead of crystals) and equivalences (instead of isometry). Condition 1.2a) goes beyond a complete classification of periodic point sets modulo isometry. Indeed, any metric $d$ satisfying 1.2a) detects all non-isometric sets $S \not\simeq Q$ by checking if $d(S,Q) \neq 0$. Conversely, detecting an isometry $S \simeq Q$ gives only a discontinuous metric $d$, e.g. $d(S,Q) = 1$ for any non-isometric $S \not\simeq Q$ and $d(S,Q) = 0$ for any $S \simeq Q$. 

4
For finite point sets under rigid motion in $\mathbb{R}^n$, Geometric Deep Learning \cite{17} experimentally looked for invariants, the persistent homology turned out to be weaker than anticipated \cite{18}, while Problem 1.2 was solved by easier and faster invariants in \cite{19,20}. In the periodic case, Problem 1.2 was solved in dimension $n = 1$ \cite{21} and for lattices in $\mathbb{R}^2$ \cite{15,22} but remained open for $n > 2$.

This paper solves Problem 1.2 by defining a continuous metric on complete invariant from the past work \cite{23}. The first step introduces a boundary tolerant metric $BT$ on local clusters around points of a periodic set $S$, which continuously changes when points cross a cluster boundary. This discontinuity at the boundary can be formally resolved by an extra factor, which smoothly goes down to 0 depending on an extra parameter. Without using extra parameters, the new metric $BT$ will be exactly expressed in terms of simpler distances.

The second step uses the Earth Mover’s Distance \cite{24} to extend $BT$ to complete invariants \cite{23} that are weighted distributions of local clusters up to rotations. The resulting metric on periodic sets in $\mathbb{R}^n$ will be approximated with a factor $\eta$, e.g. $\eta \approx 4$ in $\mathbb{R}^3$, in a time with a polynomial bound in the input size.

The third step proves the metric axioms and continuity $d(S, Q) \leq 2\varepsilon$, which also has practical importance. Indeed, if $d(S, Q)$ is approximated by a value $d$ with a factor $\eta$, we get the lower bound $\varepsilon \geq \frac{d}{2\eta}$ for the maximum displacement $\varepsilon$ of points. Such a lower bound is impossible to guarantee by analyzing only finite subsets, which can be very different in identical periodic sets, see Fig. 3.

Figure 3: \textbf{Left:} for any lattice $S$ and a fixed size of a box or a ball, one can choose many non-isometric finite subsets of different sizes. \textbf{Right:} the blue set $S$ and green set $Q$ in the line $\mathbb{R}$ have a small Hausdorff distance $d_H = \varepsilon$ but are not related by a small perturbation.
2. Past work on distances and invariants of periodic point sets

One can try comparing periodic point sets by finding an isometry of $\mathbb{R}^n$ that makes them as close as possible [26]. This approximate matching is much easier for finite sets. Hence it is very tempting to restrict any periodic point set to a large rectangular box or a cube with identified opposite sides [27] (a fixed 3D torus). However, differently located boxes or balls of any fixed size can contain non-isometric finite sets as shown in Fig. 3 (left) for the square lattice. Then extra justifications are needed to show that a comparison of periodic sets by their finite subsets does not depend on the choices of these finite subsets.

**Definition 2.1** (Hausdorff distance $d_H$, bottleneck distance $d_B$). (a) For any sets $S, Q$ in a metric space, $d_H(S, Q) = \sup_{p \in S} \inf_{q \in Q} d(p, q)$ is the directed Hausdorff distance. The Hausdorff distance is $d_H(S, Q) = \max\{d_H(S, Q), d_H(Q, S)\}$.

(b) The bottleneck distance $d_B(S, Q) = \inf_{g:S \to Q} \sup_{p \in S} d(p, g(p))$ for sets $S, Q$ of the same cardinality is minimized over bijections $g$ and maximized over $p \in S$. ■

Fig. 3 (right) shows the sets $S, Q$ consisting of blue and green points, respectively, where all green points of $Q$ are covered by small closed blue balls centered at all points of $S$ in the top right picture, and vice versa. Hence a small Hausdorff distance $d_H(S, Q)$ doesn’t guarantee that the sets $S, Q$ are related by a small perturbation of points. A non-bijective matching of points is inappropriate for real atoms that cannot disappear and reappear from thin air. Hence the bottleneck distance $d_B$ is more suitable for measuring atomic displacements than $d_H$. [10, Example 2.1] shows that the 1-dimensional lattices $\mathbb{Z}$ and $(1 + \delta)\mathbb{Z}$ have $d_B = +\infty$ for any $\delta > 0$. If any lattices have equal density (or unit cell volume), they have a finite bottleneck distance $d_B$ by [28, Theorem 1(iii)].

If we consider only periodic point sets $S, Q \subset \mathbb{R}^n$ with the same density (or unit cells of the same volume), the bottleneck distance $d_B(S, Q)$ becomes a well-defined wobbling distance [29], which is still discontinuous under perturbations by [10, Example 2.2], see the related results for non-periodic sets in [30, 31].
Another approach to comparing crystals is by Voronoi diagrams [32], which can be defined for periodic sets but remain combinatorially unstable as for finite sets. Under almost any perturbation of basis vectors in $\mathbb{R}^2$, a rectangular lattice becomes generic with a hexagonal Voronoi domain. Hence combinatorial descriptors of Voronoi domains discontinuously change under perturbations of non-generic sets as in Fig. 2. Geometric descriptors such as the area or volume can be continuously compared by the Hausdorff distance [33] and helped define two continuous metrics between lattices in $\mathbb{R}^n$ [34], though their implementation sampled finitely many rotations without approximation guarantees.

Other comparisons of periodic sets use a manually chosen number of neighbors [26] or a cut-off radius [35]. A reduction to a finite subset cannot provide a complete and continuous invariant of periodic sets because, under tiny perturbations, a primitive (minimal by volume) cell can become larger than any bounded subset of a fixed size, see Fig. 2. One can guarantee the continuity under perturbations by extra smoothing at a fixed cut-off radius so that non-matched points covertly cross a fixed boundary, e.g. [36] starts from a Gromov-Hausdorff distance between finite sets of any sizes and adds terms converging to 0 at the boundary. The continuity of this distance was shown for three motions [36, Fig. 3,4,5] but the triangle inequality still needs proof.

Crystallographers often compared periodic crystals by using reduced or conventional cells [37, section 9.3]. In $\mathbb{R}^2$, a cell with basis vectors $\vec{v}_1, \vec{v}_2$ is reduced if $|\vec{v}_1| \leq |\vec{v}_2|$ and $-1/2 \vec{v}_1^2 \leq \vec{v}_1 \cdot \vec{v}_2 \leq 0$. The vectors $\vec{v}_1 = (2a, 0)$ and $\vec{v}_2 = (2b, \pm b)$ for $b \geq a\sqrt{3}$ and both signs $\pm$ are reduced and define isometric lattices related by reflection. This ambiguity of bases can be resolved by an additional condition $\det(\vec{v}_1, \vec{v}_2) > 0$, which creates the inevitable discontinuity, see more details in [15, Fig. 4]. In $\mathbb{R}^3$, the most widely used reduced cell is Niggli’s cell [38], which has a minimum volume and all angles as close to $90^\circ$ as possible. [39] Theorem 4.2.1] expressed the complexity of cell reductions via vector lengths of a given basis. Fig. 2 shows that any primitive cell discontinuously changes under almost any perturbation of points. Niggli’s cell was known to be experimentally
discontinuous since 1965 \[40\] and perhaps clear to Eisenstein in 1850 \[41\].

General periodic point sets have density functions \[42\], which are practically computable \[43\] complete invariants in general position in \(\mathbb{R}^3\). The distance between sequences of density functions was defined in terms of two suprema over infinitely many radii \(t \in \mathbb{R}\) and indices \(k \in \mathbb{N}\), so the metric was approximated without guarantees. The density functions experimentally coincided \[42, section 5\] for the periodic sets \(S_{15} = X + Y + 15\mathbb{Z}\) and \(Q_{15} = X - Y + 15\mathbb{Z}\) for \(X = \{0, 4, 9\}\) and \(Y = \{0, 1, 3\}\), which was theoretically proved in \[44\, Example 11\]. This pair is distinguished by the faster invariants \[9\].

A distance between invariant values can be a metric on isometry classes only if the underlying invariant is complete under isometry. Otherwise, non-isometric sets can have identical invariant values with a distance of 0. Hence a complete classification should take into account a potential high complexity of periodic sets. Inspired by \[45, 46, 47\], an isometry classification was reduced \[23\] to only rotations of local clusters whose radius depends on \(S\) and can be as large as necessary to reconstruct a full set \(S\), uniquely under isometry in \(\mathbb{R}^n\).

Section 3 reminds us of a complete invariant from \[23\]. Section 4 introduces a Lipschitz continuous metric (Definition 4.4 and Theorem 4.9), whose polynomial time bounds (Corollaries 5.4, 5.10) are proved in section 5. Section 6 provides a lower bound (Theorem 6.5) for the new metric via simpler invariants. Section 7 discusses the significance of the continuous metric for detecting near-duplicates in major materials databases and for upholding scientific integrity.

### 3. Isometry classification of periodic point sets by complete invariants

This section reviews the complete invariant \[23\] based on local clusters and their symmetry groups, which were previously studied in \[45, 46\].

**Definition 3.1** (global clusters and m-regular periodic sets). For any point \(p\) in a periodic set \(S \subset \mathbb{R}^n\), the global cluster is \(C(S, p) = \{q - p : q \in S\}\). For any \(p, q \in \mathbb{R}^n\), let \(O(\mathbb{R}^n; p, q)\) be the group of all isometries of \(\mathbb{R}^n\) that
map $p$ to $q$. Global clusters $C(S,p)$ and $C(S,q)$ are called isometric if there is $f \in O(\mathbb{R}^n; p, q)$ such that $f(S) = S$. A periodic point set $S \subset \mathbb{R}^n$ is called $m$-regular if all global clusters of $S$ form exactly $m \geq 1$ isometry classes.

For any point $p \in S$, its global cluster is a view of $S$ from the position of a point $p$. We view all astronomical stars in the universe $S$ from our planet Earth at $p$. Any lattice is 1-regular since all its global clusters are related by translations. Though global clusters $C(S,p), C(S,q)$ at any different points $p, q \in S$ contain the same set $S$, they may not match under the translation shifting $p$ to $q$. The global clusters are infinite, hence distinguishing them up to isometry is not easier than original periodic sets. However, the $m$-regularity of a periodic set can be checked in terms of finite local $\alpha$-clusters below.

**Definition 3.2** *(local $\alpha$-clusters $C(S,p; \alpha)$ and symmetry groups $\text{Sym}(S,p; \alpha))$.

For a point $p$ in a periodic point set $S \subset \mathbb{R}^n$ and any $\alpha \geq 0$, the local $\alpha$-cluster $C(S,p; \alpha)$ is the set of all vectors $q - p$ such that $q \in S$ and $|q - p| \leq \alpha$. Let the group $O(\mathbb{R}^n; p)$ consist of all isometries that fix $p$. If $p = 0$ is the origin, $O(\mathbb{R}^n; 0)$ is the usual orthogonal group. The symmetry group $\text{Sym}(S,p; \alpha)$ consists of all isometries $f \in O(\mathbb{R}^n; p)$ that map $C(S,p; \alpha)$ to itself so that $f(p) = p$.

For any periodic set $S$, if $\alpha$ is smaller than the minimum distance between all points of $S$, then any $\alpha$-cluster $C(S,p; \alpha)$ is one point $\{p\}$. Its symmetry group consists of all isometries fixing the center $p$, so $\text{Sym}(S,p; \alpha) = O(\mathbb{R}^n; p)$. When $\alpha$ is increasing, the $\alpha$-clusters $C(S,p; \alpha)$ become larger and there can be fewer (not more) isometries $f \in O(\mathbb{R}^n; p)$ that bijectively map $C(S,p; \alpha)$ to itself. So the group $\text{Sym}(S,p; \alpha)$ can become smaller (not larger) and eventually stabilizes (stops changing), which will be formalized later in Definition 3.5.

Fig. 4 (left) shows the 1-regular periodic set $S_1 \subset \mathbb{R}^2$ whose all points (close to vertexs of square cells) have isometric global clusters related by translations and rotations through $90^\circ, 180^\circ, 270^\circ$. The set $S_2$ has extra points at the centers of all square cells. The local $\alpha$-clusters around these centers are not isometric to $\alpha$-clusters around the points close to cell vertexs for any $\alpha \geq 3\sqrt{2}$.
The 1-regular periodic point set $S_1$ in Fig. 4 for any $p \in S_1$ has the symmetry group $\text{Sym}(S_1, p; \alpha) = O(\mathbb{R}^2)$ for $\alpha \in [0, 4)$. Then $\text{Sym}(S_1, p; \alpha)$ stabilizes as $\mathbb{Z}^2$ with one reflection for $\alpha \geq 4$ as soon as $C(S_1, p; \alpha)$ includes one more point.

Figure 4: **Left**: in $\mathbb{R}^2$, the periodic point set $S_1$ has the square unit cell $[0, 10)^2$ containing the four points $(2, 2), (2, 8), (8, 2), (8, 8)$, so $S_1$ isn’t a lattice, but is 1-regular by Definition 3.1, and $\beta(S_1) = 6$. All local $\alpha$-clusters of $S_1$ are isometric, shown by red arrows for $\alpha = 5, 6, 8$, see Definition 3.2. **Right**: $S_2$ has the extra point $(5, 5)$ in the center of the cell $[0, 10)^2$ and is 2-regular with $\beta(S_2) = 3\sqrt{2}$, so $S_2$ has green and yellow isometry types of $\alpha$-clusters.

**Definition 3.3** (*bridge length* $\beta(S)$). For a periodic point set $S \subset \mathbb{R}^n$, the *bridge length* is a minimum distance $\beta(S) > 0$ such that any $p, q \in S$ can be connected by a sequence of points $p_0 = p, p_1, \ldots, p_k = q$ such that any two successive points $p_{i-1}, p_i$ are close so that $|p_{i-1} - p_i| \leq \beta(S)$ for $i = 1, \ldots, k$.

The theorem from [45, p. 20] proves that any 1-regular periodic point set is uniquely determined (up to isometry) by one sufficiently large $\alpha$-cluster. [46, Theorem 1.3] describes how a family of clusters uniquely determines a periodic point set up to isometry. These results motivated the concepts of the *isotree*, *stable radius*, and *isoset* in Definitions 3.4, 3.5, 3.9 respectively, leading to the isometry classification of periodic point sets via isosets in Theorem 3.10. The *isotree* in Definition 3.4 is inspired by a clustering dendrogram but points of $S$ split into isometry classes of $\alpha$-clusters at different radii $\alpha$, not at a fixed $\alpha$. 
Definition 3.4 (isotree $IT(S)$ of $\alpha$-partitions). Fix a periodic point set $S \subset \mathbb{R}^n$. Points $p, q \in S$ are $\alpha$-equivalent if their $\alpha$-clusters $C(S, p; \alpha)$ and $C(S, q; \alpha)$ are isometric so that their centers are matched. The isometry class $[C(S, p; \alpha)]$ consists of all $\alpha$-clusters isometric to $C(S, p; \alpha)$. The $\alpha$-partition $P(S; \alpha)$ is the splitting of $S$ into $\alpha$-equivalence classes of points. Call $\alpha$ singular if $P(S; \alpha) \neq P(S; \alpha - \varepsilon)$ for any small enough $\varepsilon > 0$ and represent each $\alpha$-equivalence class by a vertex of the isotree $IT(S)$. The top vertex of $IT(S)$ represents the $0$-equivalence class coinciding with the full set $S$. For any singular $\alpha < \beta$ without intermediate singular values, connect the vertices representing classes $A \in P(S; \alpha), B \in P(S; \beta)$ by an edge of the length $\beta - \alpha$ in $IT(S)$ if $B \subset A$. ■

Figure 5: Left: the 1-dimensional set $S_4 = \{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}\} + \mathbb{Z}$ has four points in the unit cell $[0, 1)$ and is 4-regular by Definition 3.1. Right: the colored disks show $\alpha$-clusters in the line $\mathbb{R}$ with radii $\alpha = 0, \frac{1}{12}, \frac{1}{6}, \frac{1}{4}, \frac{3}{4}$ and represent points in the isotree $IT(S_4)$ from Definition 3.4.

For any periodic point set $S \subset \mathbb{R}^n$, the root vertex of $IT(S)$ at $\alpha = 0$ is the single class $S$, because any 0-cluster $C(S, p; 0)$ of a point $p \in S$ consists only of its center $p$. When the radius $\alpha$ is increasing, $\alpha$-clusters $C(S, p; \alpha)$ include more points and hence may not be isometric. In other words, any $\alpha$-equivalence class from $P(S; \alpha)$ may split into two or more classes, which cannot merge at any larger $\alpha'$. Branched vertices of $IT(S)$ correspond to the values of $\alpha$ when an $\alpha$-equivalence class is split into subclasses for $\alpha'$ slightly larger than $\alpha$. So the number $|P(S; \alpha)|$ of $\alpha$-equivalence is non-decreasing in $\alpha$, see Fig. 5.
The $\alpha$-clusters of the 1-dimensional periodic point set $S_4 \subset \mathbb{R}$ in Fig. 5 are intervals in $\mathbb{R}$, shown as disks for better visibility. In Fig. 5, this class persists until $\alpha = \frac{1}{12}$, when all points $p \in S_4$ are split into two classes: one represented by 1-point cluster $\{p\}$ for $p \in \{0, \frac{1}{2}\} + \mathbb{Z}$, and another represented by 2-point clusters $\{p, p + \frac{1}{12}\}$, $p \in \{\frac{1}{4}, \frac{1}{3}\} + \mathbb{Z}$. The periodic set $S_4$ has four $\alpha$-equivalence classes for any radius $\alpha \geq \frac{1}{6}$. For any point $p \in \mathbb{Z} \subset S_4$, the symmetry group $\text{Sym}(S_4, p; \alpha) = \mathbb{Z}_2$ is generated by the reflection in $p$ for $\alpha \in [0, \frac{1}{4})$. For all $p \in S_4$, the symmetry group $\text{Sym}(S_4, p; \alpha)$ is trivial for any $\alpha \geq \frac{1}{4}$. For any periodic point set $S \subset \mathbb{R}^n$, the $\alpha$-partitions of $S$ stabilize in the sense below.

**Definition 3.5 (the minimum stable radius $\alpha(S)$).** Let $S \subset \mathbb{R}^n$ be a periodic point, $\beta \geq \beta(S)$ be an upper bound of the bridge length $\beta(S)$ from Definition 3.3. A radius $\alpha \geq \beta$ is called stable if the following conditions hold:

1. the $\alpha$-partition $P(S; \alpha)$ equals the $(\alpha - \beta)$-partition $P(S; \alpha - \beta)$;
2. the groups stabilize so that $\text{Sym}(S, p; \alpha) = \text{Sym}(S, p; \alpha - \beta)$ for any $p \in S$, i.e. any isometry $f \in \text{Sym}(S, p; \alpha - \beta)$ preserves the larger cluster $C(S, p; \alpha)$.

A minimum value of a stable radius $\alpha$ satisfying (3.5b) for $\beta = \beta(S)$ from Definition 3.3 is called the minimum stable radius and denoted by $\alpha(S)$. ■

Due to the upper bounds in Lemma 3.7(b,c), the minimum stable radius $\alpha(S) \geq 0$ exists and is achieved because $P(S; \alpha)$ and $\text{Sym}(S, p; \alpha)$ are continuous on the right (unchanged when $\alpha$ increases by a sufficiently small value).

**Example 3.6 (isosets of simple lattices).** (a) Any lattice $\Lambda \subset \mathbb{R}^n$ is 1-regular by Definition 3.1 and can be assumed to contain the origin $0$ of $\mathbb{R}^n$. Then the isoset $I(\Lambda; \alpha)$ consists of a single isometry class of a cluster $C(\Lambda, 0; \alpha)$. So the isotree $IT(\Lambda)$ is a linear path, which is horizontally drawn for the hexagonal and square lattices $\Lambda_6, \Lambda_4$ in Fig. 6. If both $\Lambda_6, \Lambda_4$ have a minimum inter-point distance 1, then the bridge length from Definition 3.3 is $\beta = 1$.

(b) For the hexagonal lattice $\Lambda_6 \subset \mathbb{R}^2$, $C(\Lambda_6, (0, 0); \alpha)$ includes points $p \neq (0, 0)$ only for $\alpha \geq 1$. The cluster $C(\Lambda_6, (0, 0); 1) = \{(0, 0), (\pm 1, 0), (\pm \frac{1}{2}, \pm \frac{\sqrt{3}}{2})\}$
appears in the 2nd step of Fig. 6 (left). The symmetry group Sym(Λ₆, (0, 0); α) becomes the dihedral group $D_6$ (all symmetries of a regular hexagon) for $α ≥ 1$. Hence any $α ≥ β + 1 = 2$ is stable. The isoset $I(Λ₆; 1)$ is the isometry class of the cluster $C(Λ₆, (0, 0); 1)$ of six vertices of the regular hexagon and its center.

(c) For the square lattice $Λ₄ ⊂ \mathbb{R}^2$, $C(Λ₄, (0, 0); α)$ has points $p \neq (0, 0)$ only for $α ≥ 1$. $C(Λ₄, (0, 0); 2) = \{(0, 0), (±1, 0), (0, ±1), (±\sqrt{2}, ±\sqrt{2}), (±2, 0), (0, ±2)\}$ includes the origin $(0, 0)$ with its 12 neighbors in the 4th step of Fig. 6 (right). The group Sym(Λ₄, (0, 0); α) becomes the dihedral group $D_4$ (all symmetries of a square) for $α ≥ 1$. So any $α ≥ β + 1 = 2$ is stable. The isoset $I(Λ₄; 1)$ is the isometry class of $C(Λ₄, (0, 0); 1)$ of four vertices of the square and its center.

For any $m$-regular periodic point set $S ⊂ \mathbb{R}^n$, the isoset $I(S; α)$ has at most $m$ isometry classes of $α$-clusters, so the isotree $IT(S)$ stabilizes with maximum $m$ branches. Though (3.5b) is stated for all points $p ∈ S$ for simplicity, it suffices to check (3.5b) only for all $p$ from a finite motif $M$ of $S$ due to periodicity. All stable radii of $S$ form the interval $[α(S), +∞)$ by Lemma A.4 in the appendix.

The periodic set $S₄$ in Fig. 5 has $β(S₄) = \frac{1}{2}$ and $α(S) = \frac{3}{4}$ since the $α$-partition and symmetry groups Sym($S₄, p; α$) are stable for $\frac{1}{4} ≤ α ≤ \frac{3}{4}$.

Condition (3.5b) doesn’t follow from condition (3.5a) due to the following example. Let $Λ$ be the 2D lattice with the basis $(1, 0)$ and $(0, β)$ for $β > 1$. Then $β$ is the bridge length of $Λ$. Condition (3.5a) is satisfied for any $α ≥ 0$, because all points of any lattice are equivalent up to translations. However, condition (3.5b) fails for any $α < β + 1$. Indeed, the $α$-cluster of the origin $(0, 0)$ contains five points $(0, 0), (±1, 0), (0, ±β)$, whose symmetries are generated by the two reflections in the axes $x, y$, but the $(α - β)$-cluster of the origin $(0, 0)$ consists of its center and has the symmetry group $O(\mathbb{R}^2)$. It is possible that condition
might imply condition (3.5a), but in practice it makes sense to verify (3.5b) only after checking much simpler condition (3.5a). Both conditions are essentially used in the proof of Isometry Classification Theorem 3.10.

Conditions (3.5ab) appeared in [46] with different notations $\rho, \rho + t$. Since many applied papers use $\rho$ for the physical density and have many types of bond distances, we replaced $t$ and $\rho + t$ with the bridge length $\beta$ and radius $\alpha$, respectively, as for growing $\alpha$-shapes in Topological Data Analysis [48].

Recall that the covering radius $R(S)$ of a periodic point set $S \subset \mathbb{R}^n$ is the minimum radius $R > 0$ such that $\bigcup_{p \in S} B(S; R) = \mathbb{R}^n$, or the largest radius of an open ball in the complement $\mathbb{R}^n - S$. For $m$-regular point sets in $\mathbb{R}^n$, an upper bound of $\alpha(S)$ can be extracted from [46, Theorem 1.3] whose proof motivated a stronger bound in Lemma 3.7(c), see comparisons in Example 3.8(c).

A periodic point set $S$ is locally antipodal if the local cluster $C(S, p; 2R(S))$ is centrally symmetric for any point $p \in S$, i.e. bijectively maps to itself under $q \mapsto 2p - q, q \in \mathbb{R}^n$. [49, Theorem 1] says that all locally antipodal Delone sets, hence all periodic sets $S$, are globally antipodal, i.e. $S$ is preserved under the isometry $q \mapsto 2p - q$ for any fixed $p \in S$, e.g. any lattice is antipodal.

**Lemma 3.7** (upper bounds for a stable radius $\alpha(S)$ and bridge length $\beta(S)$).

(a) Let $S \subset \mathbb{R}^n$ be a periodic point set with a unit cell $U$, which has the longest edge $b$ and longest diagonal $d$. Set $r(U) = \max\{b, \frac{d}{2}\}$. Then the bridge length $\beta(S)$ from Definition 3.3 has the upper bound $\min\{2R(S), r(U)\} \geq \beta(S)$.

(b) For any antipodal periodic set $S \subset \mathbb{R}^n$ whose covering radius is $R(S)$, the minimum stable radius has the upper bound $2R(S) + \beta(S) > \alpha(S)$.

(c) Let $S \subset \mathbb{R}^n$ be any periodic point set with the bridge length $\beta$. For a point $p \in S$ and a radius $\alpha_0 > 0$, let $|\text{Sym}(S, p; \alpha_0)|$ denote the size of the group $\text{Sym}(S, p; \alpha_0)$, which is finite for $\alpha_0 \geq 2R(S)$. Let $p_1, \ldots, p_m \in S$ be all points of an asymmetric unit of $S$. Set $L = \left\lceil \sum_{i=1}^{m} \left( \log_2 |\text{Sym}(S, p_i; \alpha_0)| - \log_2 |\text{Sym}(S, p_i)| \right) \right\rceil$. The minimum stable radius of $S$ from Definition 3.5 has the upper bound $\alpha_0 + (L + m)\beta \geq \alpha(S)$. For $\alpha_0 = 2R(S)$, we get $(L + m + 1)2R(S) \geq \alpha(S)$. ■
Proof. (a) The lemma in [45, section 2] proved that, in any Delone set $S$ with the covering radius $R(S)$, any two points $p, q \in S$ can be connected by a finite sequence of points $p_0 = p, p_1, \ldots, p_k = q$ such that $|p_{i−1} − p_i| \leq 2R(S)$ for $i = 1, \ldots, k$. In particular, any periodic point set $S$ has the upper bound $2R(S) \geq \beta(S)$. It remains to prove the second upper bound $r(U) \geq \beta(S)$.

For a point $p \in S$, shift the unit cell $U$ so that $p$ becomes the origin of $\mathbb{R}^n$ and a vertex of $U$, so the lattice $\Lambda$ can be considered a subset of the periodic point set $S$. Any points of $\Lambda$ can be connected by a sequence of lattice points such that any successive points have a distance not greater than the longest edge-length $b$ of $U$. Any point of a motif $M \subset U$ of $S$ is at most $d_2 \leq b$ away from a vertex of $U$, where $d$ is the length of the longest diagonal of $U$. Any points of $S$ can be connected by a sequence whose successive points are at most $r(U) = \max\{b, d_2\}$ away from each other, so $\beta(S) \leq r(U)$ by Definition 3.3.

(b) We will prove that the conditions of Definition 3.5 hold for $\alpha = 2R(S) + \beta(S)$ and $\beta = \beta(S)$. To prove condition 3.5(a), we check below that any $2R(S)$-equivalent points $p, q \in S$ are $\alpha$-equivalent for any $\alpha > 2R(S)$. The $2R(S)$-equivalence means that there is an isometry $f \in O(\mathbb{R}^n; p, q)$ such that $f(C(S, p; 2R(S))) = C(S, q; 2R(S))$. Set $Q = f(S)$. Then $f(C(S, p; 2R(S))) = C(f(S), f(p); 2R(S))$ means that $C(S, q; 2R(S)) = C(Q, q; 2R(S))$. [49, Theorem 3] implies that if antipodal periodic point sets $S, Q \subset \mathbb{R}^n$ have a common point $q$ with $C(S, q; 2R(S)) = C(Q, q; 2R(S))$, then $S = Q$. In our case, $f(S) = S$ implies that $f$ makes the points $p$ and $q = f(p)$ $\alpha$-equivalent for any $\alpha > 2R(S)$. Condition 3.5(b) says that any isometry $f \in \text{Sym}(S, p; 2R(S))$ should belong to $\text{Sym}(S, p; \alpha)$ for any point $p \in S$ and radius $\alpha > 2R(S)$. Indeed, [49, Theorem 3] implies that $Q = f(S)$ and $S$ should coincide, so $f$ isometrically maps any cluster $C(S, p; \alpha)$ to itself, hence $f \in \text{Sym}(S, p; \alpha)$.

(c) The argument from [45, p. 20] implies that, for any periodic point set $S \subset \mathbb{R}^n$ whose lattice is $n$-dimensional, the cluster $C(S, p; 2R(S))$ for any $p \in S$ is $n$-dimensional, i.e. not contained in a lower dimensional subspace. Hence the symmetry group $\text{Sym}(S, p; 2R(S))$ of this finite cluster is finite. For any initial
radius $\alpha_0 \geq 2R(S)$, we aim to find a radius $\alpha = \alpha_0 + k\beta$ such that both conditions 3.5(a,b) hold for a suitable index $k = 1, \ldots$ whose upper bound we will determine below. If condition 3.5(a) fails for some indices $j$, the number $|P(S; \alpha_0 + (k-1)\beta)|$ of $\alpha$-equivalence classes increases at least by one when $\alpha_0 + (k-1)\beta$ increases to $\alpha_0 + j\beta$. Since an asymmetric unit of $S$ consists of $m \geq 1$ points, there are at most $m - 1$ incremental values $0 = k_0 \leq k_1 \leq \ldots \leq k_{m-1}$ when $1 \leq |P(S; \alpha_0 + (k_1 - 1)\beta)| < |P(S; \alpha_0 + k_1\beta)| \leq m$ for $i = 1, \ldots, m - 1$.

In a degenerate case, if all points of $S$ are $(\alpha_0 + (k - 1)\beta)$-equivalent, this single class can split into the maximum $m > 1$ classes of $(\alpha_0 + k\beta)$-equivalence, then $k_1 = \ldots = k_{m-1} = k \geq 1$. For any successive incremental values $k_{i-1} < k_i$, the number $|P(S; \alpha_0 + k\beta)|$ of $(\alpha_0 + k\beta)$-equivalence classes is constant for $k = k_{i-1} + 1, \ldots, k_i$, so condition 3.5(a) holds for every radius $\alpha = \alpha_0 + k\beta$.

By reordering the points $p_1, \ldots, p_m$ from an asymmetric unit of $S$, we can assume that $p_1, \ldots, p_i$ represent $i$ classes of $(\alpha + k_{i-1}\beta)$-equivalence for any fixed $i = 1, \ldots, m$. Set $L(k) = \sum_{i=1}^{m} \log_2 |\text{Sym}(S, p_i; \alpha_0 + k\beta)|$. When $k$ increases, any group $\text{Sym}(S, p_i; \alpha_0 + k\beta)$ can become only smaller, not larger, so $L(k)$ is non-increasing. If $L(k-1) = L(k)$ for any $0 < k \neq k_1, \ldots, k_{m-1}$, both conditions 3.5(a,b) hold, so $\alpha_0 + k\beta$ is a stable radius. We will find an upper bound for a minimum value of such $k$. If condition 3.5(b) fails for all radii $\alpha = \alpha_0 + k\beta$ with $k = k_{i-1} + 1, \ldots, k_i$, then at least one of the groups $\text{Sym}(S, p; \alpha_k + j\beta)$ for $p \in \{p_1, \ldots, p_i\}$ is a proper subgroup of $\text{Sym}(S, p; \alpha_0 + (k - 1)\beta)$. The size of a proper subgroup is at most twice smaller than the size of the group, so

$$\log_2 |\text{Sym}(S, p; \alpha_0 + k\beta)| \leq \log_2 |\text{Sym}(S, p; \alpha_0 + (k - 1)\beta)| - 1, k = k_{i-1} + 1, \ldots, k_i.$$

Hence the sum $L(k)$ decreases at least by 1 for any failure of condition 3.5(b) from $L(0) = \sum_{i=1}^{m} \log_2 |\text{Sym}(S, p_i; \alpha_0)|$ to $L(+\infty) = \sum_{i=1}^{m} \log_2 |\text{Sym}(S, p_i)|$, where $\text{Sym}(S, p_i)$ is the symmetry group of the global cluster $C(S; p_i)$. Adding $m - 1$ potential failures of condition 3.5(a) for $\alpha_0 + k_i\beta$ with $i = 1, \ldots, m - 1$, the radius $\alpha_0 + k\beta$ cannot be stable for a maximum $L + m - 1$ values of $k$, where

$$L = [L(0) - L(+\infty)] = \left[ \sum_{i=1}^{m} \left( \log_2 |\text{Sym}(S, p_i; \alpha_0)| - \log_2 |\text{Sym}(S, p_i)| \right) \right].$$

16
Then any $\alpha = \alpha_0 + k\beta$ with $k \geq L + m$ is stable, so $\alpha(S) \leq \alpha_0 + (L + m)\beta$. To get $\alpha(S) \leq (L + m + 1)2R(S)$, set $\alpha_0 = 2R(S)$ and use $\beta \leq 2R(S)$ from (a). □

The upper bound in Lemma 3.7(a) holds for any unit cell of $S$. If a cell is non-reduced and too long, its reduced form can have smaller bounds for $\beta(S)$.

**Example 3.8** (upper bounds for $\alpha(S)$ and $\beta(S)$). Let $\Lambda(b) \subset \mathbb{R}^n$ be a lattice whose unit cell is a rectangular box with the longest edge $b$.

(a) In Lemma 3.7(a), the upper bound $b \geq \beta(S)$ is tight because $\beta(\Lambda(b)) = b$.

(b) In Lemma 3.7(b), the upper bound $2R(S) + \beta(S) \geq \alpha(S)$ is also tight for $\Lambda(b)$. Indeed, a cluster $C(\Lambda(b), 0; \alpha)$ is $n$-dimensional only for $\alpha \geq b$, so the group $\text{Sym}(\Lambda(b), 0; \alpha)$ stabilizes at $\alpha = b$, hence $\alpha(S) = b + \beta(\Lambda(b)) = 2b$ is the minimum stable radius. The covering radius $R(\Lambda(b))$ is half of the longest diagonal of the rectangular cell $U$. When $b \to +\infty$ and all other sizes of $U$ remain fixed, the upper bound $2R(\Lambda(b)) + \beta(\Lambda(b)) \geq \alpha(S)$ approaches $2b \geq \alpha(S)$.

(c) Lemma 3.7(c) was motivated by [46, Theorem 1.3], which implies the upper bound $\beta(S) + 2m(n^2 + 1)\log_2(2 + R(S)/r(S)) > \alpha(S)$ for $m$-regular point sets. Let $\Lambda \subset \mathbb{R}^2$ be a lattice whose unit cell is a rhombus with sides 1. Then $m = 1$, $n = 2$, $r(\Lambda) = 0.5$, $\beta(\Lambda) = 1$, and $\alpha(\Lambda) = 2$. If $\Lambda$ deforms from a square lattice to a hexagonal lattice, the covering radius $R(\Lambda)$ varies in the range $[\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{2}}]$. The past bound above gives the estimate $1 + 2(2^2 + 1)\log_2(2 + \frac{2}{\sqrt{3}}) \approx 17.6 > \alpha(\Lambda) = 2$.

For any lattice $\Lambda$ in this family, the symmetry group $\text{Sym}(\Lambda, 0) = \text{Sym}(\Lambda, 0; 1)$ stabilizes at $\alpha_0 = 1$. Lemma 3.7(c) for $\alpha_0 = 1$ gives $L = \log_2(2) - \log_2(2) = 0$, so the upper bound $\alpha_0 + (L + m)\beta(S) \geq \alpha(S)$ is tight: $2 \geq \alpha(\Lambda)$. In practice, if $L$ is large because some local clusters $C(S; p; \alpha_0)$ have too many symmetries, one can increase the radius $\alpha_0$ to reduce $L$ for a better bound of $\alpha(S)$. □

Definition 3.9 reminds of the *isoret*, which was initially introduced in [23, Definition 9]. We also cover the case of rigid motion and prove Completeness Theorem 3.10 in the appendix in more detail than in [23, Theorem 9].

**Definition 3.9** (*isoret* $I(S; \alpha)$ at a radius $\alpha \geq 0$). Let a periodic point set $S \subset \mathbb{R}^n$ have a motif $M$ of $m$ points. Split all points $p \in M$ into $\alpha$-equivalence classes.
classes. Each \(\alpha\)-equivalence class consisting of (say) \(k\) points in \(M\) can be associated with the isometry class \(\sigma = [C(S, p; \alpha)]\) of an \(\alpha\)-cluster centered at one of these \(k\) points \(p \in M\). The weight of \(\sigma\) is \(w = k/m\). The isoset \(I(S; \alpha)\) is the unordered set (weighted distribution) of all isometry classes \((\sigma; w)\) with weights \(w\) for all points \(p\) in the motif \(M\). If we consider only orientation-preserving isometries, the oriented isoset will be denoted by \(I^o(S; \alpha)\).

All points \(p\) of a lattice \(\Lambda \subset \mathbb{R}^n\) from one \(\alpha\)-equivalence class for any radius \(\alpha \geq 0\) because all \(\alpha\)-clusters \(C(\Lambda, p; \alpha)\) are isometrically equivalent to each other by translations. Hence the isoset \(I(\Lambda; \alpha)\) is one isometry class of weight 1 for \(\alpha \geq 0\), see examples in Fig. 7. All isometry classes \(\sigma\) in \(I(S; \alpha)\) are in a 1-1 correspondence with all \(\alpha\)-equivalence classes in the \(\alpha\)-partition \(P(S; \alpha)\) from Definition 3.4. So \(I(S; \alpha)\) without weights can be viewed as a set of points in the isotree \(IT(S)\) at the radius \(\alpha\). The size of the isoset \(I(S; \alpha)\) equals the number \(|P(S; \alpha)|\) of \(\alpha\)-equivalence classes in the \(\alpha\)-partition. Formally, \(I(S; \alpha)\) depends on \(\alpha\) because \(\alpha\)-clusters grow in \(\alpha\). To distinguish any \(S, Q \subset \mathbb{R}^n\) up to isometry, we will compare their isosets at a maximum stable radius of \(S, Q\).

An equality \(\sigma = \xi\) between isometry classes of clusters means that some (hence any) clusters \(C(S, p; \alpha)\) and \(C(Q, q; \alpha)\) representing \(\sigma, \xi\), respectively, are related by \(f \in O(\mathbb{R}^n; p, q)\), which will be algorithmically tested in Corollary 5.4.

**Theorem 3.10** (isometry classification of periodic point sets). For any periodic point sets \(S, Q \subset \mathbb{R}^n\), let \(\alpha\) be a common stable radius satisfying Definition 3.5 for an upper bound \(\beta\) of the bridge lengths \(\beta(S), \beta(Q)\). Then \(S, Q\) are isometric if and only if there is a bijection \(\varphi: I(S; \alpha) \to I(Q; \alpha)\) respecting all weights. ■

Theorem 3.10 was inspired by [46, Theorem 1.3] saying that, for a multi-regular point set \(X\), “the only Delone sets \(Y\) all of whose \(\rho\)-stars are isometric to \(\rho\)-stars of \(X\) are sets globally isometric to \(X\)”. After renaming \(\rho\)-stars as \(\alpha\)-clusters, we collected their isometry classes (with weights) into the isoset to rephrase [46, Theorem 1.3] as a complete classification of all periodic point sets by their isoset invariants in Theorem 3.10. If we consider only orientation-preserving isometries, an oriented analog of Theorem 3.10 classifies all periodic...
point sets modulo *rigid motion* defined as a composition of translations and rotations in $\mathbb{R}^n$ by the oriented isoset $I^*(S; \alpha)$ in Definition 3.9.

The $\alpha$-equivalence and isoset in Definition 3.9 can be refined by labels such as chemical elements, which keeps Theorem 3.10 valid for labeled points.

When comparing sets from a finite database, it suffices to build their isosets only up to a common upper bound of a stable radius $\alpha$ in Lemma 3.7(c).

4. Continuous metrics on isometry classes of periodic sets in $\mathbb{R}^n$

This section proves the continuity of the isoset $I(S; \alpha)$ in Theorem 4.9 by using the Earth Mover’s Distance (EMD) from Definition 4.4. For a point $p \in \mathbb{R}^n$ and a radius $\varepsilon$, the closed ball $\bar{B}(p; \varepsilon) = \{ q \in \mathbb{R}^n : |q - p| \leq \varepsilon \}$ has the boundary $(n - 1)$-dimensional sphere $\partial \bar{B}(p; \varepsilon) \subset \mathbb{R}^n$. The $\varepsilon$-offset of any set $C \subset \mathbb{R}^n$ is the Minkowski sum $C + \bar{B}(0; \varepsilon) = \{ p + q : p \in C, q \in \bar{B}(0; \varepsilon) \}$.

Then the directed Hausdorff distance from Definition 2.1(a) $d_H(C, D)$ is the minimum radius $\varepsilon \geq 0$ such that $C \subseteq D + \bar{B}(0; \varepsilon)$. Definition 4.1 introduces the crucial new metric, which will be explicitly computed in Lemma 5.6.

**Definition 4.1** (boundary tolerant metric BT on isometry classes of clusters). For a radius $\alpha$ and periodic point sets $S, Q \subset \mathbb{R}^n$, let clusters $C(S, p; \alpha), C(Q, q; \alpha)$ represent isometry classes $\sigma \in I(S; \alpha), \xi \in I(Q; \alpha)$, respectively. The boundary tolerant metric $BT(\sigma, \xi)$ is defined as the minimum $\varepsilon \geq 0$ such that

$$C(Q, q; \alpha - \varepsilon) \subseteq f(C(S, p; \alpha)) + \bar{B}(0; \varepsilon)$$

for some $f \in O(\mathbb{R}^n; p, q)$, and

$$C(S, p; \alpha - \varepsilon) \subseteq g(C(Q, q; \alpha)) + \bar{B}(0; \varepsilon)$$

for some $g \in O(\mathbb{R}^n; q, p)$.

**Lemma 4.2** (correctness of BT). The metric $BT(\sigma, \xi)$ in Definition 4.1 is independent of cluster representatives and satisfies the metric axioms below:

$$BT(\sigma, \xi) = 0$$

if and only if $\sigma = \xi$ as isometry classes of $\alpha$-clusters;

symmetry : $BT(\sigma, \xi) = BT(\xi, \sigma)$ for any isometry classes of $\alpha$-clusters;

triangle inequality : $BT(\sigma, \xi) \leq BT(\sigma, \zeta) + BT(\zeta, \xi)$ for any $\sigma, \xi, \zeta$. 

19
Example 4.3 (square lattice vs hexagonal). The isoset $I(\Lambda; \alpha)$ of any lattice $\Lambda \subset \mathbb{R}^n$ containing the origin 0 consists of a single isometry class $[C(\Lambda, 0; \alpha)]$, see Example 3.6. For the square (hexagonal) lattice with minimum inter-point distance 1 in Fig. 7, the cluster $C(\Lambda, 0; \alpha)$ consists of only 0 for $\alpha < 1$ and includes four (six) nearest neighbors of 0 for $\alpha \geq 1$. Hence $\text{Sym}(\Lambda, 0; \alpha)$ stabilizes as the symmetry group of the square (regular hexagon) for $\alpha \geq 1$. The lattices have the minimum stable radius $\alpha(\Lambda) = 2$ and $\beta(\Lambda) = 1$ by Example 3.8(c).

Figure 7: Example 4.3 computes the metric $\text{BT}$ from Definition 4.1 for the isometry classes of the 2-clusters in the square and hexagonal lattices $\Lambda_4, \Lambda_6$. 1st: for $\varepsilon_1 = \sqrt{2} - \sqrt{3} \approx 0.52$, the shrunken square cluster $C(\Lambda_4, 0; 2 - \varepsilon)$ is covered by the yellow $\varepsilon$-offset of $C(\Lambda_6, 0; 2)$. 2nd: for $\varepsilon_0 = \sqrt{2} - 1 \approx 0.41$, the shrunken cluster $C(\Lambda_4, 0; 2 - \varepsilon_0)$ is rotated through $-15^\circ$ (clockwise) and covered by the $\varepsilon_0$-offset of $C(\Lambda_6, 0; 2)$. 3rd: $C(\Lambda_4, 0; 2 - \varepsilon_0)$ is rotated through $15^\circ$ (counter-clockwise) and covered by the $\varepsilon_0$-offset of $C(\Lambda_6, 0; 2)$. 4th: $C(\Lambda_6, 0; 2 - \varepsilon_0)$ is covered by the blue $\varepsilon$-offset of $C(\Lambda_4, 0; 2)$ rotated through $15^\circ$. Finally, $\text{BT} = \varepsilon_0 = \sqrt{2} - 1$.

Non-isometric periodic sets $S, Q$ such as perturbations in Fig. 2 can have isosets of different numbers of isometry classes. A distance between these weighted distributions of different sizes can be measured by EMD below.

Definition 4.4 (Earth Mover’s Distance on isosets). Let periodic point sets $S, Q \subset \mathbb{R}^n$ have a common stable radius $\alpha$ and isosets $I(S; \alpha) = \{(\sigma_i, w_i)\}$ and $I(Q; \alpha) = \{(\xi_j, v_j)\}$, where $i = 1, \ldots, m(S)$ and $j = 1, \ldots, m(Q)$. The Earth Mover’s Distance [24] is $\text{EMD}(I(S; \alpha), I(Q; \alpha)) = \sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} \text{BT}(\sigma_i, \xi_j)$ minimized over flows $f_{ij} \in [0, 1]$ subject to $\sum_{j=1}^{m(Q)} f_{ij} \leq w_i$ for $i = 1, \ldots, m(S)$, $\sum_{i=1}^{m(S)} f_{ij} \leq v_j$ for $j = 1, \ldots, m(Q)$, and $\sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} = 1$. □

Fig. 7 illustrates the computations whose extra details are in Example A.5 □
**Lemma 4.5** (EMD is a metric on isosets). The Earth Mover’s Distance from Definition 4.4 satisfies the metric axioms for all \( \alpha \) and periodic sets \( S, Q, T \).

\[
\begin{align*}
(4.5a) \quad & \text{EMD}(I(S; \alpha), I(Q; \alpha)) = 0 \iff I(S; \alpha) = I(Q; \alpha); \\
(4.5b) \quad & \text{EMD}(I(S; \alpha), I(Q; \alpha)) = \text{EMD}(I(Q; \alpha), I(S; \alpha)); \\
(4.5c) \quad & \text{EMD}(I(S; \alpha), I(Q; \alpha)) + \text{EMD}(I(Q; \alpha), I(T; \alpha)) \geq \text{EMD}(I(S; \alpha), I(T; \alpha)).
\end{align*}
\]

**Example 4.6** (EMD for lattices with \( d_B = +\infty \)). Example 2.1 showed that the lattices \( S = \mathbb{Z} \) and \( Q = (1 + \delta)\mathbb{Z} \) have the bottleneck distance \( d_B(S, Q) = +\infty \) for any small \( \delta > 0 \). We show that \( S, Q \) have Earth Mover’s Distance \( \text{EMD} = 2\delta \) at their common stable radius \( \alpha = 2 + 2\delta \). The bridge lengths are \( \beta(S) = 1 \) and \( \beta(Q) = 1 + \delta \). The \( \alpha \)-cluster \( C(S, 0; \alpha) \) contains non-zero points for \( \alpha \geq 1 \), e.g. \( C(S, 0; 1) = \{0, \pm 1\} \). The symmetry group \( \text{Sym}(S, 0; \alpha) = \mathbb{Z}_2 \) includes a non-trivial reflection with respect to 0 for all \( \alpha \geq 1 \), so the stable radius of \( S \) is any \( \alpha \geq \beta + 1 = 2 \). Similarly, \( Q \) has \( \beta(Q) = 1 + \delta \) and stable radii \( \alpha \geq 2(1 + \delta) \). The Earth Mover’s Distance between \( I(S; \alpha) \) and \( I(Q; \alpha) \) at the common stable radius \( \alpha = 2 + 2\delta \) equals the metric \( \text{BT} \) between the only \( \alpha \)-clusters \( C(S, 0; \alpha) = \{0, \pm 1, \pm 2\} \) and \( C(Q, 0; \alpha) = \{0, \pm(1+\delta), \pm(2+\delta)\} \).

By Definition 4.1, we look for a minimum \( \varepsilon > 0 \) such that the cluster \( C(S, 0; \alpha - \varepsilon) \) is covered by \( \varepsilon \)-offsets of \( \pm(1 + \delta), \pm(2 + \delta) \) and vice versa. If \( \varepsilon < 2\delta < \frac{1}{2} \), the points \( \pm 2 \in C(S, 0; \alpha - \varepsilon) \) cannot be \( \varepsilon \)-close to \( \pm(1 + \delta), \pm(2 + \delta) \), but \( \varepsilon = 2\delta \) is large enough. The cluster \( C(Q, 0; \alpha - 2\delta) = \{0, \pm(1+\delta)\} \) is covered by the \( 2\delta \)-offset of \( C(S, 0; \alpha) = \{0, \pm 1, \pm 2\} \), so \( \text{EMD}(I(S; \alpha), I(Q; \alpha)) = 2\delta \). □

**Definition 4.7** (packing radius). For a discrete set \( Q \subset \mathbb{R}^n \), the **packing radius** \( r(Q) \) is the minimum half-distance between any points of \( Q \). Also, \( r(Q) \) is the maximum radius \( r \) such that the open balls \( B(p; r) \) are disjoint for all \( p \in Q \). □

Lemma 4.8 is proved in the appendix and is needed for Theorem 4.9.

**Lemma 4.8.** Let periodic point sets \( S, Q \subset \mathbb{R}^n \) have bottleneck distance \( d_B(S, Q) < r(Q) \), where \( r(Q) \) is the packing radius. Then \( S, Q \) have a common lattice \( \Lambda \) with a unit cell \( U \) such that \( S = \Lambda + (U \cap S) \) and \( Q = \Lambda + (U \cap Q) \). □
For rigid motion instead of general isometry, Definition 4.1 of a boundary tolerant metric BT is updated to BT\(^o\) by considering only orientation-preserving isometries from SO(\(\mathbb{R}^n\); p, q), which also makes the continuity below valid for oriented isosets \(I^o(S; \alpha)\) under EMD using BT\(^o\) instead of BT in Definition 4.4.

**Theorem 4.9** (continuity of isosets under perturbations). Let periodic point sets \(S, Q \subset \mathbb{R}^n\) have a bottleneck distance \(d_B(S, Q) < r(Q)\), where \(r(Q)\) is the packing radius in Definition 4.7. Then the isosets \(I(S; \alpha), I(Q; \alpha)\) are close in the Earth Mover’s Distance: \(\text{EMD}(I(S; \alpha), I(Q; \alpha)) \leq 2d_B(S, Q)\) for \(\alpha \geq 0\). ■

**Proof.** By Lemma 4.8 the given periodic point sets \(S, Q\) have a common unit cell \(U\). Let \(g: S \rightarrow Q\) be a bijection such that \(|p - g(p)| \leq \varepsilon = d_B(S, Q) = \inf_{g: S \rightarrow Q} \sup_{p \in S} |p - g(p)|\) for all points \(p \in S\). Since the bottleneck distance \(\varepsilon < r(Q)\) is small, the bijective image \(g(p)\) of any point \(p \in S\) is a unique \(\varepsilon\)-close point of \(Q\) and vice versa. Hence we can assume that the common unit cell \(U \subset \mathbb{R}^n\) contains the same number (say, \(m\)) points from \(S\) and \(Q\). Expand the initial \(m(S)\) isometry classes \((\sigma_i, w_i)\) \(\in I(S; \alpha)\) to \(m\) isometry classes (with equal weights \(\frac{1}{m}\)) represented by clusters \(C(S, p; \alpha)\) for \(m\) points \(p \in S \cap U\). If the \(i\)-th initial isometry class had a weight \(w_i = \frac{k_i}{m}\), \(i = 1, \ldots, m(S)\), the expanded isoset contains \(k_i\) equal isometry classes of weight \(\frac{1}{m}\). For example, the 1-regular set \(S_1\) in Fig. 4 has the isoset consisting of a single class \([C(S_1, p; \alpha)]\), which is expanded to four identical classes of weight \(\frac{1}{4}\) for the four points in the motif.

The isoset \(I(Q; \alpha)\) is similarly expanded to \(m\) isometry classes of weight \(\frac{1}{m}\).

For any point \(p \in S \cap U\), the image \(g(p) \in Q\) has a unique point \(h(p) \in Q \cap U\) such that \(h(p)\) is equivalent to \(g(p)\) modulo the lattice of \(Q\). Then the \(\alpha\)-clusters of \(g(p)\) and \(h(p)\) in \(Q\) are isometric for any \(\alpha \geq 0\). The bijection \(p \mapsto h(p)\) between the expanded motifs of \(S, Q\) induces the bijection between the expanded sets of \(m\) isometry classes. Each correspondence \(\sigma_i \mapsto \xi_l\) in the latter bijection can be visualized as the flow \(f_{ll} = \frac{1}{m}\) for \(l = 1, \ldots, m\), so \(\sum_{l=1}^m f_{ll} = 1\).

To show that the Earth Mover’s Distance (EMD) between any initial isoset and its expansion is 0, we collapse all identical isometry classes in the expanded
isosets, but keep the arrows with the flows above. Only if both tail and head of
two (or more) arrows are identical, we collapse these arrows into one arrow that
gets the total weight. All equal weights \( \frac{1}{m} \) correctly add up at heads and tails
of final arrows to the initial weights \( w, v \) of isometry classes. So the total sum
of flows is \( \sum_{i=1}^{m} \sum_{j=1}^{m} f_{ij} = 1 \) as required by Definition 4.4. It suffices to consider
below the EMD only for the expanded isosets of exactly \( m \) classes.

We will estimate the boundary tolerant metric between isometry classes \( \sigma, \xi \)
whose centers \( p, g(p) \) are \( \varepsilon \)-close within the common unit cell \( U \). For any
fixed point \( p \in S \cap U \), shift \( S \) by the vector \( g(p) - p \). This shift makes \( p \in S \)
and \( g(p) \in Q \) identical and keeps all pairs \( q, g(q) \) for \( q \in C(S, p; \alpha) \) within \( 2\varepsilon \)
of each other. Using the identity map \( f \) in Definition 4.1, we get the upper
bound \( BT([C(S, p; \alpha)], [C(Q, g(p); \alpha)]) \leq 2\varepsilon \). Then
\( \text{EMD}(I(S; \alpha), I(Q; \alpha)) \leq \sum_{l=1}^{m} f_{ll} BT([C(S, p; \alpha)], [C(Q, g(p); \alpha)]) \leq 2\varepsilon \sum_{l=1}^{m} f_{ll} = 2\varepsilon \) as required.

Corollary 4.10a justifies that the EMD satisfies all metric axioms for periodic
point sets that have a stable radius \( \alpha \). Corollary 4.10b avoids this dependence
on \( \alpha \) and scales any periodic point set \( S \) to the minimum stable radius \( \alpha(S) = 1 \).

**Corollary 4.10.** (a) For \( \alpha > 0 \), \( \text{EMD}(I(S; \alpha), I(Q; \alpha)) \) is a metric on the space
of isometry classes of all periodic point sets with a stable radius \( \alpha \) in \( \mathbb{R}^n \).

(b) For a periodic point set \( S \subset \mathbb{R}^n \) let \( S/r(S) \subset \mathbb{R}^n \) denote \( S \) after uniformly dividing all vectors by the packing radius \( r(S) \). Then \( |r(S) - r(Q)| + \text{EMD}(I(S/r(S); 1), I(Q/r(Q); 1)) \) is the metric on all periodic point sets.

**Proof.** (a) Lemma 4.5 proved the metric axioms for the EMD on isosets. The
equality \( I(S; \alpha) = I(Q; \alpha) \) is equivalent to isometry \( S \simeq Q \) by Theorem 3.10

(b) By part (a), \( \text{EMD}(I(S/r(S); 1), I(Q/r(Q); 1)) \) satisfies the symmetry and
triangle inequality, which are preserved by adding the Euclidean distance \( d = |r(S) - r(Q)| \) between the packing radii. The equality \( \text{EMD} = 0 \) means that
\( S/r(S) \simeq Q/r(Q) \) are isometric. Hence \( S, Q \) are isometric up to a uniform
factor. Adding the distance \( d = |r(S) - r(Q)| \) guarantees that the sum becomes
zero only if \( r(S) = r(Q) \), so the given sets \( S, Q \) should be truly isometric.
The metric $\text{EMD}(I(S; \alpha), I(Q; \alpha))$ is measured in the same units as atomic coordinates, say in angstroms: $1\text{Å} = 10^{-10}\text{m}$, and hence is physically meaningful. Since crystals are practically compared within a finite dataset, we can take any common upper bound of $\alpha(S)$ from Lemma 3.7 also in Corollary 4.10(b).

5. Algorithms to test isometry and to approximate metrics on isosets

This section describes time complexities for computing the complete invariant isoset (Theorem 5.3), comparing isosets (Corollary 5.4), approximating the boundary-tolerant metric BT and Earth Mover’s Distance on isosets (Corollary 5.10). All estimates will use the geometric complexity $\text{GC}(S)$ below.

**Definition 5.1** (geometric complexity $\text{GC}$). Let a periodic point set $S \subset \mathbb{R}^n$ have an asymmetric unit of $m$ points in a cell $U$ of volume $\text{vol}[U]$. Let $L$ be the symmetry characteristic for $\alpha_0 = 2R(S)$ in Lemma 3.7(c), where $R(S)$ is the covering radius. The geometric complexity is $\text{GC}(S) = \frac{(10(L+m+2))R(S)/n}{2\text{vol}[U]}$.

Let $V_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}$ be the volume of the unit ball in $\mathbb{R}^n$, where the Gamma function $\Gamma$ has $\Gamma(k) = (k-1)!$ and $\Gamma(\frac{5}{2} + 1) = \sqrt{\pi}(k - \frac{1}{2})(k - \frac{3}{2})\cdots \frac{1}{2}$ for any integer $k \geq 1$. Set $\nu(U, \alpha, n) = \frac{(\alpha+\delta)nV_n}{\text{vol}[U]}$, where $\delta = \sup_{p,q \in U} |p - q|$ is a longest diagonal of a unit cell $U$. All complexities assume the real Random-Access Machine (RAM) model and a fixed dimension $n$ of Euclidean space $\mathbb{R}^n$.

The main input size of a periodic set is the number $m$ of motif points because the length of a standard Crystallographic Information File is linear in $m$. For a fixed dimension $n$, the big $O$ notation $O(m^n)$ in all complexities means a function $t(m)$ such that $t(m) \leq Cm^n$ for a fixed constant $C$ independent of $m$. We will include all other parameters depending on a periodic point set $S$.

**Lemma 5.2** (a local cluster). Let a periodic point set $S \subset \mathbb{R}^n$ have $m$ points in a unit cell $U$. For any stable radius $\alpha \geq 0$ and $p \in M = S \cap U$, the cluster $C(S, p; \alpha)$ has at most $k = \nu m$ points and can be found in time $\nu O(m)$, where $\nu \leq \text{GC}(S)$ for geometric complexity $\text{GC}(S)$ from Definition 5.1.
To verify a congruence (isometry) of finite sets $A, B$ directed rotationally invariant, the Lemma 5.2 computes the distance $d_R$. Theorem 5.3 first moves the centers of mass of $A, B$ through $O$ to the origin and then follows to check if the shifted clusters are related by an isometry $f \in O(\mathbb{R}^n; 0)$ in time $O(k^{[n/3]} \log k)$. The isoset $I(S; \alpha)$ is obtained after identifying isometric clusters for $m$ points through $O(m^2)$ pairwise comparisons. The total time is $O(m^2)k^{[n/3]} \log k$. ■

**Corollary 5.4** (comparing isosets). One can check if any periodic point sets $S, Q \subset \mathbb{R}^n$ with motifs of at most $m$ points are isometric in time $O(m^2)k^{[n/3]} \log k$, where $k = \nu m$ for $\nu \leq \max\{\text{GC}(S), \text{GC}(Q)\}$. ■

**Theorem 5.3** (computing an isoset). For any periodic point set $S \subset \mathbb{R}^n$ given by a motif $M$ of $m$ points in a unit cell $U$, the isoset $I(S; \alpha)$ at a stable radius $\alpha$ can be found in time $O(m^2)k^{[n/3]} \log k$, where $k = \nu m$ for $\nu \leq \text{GC}(S)$. ■

**Proof.** Lemma 5.2 computes the $\alpha$-clusters of $m$ points $p \in M$ in time $O(k)$. To verify a congruence (isometry) of finite sets $A, B \subset \mathbb{R}^n$, the algorithm from [50] first moves the centers of mass of $A, B$ to $0 \in \mathbb{R}^n$. We instead move the centers of given clusters $A, B$ to the origin and then follow [50] to check if the shifted clusters are related by an isometry $f \in O(\mathbb{R}^n; 0)$ in time $O(k^{[n/3]} \log k)$. The isoset $I(S; \alpha)$ is obtained after identifying isometric clusters for $m$ points through $O(m^2)$ pairwise comparisons. The total time is $O(m^2)k^{[n/3]} \log k$. ■

**Definition 5.5** (rotationally invariant distance $d_R$). For any sets $C, D \subset \mathbb{R}^n$, the directed rotationally invariant distance $d_R(C, D) = \min_{f \in O(\mathbb{R}^n)} d_R(f(C), D)$ is minimized over all maps $f \in O(\mathbb{R}^n; 0)$, which fix the origin $0 \in \mathbb{R}^n$. ■

Definition 5.5 Lemma 5.6 and hence all further results similarly work for rigid motion by restricting all maps to the special orthogonal group $\text{SO}(\mathbb{R}^n; 0)$.

**Lemma 5.6** (max-min formula for $d_R$). For any finite sets $C, D \subset \mathbb{R}^n$, order all $p_1, \ldots, p_k \in C$ and $q_1, \ldots, q_k \in D$ by distance to the origin. For any $\alpha \geq \max\{|p_k|, |q_k|\}$, the distance $d_R(C \cup \partial B(0; \alpha), D \cup \partial B(0; \alpha))$ from Definition 5.5 equals $d_R(C, D)$ defined as $\max_{i=1, \ldots, k} \min\{\alpha - |p_i|, d_R(p_1, \ldots, p_i), D\}$. ■

**Example 5.7** (max-min formula). Consider the ‘rotational’ subcluster $C$ of the points $p_1 = (0, 1), p_2 = (1, 1), p_3 = (-1, 1), p_4 = (0, 2)$ from the square lattice.
\( \Lambda_4 \) in Fig. 7 Let \( \alpha = 2 \) and \( D = C(\Lambda_6, 0; 2) \) be the 2-cluster of the hexagonal lattice \( \Lambda_6 \). Then \( d_R(p_1, D) = 0 \) because \( p_1 \) can be rotated to \((1, 0) \in D \). Then \( d_R(p_1, D) = 0 \) because \( p_1, p_2 \) can be rotated to \((1, \sqrt{3}) \in D \) and \((\sqrt{3}, 1) \), which is at the distance \( \sqrt{3} - \sqrt{2} \) from \((\sqrt{3}, \sqrt{2}) \in D \). Example 4.3 confirms that \( d_R(p_1, D) = \sqrt{2} - 1 \). For \( i = 1 \), \( \min (\alpha - |p_1|, d_R(p_1, D)) = \min (2 - 1, 0) = 0 \). For \( i = 2 \), \( \min (\alpha - |p_2|, d_R(p_1, D)) = \min (2 - \sqrt{2}, \sqrt{3} - \sqrt{2}) = \sqrt{3} - \sqrt{2} \). For \( i = 3 \), \( \min (\alpha - |p_3|, d_R(p_1, D)) = \min (2 - \sqrt{2}, \sqrt{2} - 1) = \sqrt{2} - 1 \). For \( i = 4 \), \( \min (\alpha - |p_4|, d_R(C, D)) = 0 \) since \( \alpha = 2 = |p_4| \). The maximum of the above values is \( \sqrt{2} - 1 \), so Example 4.3 fits Lemma 5.6.

Lemma 5.8 extends [61] section 2.3 from \( n = 3 \) to any dimension \( n > 1 \).

**Lemma 5.8** (approximating \( d_R \)). For sets \( C, D \subset \mathbb{R}^n \) of at most \( k \) points, \( d_R(C, D) \) in Definition 5.5 is approximated with a factor \( \eta = \frac{n^2 - n + 2}{2} (1 + \delta) \) for \( \delta > 0 \) in time \( O(c_3 k^n \log k) \), where \( c_3 \leq \lceil n/3 \rceil^3 k^n \) is independent of \( k \). ■

**Proof.** Let \( p_1 \in C \) be a point that has a maximum distance to the origin. If there are several points at the same maximum distance, choose any of them. Similar choices below do not affect the estimates. For any \( 1 < i < n \), let \( p_i \in C \) be a point that has a maximum perpendicular distance to the linear subspace spanned by the vectors \( \vec{p}_1, \ldots, \vec{p}_{i-1} \). Let \( f \in O(\mathbb{R}^n) \) be an optimal map that gives \( \min_{f \in O(\mathbb{R}^n)} d_R(f(C), D) \) in Definition 2.1a, so the optimal distance is \( d_o = d_R(f(C), D) \). For simplicity, one can assume that \( f \) is the identity, then \( d_o = d_R(C, D) \), else any \( p \in C \) should be replaced by \( f(p) \) below. For each \( p_i \in C, i = 1, \ldots, n - 1 \), choose its closest neighbor \( q_i \in D \) with \( |p_i - q_i| \leq d_o \).

The key idea is to replace the above minimization over infinitely many \( f \in O(\mathbb{R}^n) \) by a finite minimization over compositions \( f_{n-1} \circ \cdots \circ f_1 \in O(\mathbb{R}^n) \) depending on finitely many unknown points \( q_1, \ldots, q_{n-1} \in D \), which can be exhaustively checked in time \( O(k^{n-1}) \). If the point \( p_1 \) belongs to the line \( L(q_1) \) through \( \vec{q}_1 \), set \( f_1[q_1] \) to be the identity map. Otherwise, let \( f_1[q_1] \in SO(\mathbb{R}^n) \) fix the linear subspace orthogonal to the plane spanned by \( \vec{p}_1, \vec{q}_1 \), and then rotate the point \( p_1 \) to \( L(q_1) \) through the smallest possible angle. Since \( p_1 \) is a furthest
point of $C$ from the origin 0 and $|p_1 - q_1| \leq d_o$, the rotation $f_1[q_1]$ moves $p_1$, hence any other point of $C$, by at most $d_o$. Then any point in $f_1[q_1](C)$ is at most $2d_o$ away from its closest neighbor in $D$, so $d_H(f_1[q_1](C), D) \leq 2d_o$.

For any $1 < i < n$, if $p_i$ belongs to the linear subspace $L(p_1, \ldots, p_{i-1}, q_i)$ spanned by $\vec{p}_1, \ldots, \vec{p}_{i-1}, \vec{q}_i$, set $f_1[q_i]$ to be the identity map. Otherwise, let the rotation $f_1[q_i] \in SO(\mathbb{R}^n)$ fix the linear subspace orthogonal to $\vec{p}_1, \ldots, \vec{p}_{i-1}, \vec{q}_i$, and rotate $p_i$ to $L(p_1, \ldots, p_{i-1}, q_i)$ through the smallest possible angle. Since $f_1[q_i](p_2)$ is at most $2d_o$ away from $q_2 \in D$, the map $f_2[q_2]$ moves $f_1[q_1](p_2)$, hence any other point of $f_1[q_1](C)$, by at most $2d_o$. Since $p_2$ had a maximum perpendicular distance from the line through $\vec{p}_1$, the composition $f_2[q_2] \circ f_1[q_1]$ moves any point of $C$ by at most $d_o + 2d_o = 3d_o$. For any $2 < i < n$, the composition $f_{n-1}[q_{n-1}] \circ \ldots \circ f_1[q_1]$ moves any point of $C$ by at most $d_o + 2d_o + \ldots + (n-1)d_o = \frac{1}{2}n(n-1)d_o$. Since $D$ was covered by the $d_o$-offset of $C$, we get the upper bound $d_H(C', D) \leq \frac{n^2 - n + 2}{2}d_o$ for $C' = f_{n-1}[q_{n-1}] \circ \ldots \circ f_1[q_1](C)$.

If we minimize the left hand side over all $q_1, \ldots, q_{n-1} \in D$, the upper bound remains the same: $\min_{q_1, \ldots, q_{n-1} \in D} d_H(C', D) \leq \frac{n^2 - n + 2}{2}d_o$. The points $p_1, \ldots, p_{n-1} \in C$ are found in time $O(kn)$. The algorithm from [52] preprocesses the set $D \subset \mathbb{R}^n$ of $k$ points in time $O(nk \log k)$ and for any point $p \in C'$ finds its $(1 + \delta)$-approximate nearest neighbor in $D$ in time $O(c_3 k \log k)$. Hence $d_H(C', D) = \max_{p \in C'} \min_{q \in D} |p - q|$ can be $(1 + \delta)$-approximated in time $O(c_3 k \log k)$. The minimization over $q_1, \ldots, q_{n-1} \in D$ gives the final time $O(c_3 k^n \log k)$.

The proof of Lemma 5.8 uses only orientation-preserving isometries from $SO(\mathbb{R}^n, 0)$. Hence the upper bounds from Lemma 5.8, Theorem 5.9 and Corollary 5.10 work for both cases of rigid motion and general isometry.

**Theorem 5.9** (approximating BT). Let periodic point sets $S, Q \subset \mathbb{R}^n$ have isometry classes $\sigma, \xi$ represented by clusters $C, D$, respectively, which have at most $k$ points. Then $BT(\sigma, \xi)$ from Definition 4.1 can be approximated with a factor $\eta = \frac{n^2 - n + 2}{2}(1 + \delta)$ for any $\delta > 0$ in time $O(c_3 k^{n+1} \log k)$.

**Proof.** $BT(\sigma, \xi) = \max\{d_{\bar{M}}(C, D), d_{\bar{M}}(D, C)\}$, where $d_{\bar{M}}$ is expressed via $k$ dis-
Corollary 5.10 (approximating EMD). Let $S, Q \subset \mathbb{R}^n$ be any periodic point sets with motifs of a maximum size $m$. The metric $\text{EMD}(I(S; \alpha), I(Q; \alpha))$ can be approximated with a factor $\eta = \frac{n^2 - n + 2}{2}(1 + \delta)$ for any $\alpha, \delta > 0$ in time $O(c_\delta m^{n+3}\nu^{n+1} \log(\nu m))$, where $\nu \leq \max\{\text{GC}(S), \text{GC}(Q)\}$. 

Proof. Since $S, Q$ have at most $m$ points in their motifs, their isosets at any radius $\alpha$ have at most $m$ isometry classes. By Theorem 5.9 the distance $\text{BT}(\sigma, \xi)$ between any classes $\sigma \in I(S; \alpha)$ and $\xi \in I(Q; \alpha)$ of $\alpha$-clusters up to $k$ points can be approximated with a factor $\eta$ in time $O(c_\delta k^{n+1} \log k)$. By Lemma 5.2 the maximum number of points is $k = \nu m$, where $\nu \leq \max\{\text{GC}(S), \text{GC}(Q)\}$. Since Definition 4.4 uses normalized distributions, $\eta$ emerges as a multiplicative upper bound in $\text{EMD}(I(S; \alpha), I(Q; \alpha))$. After computing $O(m^2)$ pairwise distances between $\alpha$-clusters, the exact EMD can be found in time $O(m^3 \log m)$ [53]. So the total time becomes $O(c_\delta m^{n+3}\nu^{n+1} \log(\nu m))$. The EMD can be approximated [54, section 3] with a constant factor in time $O(m)$.  

6. A lower bound for continuous metrics via simpler invariants

Theorem 6.5 gives a lower bound for EMD in terms of the simpler invariant

**Pointwise Distance Distribution** [10]: PDD$(S; k)$ of a periodic point set $S \subset \mathbb{R}^n$ is the matrix of $m$ lexicographically ordered rows of distances $d_{i1} \leq \ldots \leq d_{ik}$ from a motif point $p_i$, $i = 1, \ldots, m$, to its $k$ nearest neighbors in the full set $S$, see Definition 6.1 below. If $S$ is a lattice or a 1-regular set, then all points are isometrically equivalent, so they have the same distances to all their neighbors. In this case, PDD$(S; k)$ is a single row of $k$ distances, which is the vector AMD$(S; k)$ of Average Minimum Distances [9].

**Definition 6.1** (Pointwise Distance Distribution PDD). Let a periodic set $S = \Lambda + M$ have points $p_1, \ldots, p_m$ in a unit cell. For $k \geq 1$, consider the $m \times k$ matrix $D(S; k)$, whose $i$-th row consists of the ordered Euclidean distances $d_{i1} \leq \cdots \leq d_{ik}$ in Lemma 5.6. Because $d_R$ is approximated with a required factor in time $O(c_\delta k^{n} \log k)$ by Lemma 5.8, the total time is $O(c_\delta k^{n+1} \log k)$.  

$d_{ik}$ from $p_i$ to its first $k$ nearest neighbors in the full set $S$. The rows of $D(S; k)$ are lexicographically ordered as follows. A row $(d_{i1}, \ldots, d_{ik})$ is smaller than $(d_{j1}, \ldots, d_{jk})$ if the first (possibly none) distances coincide: $d_{i1} = d_{j1}, \ldots, d_{il} = d_{jl}$ for $l \in \{1, \ldots, k - 1\}$ and the next $(l + 1)$-st distances satisfy $d_{i,l+1} < d_{j,l+1}$.

If $w$ rows are identical to each other, these rows are collapsed to one row with the weight $w/m$. Put this weight in the extra first column. The final matrix of $k + 1$ columns is the Pointwise Distance Distribution $PDD(S; k)$. The Average Minimum Distance $AMD(S; k)$ is the vector $(AMD_1, \ldots, AMD_k)$, where $AMD_i$ is the weighted average of the $(i + 1)$-st column of $PDD(S; k)$.

**Theorem 6.2** (isometry invariance of PDD). For any finite or periodic set $S \subset \mathbb{R}^n$, $PDD(S; k)$ in Definition 6.1 is an isometry invariant of $S$ for $k \geq 1$.

Theorem 6.2 and continuity of PDD in the metric from Definition 6.3 follows from more general results in [10]. The distance $|R_i(S) - R_j(Q)|$ between rows of PDD matrices below is measured in the $L_\infty$ metric.

**Definition 6.3** (Earth Mover’s Distance on Pointwise Distance Distributions). Let finite or periodic sets $S, Q \subset \mathbb{R}^n$ have $PDD(S; k)$ and $PDD(Q; k)$ with weighted rows $R_i(S)$, $i = 1, \ldots, m(S)$ and $R_j(Q)$, $j = 1, \ldots, m(Q)$, respectively. A full flow from $PDD(S; k)$ to $PDD(Q; k)$ is an $m(S) \times m(Q)$ matrix whose element $f_{ij} \in [0, 1]$ is called a partial flow from $R_i(S)$ to $R_j(Q)$. The Earth Mover’s Distance is the minimum value of the cost $EMD(I(S), I(Q)) = \sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} |R_i(S) - R_j(Q)|$ over variable ‘flows’ $f_{ij} \in [0, 1]$ subject to $\sum_{j=1}^{m(Q)} f_{ij} \leq w_i$ for $i = 1, \ldots, m(S)$, $\sum_{i=1}^{m(S)} f_{ij} \leq u_j$ for $j = 1, \ldots, m(Q)$, and $\sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} = 1$.

Lemma 6.4 is a partial case of Theorem 6.5 for 1-regular point sets $S, Q$.

**Lemma 6.4** (lower bound for the tolerant distance $BT$). Let $S, Q \subset \mathbb{R}^n$ be periodic point sets with a common stable radius $\alpha$. Choose any points $p \in S$ and $q \in Q$. Let the distance between isometry classes of $\alpha$-clusters $\varepsilon = BT([C(S, p; \alpha)], [C(Q, q; \alpha)])$ be smaller than a minimum half-distance between any points within $S$ and within $Q$. Let $k$ be a minimum number of points of
S, Q in the clusters C(S, p; α − ε) and C(Q, q; α − ε). Then the L∞ distance between the rows of the points p, q in PDD(S; k), PDD(Q; k) is at most ε. ■

**Theorem 6.5** (lower bound for EMD). Let S, Q ⊂ R^n be periodic sets with a common stable radius α. Let ε = EMD(I(S; α), I(Q; α)) and k be a maximum number of points of S, Q in their (α − ε)-clusters. If ε is less than a half-distance between any points of S, Q, then EMD(PDD(S; k), PDD(Q; k)) ≤ ε. ■

**Proof.** To prove that EMD(PDD(S; k), PDD(Q; k)) ≤ ε = EMD(I(S; α), I(Q; α)), we choose optimal ‘flows’ f_{ij} ∈ [0, 1], i = 1, . . . , m(S) and j = 1, . . . , m(Q), that minimise the right hand side in Definition 4.4. For any motif points p_i ∈ S and q_j ∈ Q, let R_i(S) and R_j(Q) be their rows in PDD(S; k), PDD(Q; k), respectively. Lemma 6.4 gives |R_i(S) − R_j(Q)| ≤ BT([C(S, p_i; α)], [C(Q, q_j; α)]). These inequalities for all i, j and the same f_{ij} give \( \sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} |R_i(S) − R_j(Q)| \leq m(S) m(Q) \sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} BT(\sigma_i, \xi_j) = \varepsilon \) by the choice of f_{ij} for EMD(I(S; α), I(Q; α)). The left hand side of the last inequality can become only smaller when minimizing over f_{ij}. Then EMD(PDD(S; k), PDD(Q; k)) ≤ ε. ■

7. **Significance of complete continuous invariants for data integrity**

Sections 3 and 4 prepared the main complexity results in section 5: algorithms for computing and comparing isosets (Theorems 5.3, Corollary 5.4), and approximating the new boundary tolerant metric BT (Theorem 5.9) and EMD on isosets (Corollary 5.10). The proofs focused on polynomial bounds in terms of the motif size m = |S| of a periodic point set S because the input size of a Crystallographic Information File is linear in m, e.g. any lattice has m = 1.

The factors depending on a dimension and geometric complexity GC(S) are inevitable due to the curse of dimensionality and the infinite nature of crystals. In practice, crystal symmetries reduce a motif to a smaller asymmetric part, which usually has less than 20 atoms even for large molecules in the CSD. The lower bound via faster PDD invariants in Theorem 6.5 justifies applying the algorithm of Corollary 5.10 only for a final confirmation of near-duplicates.
The main novelty is the boundary tolerant metric in Definition 4.1 that has made the complete invariant isoset Lipschitz continuous (Theorem 4.9) without extra parameters that are needed to smooth past descriptors such as powder diffraction patterns and atomic environments with fixed cut-off radii. Because the isoset is the only Lipschitz continuous invariant whose completeness under isometry was proved for all periodic point sets in $\mathbb{R}^n$, the isoset was used to confirm the duplicates in the CSD [9, section 7] and GNoME [13, Tables 1-2].

The resulting Crystal Isometry Principle (CRISP) says that all non-isometric periodic crystals should have non-isometric sets of atomic centers) and implies that all known and not yet discovered periodic crystals live in a common Crystal Isometry Space (CRIS) whose first continuous maps appeared in [22][55].

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A. Appendix A: detailed proofs of all auxiliary results

This appendix includes more detailed and updated proofs of [23, Lemmas 7 and 11-13]. Fig. 8 visualizes the logical connections between main results. Fig. 9 additionally illustrates the isosets for the periodic sets $S_1, S_2$ in Fig. 4.

**Figure 8:** Key definitions and main Theorems 4.9, 6.5 about the continuous metrics on complete invariant isosets with time complexities of algorithms in Corollaries 5.4, 5.10.

**Figure 9:** Left: The isotree IT($S_1$) from Definition 3.4 of the 1-regular set $S_1$ in Fig. 4 for any $\alpha \geq 0$ has one isometry class of $\alpha$-clusters up to rotation. Right: the isotree IT($S_2$) of the 2-regular set $S_2$ in Fig. 4 stabilizes with two non-isometric classes of $\alpha$-clusters for $\alpha \geq 4$.

**Lemma A.1** (isotree properties). The isotree IT($S$) has the properties below:

(A.1a) for $\alpha = 0$, the $\alpha$-partition $P(S; 0)$ consists of one class;

(A.1b) if $\alpha < \alpha'$, then $\text{Sym}(S, p; \alpha') \subseteq \text{Sym}(S, p; \alpha)$ for any point $p \in S$;

(A.1c) if $\alpha < \alpha'$, the $\alpha'$-partition $P(S; \alpha')$ refines $P(S; \alpha)$, i.e. any $\alpha'$-equivalence class from $P(S; \alpha')$ is included into an $\alpha$-equivalence class from the partition $P(S; \alpha)$. So the cluster count $|P(S; \alpha)|$ is non-strictly increasing in $\alpha$. ■
Figure 10: Logical steps towards main Theorems 4.9, 6.5 and Corollaries 5.4 and 5.10.

Proof. (A.1a) Let $\alpha \geq 0$ be smaller than the minimum distance $2r(S)$ between any points of $S$. Then any cluster $C(S, p; \alpha)$ is the single-point set $\{p\}$. All these 1-point clusters are isometric to each other. So $|P(S; \alpha)| = 1$ for $\alpha < 2r(S)$.

(A.1b) For any $p \in S$, the inclusion of clusters $C(S, p; \alpha) \subseteq C(S, p; \alpha')$ implies that any isometry $f \in O(\mathbb{R}^n; p)$ that isometrically maps the larger cluster $C(S, p; \alpha')$ to itself also maps the smaller cluster $C(S, p; \alpha)$ to itself. Hence any element of $\text{Sym}(S, p; \alpha') \subseteq O(\mathbb{R}^n; p)$ belongs to $\text{Sym}(S, p; \alpha)$.

(A.1c) If points $p, q \in S$ are $\alpha'$-equivalent at the larger radius $\alpha'$, i.e. the clusters $C(S, p; \alpha')$ and $C(S, q; \alpha')$ are related by an isometry from $O(\mathbb{R}^n; p, q)$, then $p, q$ are $\alpha$-equivalent at the smaller radius $\alpha$. Hence any $\alpha'$-equivalence class of points in $S$ is a subset of an $\alpha$-equivalence class in $S$.

The proofs of Lemmas A.2, A.3, and Theorem 3.10 follow [45], [46, section 4], and extend to the oriented case by taking orientation-preserving isometries.

Lemma A.2 (local extension). Let $S, Q \subset \mathbb{R}^n$ be periodic point sets and $\text{Sym}(S, p; \alpha - \beta) = \text{Sym}(S, p; \alpha)$ for some $p \in S$ and $\alpha > \beta$. Assume that there is an isometry $g \in O(\mathbb{R}^n; p, q)$ such that $g(p) = q$ and $g(C(S, p; \alpha)) = C(Q, q; \alpha)$. Let $f \in O(\mathbb{R}^n; p, q)$ be any isometry such that $f(C(S, p; \alpha - \beta)) = C(Q, q; \alpha - \beta)$. Then $f$ isometrically maps the larger clusters: $f(C(S, p; \alpha)) = C(Q, q; \alpha)$. ■
Proof. The isometries $f, g$ may not coincide on the subcluster $C(S, p; \alpha - \beta)$. The composition $h = f^{-1} \circ g$ fixes $p$ and isometrically maps $C(S, p; \alpha - \beta)$ to itself, so $h \in \text{Sym}(S, p; \alpha - \beta)$. The condition $\text{Sym}(S, p; \alpha - \beta) = \text{Sym}(S, p; \alpha)$ implies that $h \in \text{Sym}(S, p; \alpha)$, so the isometry $h \in O(\mathbb{R}^n; p)$ isometrically maps the larger cluster $C(S, p; \alpha)$ to itself. Then the given isometry $f = g \circ h^{-1}$ isometrically maps $C(S, p; \alpha)$ to $f(C(S, p; \alpha)) = g(C(S, p; \alpha)) = C(Q, q; \alpha)$. □

Lemma A.3 (global extension). Let periodic point sets $S, Q \subset \mathbb{R}^n$ have a common stable radius $\alpha$ satisfying Definition 3.5 for an upper bound $\beta$ of the bridge lengths $\beta(S), \beta(Q)$. Let $I(S; \alpha) = I(Q; \alpha)$ and $f \in O(\mathbb{R}^n; p, q)$ be any isometry such that $f(p) = q$ and $f(C(S, p; \alpha)) = C(Q, q; \alpha)$. Then $f(S) = Q$. □

Proof. To show that $f(S) \subset Q$, it suffices to check that the image $f(a)$ of any point $a \in S$ belongs to $Q$. By Definition 3.3 the points $p, a \in S$ are connected by a sequence of points $p = a_0, a_1, \ldots, a_k = a \in S$ such that the distances $|a_{i-1} - a_i|$ between any successive points have the upper bound $\beta$ for $i = 1, \ldots, k$.

We will prove that $f(C(S, a_k; \alpha)) = C(Q, f(a_k); \alpha)$ by induction on $k$, where the base $k = 0$ is given. The induction step below goes from $i$ to $i + 1$.

The ball $\bar{B}(a_i; \alpha)$ contains the smaller ball $\hat{B}(a_{i+1}; \alpha - \beta)$ around the closely located center $a_{i+1}$. Indeed, since $|a_{i+1} - a_i| \leq \beta$, the triangle inequality for the Euclidean distance implies that any point $a'_{i+1} \in \hat{B}(a_{i+1}; \alpha - \beta)$ with $|a'_{i+1} - a_i| \leq \alpha - \beta$ satisfies $|a'_{i+1} - a_i| \leq |a'_{i+1} - a_{i+1}| + |a_{i+1} - a_i| \leq (\alpha - \beta) + \beta = \alpha$, so $\hat{B}(a_{i+1}; \alpha - \beta) \subset \bar{B}(a_i; \alpha)$. Then the inductive assumption $f(C(S, a_i; \alpha)) = C(Q, f(a_i); \alpha)$ gives $f(C(S, a_{i+1}; \alpha - \beta)) = f(C(S, a_i; \alpha)) \cap f(\hat{B}(a_{i+1}; \alpha - \beta)) = C(Q, f(a_i); \alpha) \cap \hat{B}(f(a_{i+1}); \alpha - \beta) = C(Q, f(a_{i+1}); \alpha - \beta)$.

Due to $I(S; \alpha) = I(Q; \alpha)$, the isometry class of $C(S, a_{i+1}; \alpha)$ equals an isometry class of $C(Q, b_{i+1}; \alpha)$ for some point $b_{i+1} \in Q$, i.e. there is an isometry $g \in O(\mathbb{R}^n; a_{i+1}, b_{i+1})$ such that $g(C(S, a_{i+1}; \alpha)) = C(Q, b_{i+1}; \alpha)$. Since $f \circ g^{-1} \in O(\mathbb{R}^n; b_{i+1})$ isometrically maps $C(Q, b_{i+1}; \alpha - \beta)$ to $C(Q, f(a_{i+1}); \alpha - \beta)$, the points $b_{i+1}, f(a_{i+1}) \in Q$ are in the same $(\alpha - \beta)$-equivalence class of $Q$. 

38
By condition (3.5b), the splitting of the periodic point set \( Q \subset \mathbb{R}^n \) into \( \alpha \)-equivalence classes coincides with its splitting into \((\alpha - \beta)\)-equivalence classes. Hence the points \( b_{i+1}, f(a_{i+1}) \in Q \) are in the same \( \alpha \)-equivalence class of \( Q \). Then \( C(Q, f(a_{i+1}); \alpha) \) is isometric to \( C(Q, b_{i+1}; \alpha) = g(C(S, a_{i+1}; \alpha)) \).

Now we can apply Lemma \( \text{A.2} \) for \( p = a_{i+1}, q = f(a_{i+1}) \) and conclude that the given isometry \( f \), which satisfies \( f(C(S, a_{i+1}; \alpha - \beta)) = C(Q, f(a_{i+1}); \alpha - \beta) \), isometrically maps the larger clusters: \( f(C(S, a_{i+1}; \alpha)) = C(Q, f(a_{i+1}); \alpha) \). The induction step is finished. The inclusion \( f^{-1}(Q) \subset S \) is proved similarly. \( \square \)

**Lemma A.4** (all stable radii \( \alpha \geq \alpha(S) \)). If \( \alpha \) is a stable radius of a periodic point set \( S \subset \mathbb{R}^n \), then so is any larger radius \( \alpha' > \alpha \). Then all stable radii form the interval \([\alpha(S), +\infty) \), where \( \alpha(S) \) is the minimum stable radius of \( S \). \( \blacksquare \)

**Proof.** Due to Lemma (A.1bc), conditions (3.5b) imply that the \( \alpha' \)-partition \( P(S; \alpha') \) and the symmetry groups \( \text{Sym}(S, p; \alpha') \) remain the same for all \( \alpha' \in [\alpha - \beta(S), \alpha] \), where \( \beta(S) \) is the bridle length. We need to show that they remain the same for any \( \alpha' > \alpha \) and will apply Lemma \( \text{A.3} \) for \( S = Q \) and \( \beta = \beta(S) \). Let points \( p, q \in S \) be \( \alpha \)-equivalent, i.e. there is an isometry \( f \in O(\mathbb{R}^n; p, q) \) such that \( f(C(S, p; \alpha)) = C(S, q; \alpha) \). By Lemma \( \text{A.3} \) \( f \) isometrically maps the full set \( S \) to itself. Then all larger \( \alpha' \)-clusters of \( p, q \) are matched by \( f \), so \( p, q \) are \( \alpha' \)-equivalent and \( P(S; \alpha) = P(S, \alpha') \). Similarly, any isometry \( f \in \text{Sym}(S, p; \alpha) \) by Lemma \( \text{A.3} \) for \( S = Q \) and \( p = q \), isometrically maps the full set \( S \) to itself. Then \( \text{Sym}(S, p; \alpha') \) coincides with \( \text{Sym}(S, p; \alpha) \) for any \( \alpha' > \alpha \). \( \square \)

**Proof of Theorem 3.10.** The part only if \( \Rightarrow \). Let \( f \) be an isometry of \( \mathbb{R}^n \), which isometrically maps one periodic point set \( S \) to another \( Q \). For any point \( p \) in a motif \( M(S) \) of \( S \), the image \( f(p) \in Q \) is equivalent to a unique point \( g(p) \) in a motif \( M(Q) \) of \( Q \) modulo a translation along a vector from the lattice of \( Q \).

Then, for any \( p \in M(S) \) and \( \alpha \geq 0 \), the clusters \( C(S, p; \alpha) \) and \( C(Q, g(p); \alpha) \) are related by an isometry of \( \mathbb{R}^n \). Hence the bijection \( g : M(S) \to M(Q) \) induces a bijection \( I(S; \alpha) \to I(Q; \alpha) \) between all isometry classes with weights.

39
The part if $\iff$. Fix a point $p \in S$. The cluster $C(S, p; \alpha)$ represents a class $\sigma \in I(S; \alpha)$. Due to $I(S; \alpha) = I(Q; \alpha)$, the class $\sigma$ equals some $\xi \in I(Q; \alpha)$. Hence there is an isometry $f$ of $\mathbb{R}^n$ such that the cluster $f(C(S, p; \alpha)) = C(Q, f(p); \alpha)$ represents $\xi$. By Lemma A.3, $f$ isometrically maps $S$ to $Q$. \hfill \Box

**Proof of Lemma 4.2.** Since the group $O(\mathbb{R}^n; p, q)$ is compact, the minimum $\varepsilon \geq 0$ is achieved in the inclusions from (4.1b) for some isometries $f \in O(\mathbb{R}^n; p, q)$ and $g \in O(\mathbb{R}^n; q, p)$. Then, for any clusters $C(S, \tilde{p}; \alpha)$ and $C(Q, \tilde{q}; \alpha)$ isometric to $C(S, p; \alpha)$ and $C(Q, q; \alpha)$ via $f_S \in O(\mathbb{R}^n; \tilde{p}, p)$ and $g_Q \in O(\mathbb{R}^n; \tilde{q}, q)$, respectively, the same minimum $\varepsilon \geq 0$ is achieved in the following inclusions (and vice versa), which proves the independence of $\text{BT}(\sigma, \xi)$ under a choice of clusters.

$$C(Q, \tilde{q}; \alpha - \varepsilon) \subseteq \tilde{f}(C(S, \tilde{p}; \alpha)) + \tilde{B}(0; \varepsilon)$$

$$C(S, \tilde{p}; \alpha - \varepsilon) \subseteq \tilde{g}(C(Q, \tilde{q}; \alpha)) + \tilde{B}(0; \varepsilon)$$

$$\text{where } \tilde{f} = g_Q^{-1} \circ f \circ f_S \in O(\mathbb{R}^n; \tilde{p}, \tilde{q}),$$

$$\text{and } \tilde{g} = f_S^{-1} \circ g \circ g_Q \in O(\mathbb{R}^n; \tilde{p}, \tilde{q}).$$

Now we prove the coincidence axiom. By Definition 4.1, $\text{BT}(\sigma, \xi) = 0$ means that some representatives of given classes $\sigma, \xi$ satisfy $C(Q, q; \alpha) \subseteq f(C(S, p; \alpha))$ for some $f \in O(\mathbb{R}^n; p, q)$ and $C(S, p; \alpha) \subseteq g(C(Q, q; \alpha))$ for some $g \in O(\mathbb{R}^n; q, p)$. Combining these inclusions, we get $C(Q, q; \alpha) \subseteq f \circ g(C(Q, q; \alpha))$. Since $f \circ g \in O(\mathbb{R}^n; q)$ is an isometry fixing $q$ and both clusters in the inclusion above consist of the same number of points the surjection $a \mapsto f \circ g(a)$ for $a \in C(Q, q; \alpha)$ should bijective, so $C(Q, q; \alpha) = f \circ g(C(Q, q; \alpha))$. Then the initial inclusions are equalities. Hence $C(S, p; \alpha), C(Q, a; \alpha)$ are related by the isometry $f \in O(\mathbb{R}^n; p, q)$, so $\sigma = \xi$. The symmetry axiom holds because the inclusions in condition (4.1b) are symmetric to each other under swapping the arguments.

To prove the triangle inequality, let clusters $C(S, p; \alpha), C(Q, f(p); \alpha), C(T, g \circ f(p); \alpha)$ represent $\sigma, \xi, \zeta$, respectively, so that $\varepsilon_1 = \text{BT}(\sigma, \xi)$ and $\varepsilon_2 = \text{BT}(\xi, \zeta)$ are achieved for inclusions $C(Q, f(p); \alpha - \varepsilon_1) \subseteq f(C(S, p; \alpha)) + \tilde{B}(0; \varepsilon_1)$ and $C(T, g \circ f(p); \alpha - \varepsilon_2) \subseteq g(C(Q, f(p); \alpha)) + \tilde{B}(0; \varepsilon_2)$ for isometries $f, g$ of $\mathbb{R}^n$.

The last inclusion gives $C(T, g \circ f(p); \alpha - \varepsilon_1 - \varepsilon_2) \subseteq g(C(Q, f(p); \alpha - \varepsilon_1)) + \tilde{B}(0; \varepsilon_2)$ because we can reduce the radius $\alpha$ in the cluster $g(C(Q, f(p); \alpha))$ to $\alpha - \varepsilon_1$. Indeed, if a point $t \in C(T, g \circ f(p); \alpha - \varepsilon_1 - \varepsilon_2)$ is covered by a closed
ball \( B(q; \varepsilon_2) \) for some \( q \in g(C(Q, f(p); \alpha)) \), then \( |q - t| \leq \varepsilon_2 \) and

\[
|q - g \circ f(p)| \leq |q - t| + |t - g \circ f(p)| \leq \varepsilon_2 + (\alpha - \varepsilon_1 - \varepsilon_2) = \alpha - \varepsilon_1.
\]

Hence \( q \) belongs to the smaller cluster \( g(C(Q, f(p); \alpha - \varepsilon_1)) \) as required. Now we apply the isometry \( g \) to the inclusion \( C(Q, f(p); \alpha - \varepsilon_1) \subseteq f(C(S, p; \alpha)) + \overline{B}(0; \varepsilon_1) \) to get \( C(T, g \circ f(p); \alpha - \varepsilon_1 - \varepsilon_2) \subseteq g(C(Q, f(p); \alpha - \varepsilon_1)) + \overline{B}(0; \varepsilon_2) \subseteq g \circ f(C(S, p; \alpha)) + \overline{B}(0; \varepsilon_1 + \varepsilon_2) \) as \((q + \overline{B}(0; \varepsilon_1)) + \overline{B}(0; \varepsilon_2) = q + \overline{B}(0; \varepsilon_1 + \varepsilon_2)\).

Swapping the roles of \( S, T \) in the arguments above, we similarly prove that if \( C(S, p; \alpha - \varepsilon_1) \subseteq f(C(Q, f^{-1}(p); \alpha)) + \overline{B}(0; \varepsilon_1) \) and \( C(Q, f^{-1}(p); \alpha - \varepsilon_2) \subseteq g(C(T, g^{-1} \circ f^{-1}(p); \alpha)) + \overline{B}(0; \varepsilon_2) \) for some isometries \( f, g \) of \( \mathbb{R}^n \), then

\[
C(S, p; \alpha - \varepsilon_1 - \varepsilon_2) \subseteq f \circ g(C(T, g^{-1} \circ f^{-1}(p); \alpha)) + \overline{B}(0; \varepsilon_1 + \varepsilon_2).
\]

Definition \ref{def:BT} implies that \( BT(\sigma, \zeta) \leq \varepsilon_1 + \varepsilon_2 = BT(\sigma, \xi) + BT(\xi, \zeta) \).

**Proof of Lemma \ref{lem:triangle}**. The symmetry axiom holds because Definition \ref{def:isometry} is symmetric under swapping \( S, Q \). The triangle axiom was proved for any weighted distributions in \cite[Appendix A]{24}. It remains to prove that if \( EMD(I(S; \alpha), I(Q; \alpha)) = 0 \) then \( I(S; \alpha) = I(Q; \alpha) \) as isosets. Indeed, \( \sum_{i=1}^{m(S)} \sum_{j=1}^{m(Q)} f_{ij} BT(\sigma_i, \xi_j) = 0 \) means that if any \( f_{ij} > 0 \) then \( BT(\sigma_i, \xi_j) = 0 \), so \( \sigma_i = \xi_j \) by the coincidence axiom of \( BT \) from Lemma \ref{lem:coincidence}. Hence any flow \( f_{ij} > 0 \) is always between equal isometry classes. The conditions on weights of \( \sigma_i, \xi_j \) in Definition \ref{def:isometry} imply that every class \( \sigma_i \) should ‘flow’ to its equal class \( \xi_j \) of the same weight. These flows define a bijection \( I(S; \alpha) \rightarrow I(Q; \alpha) \) of isometry classes respecting all weights.

**Proof of Lemma \ref{lem:Bottleneck}**. Choose the origin \( 0 \in \mathbb{R}^n \) at a point of \( S \). Applying translations, we can assume that primitive unit cells \( U(S), U(Q) \) of the given periodic sets \( S, Q \) have a vertex at the origin \( 0 \). Then \( S = \Lambda(S) + (U(S) \cap S) \) and \( Q = \Lambda(Q) + (U(Q) \cap Q) \), where \( \Lambda(S), \Lambda(Q) \) are lattices of \( S, Q \), respectively.

We are given that every point of \( Q \) is \( d_B(S, Q) \)-close to a point of \( S \), where the bottleneck distance \( d_B(S, Q) \) is strictly less than the packing radius \( r(Q) \).
Assume by contradiction that $S,Q$ have no common lattice. Then there is a point $p \in \Lambda(S)$ whose all integer multiples $kp \in \Lambda(S)$ do not belong to $\Lambda(Q)$ for $k \in \mathbb{Z} - \{0\}$. Any such multiple $kp$ can be translated by a vector of $\Lambda(Q)$ to a point $q(k)$ in the unit cell $U(Q)$ so that $kp \equiv q(k) \pmod{\Lambda(Q)}$. Since the cell $U(Q)$ contains infinitely many points $q(k)$, one can find a pair $q(i) \neq q(j)$ at a distance less than $\delta = r(Q) - d_B(S,Q) > 0$. For any $m \in \mathbb{Z}$, the following points are equivalent modulo (translations along the vectors of) the lattice $\Lambda(Q)$.

$$q(i + m(j - i)) \equiv (i + m(j - i))p = ip + m(jp - ip) \equiv q(i) + m(q(j) - q(i)).$$

These points for $m \in \mathbb{Z}$ lie in a straight line with gaps $|q(j) - q(i)| < \delta$. The open balls with the packing radius $r(Q)$ and centers at all points of $Q$ do not overlap. Hence all closed balls with the radius $d_B(S,Q) < r(Q)$ and the same centers are at least $2\delta$ away from each other. Due to $|q(j) - q(i)| < \delta = r(Q) - d_B(S,Q)$, there is $m \in \mathbb{Z}$ such that $q(i) + m(q(j) - q(i))$ is outside the union $Q + B(0;d_B(S,Q))$ of all these smaller balls. Then $q(i) + m(q(j) - q(i))$ has a distance more than $d_B(S,Q)$ from any point of $Q$. The translations along all vectors of the lattice $\Lambda(Q)$ preserve the union of balls $Q + B(0;d_B(S,Q))$. Then the point $(i + m(j - i))p \in S$, which is equivalent to $q(i) + m(q(j) - q(i))$ modulo $\Lambda(Q)$, has a distance more than $d_B(S,Q)$ from any point of $Q$. This conclusion contradicts Definition 2.1(b) of the bottleneck distance $d_B(S,Q)$.

**Example A.5** (detailed computations for Example 4.3). Fig. 7 shows the stable 2-clusters $C(\Lambda_4,0;2)$ and $C(\Lambda_6,0;2)$ of the square ($\Lambda_4$) and hexagonal ($\Lambda_6$) lattices. Without rotations, the 1st picture of Fig. 7 shows the directed Hausdorff distance $d_R = \sqrt{(1 - \frac{\sqrt{3}}{2})^2 + (\frac{1}{2})^2} = \sqrt{2 - \sqrt{3}} \approx 0.52$ between clusters with the added boundary circle $\partial B(0;2)$. Due to high symmetry, it suffices to consider rotations of the square vertex $(1,1)$ for angles $\gamma \in [45^\circ,60^\circ]$ because all other ranges can be isometrically mapped to this range for another vertex of the square. We find the squared distances $s_1(\gamma)$ and $s_2(\gamma)$ from the vertex $(\sqrt{2} \cos \gamma, \sqrt{2} \sin \gamma)$ rotated from $(1,1)$ at $\gamma = 45^\circ$ through the angle $\gamma - 45^\circ$ to its closest neighbors $(\frac{1}{2}, \frac{\sqrt{3}}{2})$ and $(\frac{3}{2}, \frac{\sqrt{3}}{2})$ in $C(\Lambda_6,0;2).$
We prove by induction on $k$.

Proof. C points of the hexagonal cluster numbers with the same indices are $c$ $C$ of the square cluster $q$ $q$ in the original unordered lists so that $|c_i - d_j| \leq \varepsilon$, $i = 1, \ldots, k$. The numbers with the same indices are $\varepsilon$-close, so $|c_i - d_i| \leq \varepsilon$ for all $i = 1, \ldots, k$.

Proof. We prove by induction on $k$, where the base $k = 1$ is trivial. The inductive step will reduce $k$ to $k - 1$. Without loss of generality assume that $c_1 \leq d_1$. Let these numbers have $\varepsilon$-neighbors $d_i = d_i$ and $c_i = c_j$, respectively in the original unordered lists so that $|c_i - d_i| \leq \varepsilon$ and $|d_i - c_j| \leq \varepsilon$. Due to $c_1 \leq d_1$, the former inequality above implies that $\varepsilon \geq |c_1 - d_1| = d_i - c_i \geq d_1 - c_1 \geq 0$, so the minimum numbers are $\varepsilon$-close: $|c_1 - d_i| \leq \varepsilon$. The same inequality similarly implies that $\varepsilon \geq d_i - c_i \geq d_i - c_j$. If $d_i - c_j \geq 0$, the last inequality means that $d_i, c_j$ are $\varepsilon$-close, so $|d_i - c_j| \leq \varepsilon$. If $d_i < c_j$, the latter

$$s_1(\gamma) = \left| (\sqrt{2} \cos \gamma, \sqrt{2} \sin \gamma) - \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \right|^2 = \left( \sqrt{2} \cos \gamma - \frac{1}{2} \right)^2 + \left( \sqrt{2} \sin \gamma - \frac{\sqrt{3}}{2} \right)^2 = 3 - \sqrt{2} \cos \gamma - \sqrt{6} \sin \gamma, \quad \frac{ds_1}{d\gamma} = \sqrt{2} \sin \gamma - \sqrt{6} \cos \gamma = 0, \tan \gamma = \sqrt{3}, \gamma = 60^\circ \text{, } s_1 = (\sqrt{2} - 1)^2 \text{ is minimal for the points in } y = \sqrt{3}x \text{ at distances } 1, \sqrt{2} \text{ from } 0.$$

$$s_2(\gamma) = \left| (\sqrt{2} \cos \gamma, \sqrt{2} \sin \gamma) - \left( \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2} \right) \right|^2 = \left( \sqrt{2} \cos \gamma - \frac{\sqrt{3}}{2} \right)^2 + \left( \sqrt{2} \sin \gamma - \frac{\sqrt{3}}{2} \right)^2 = 5 - 3\sqrt{2} \cos \gamma - \sqrt{6} \sin \gamma, \quad \frac{ds_2}{d\gamma} = 3\sqrt{2} \sin \gamma - \sqrt{6} \cos \gamma = 0, \gamma = 30^\circ, \quad s_2 = (\sqrt{3} - \sqrt{2})^2 \text{ is minimal for the points in } y = \frac{\sqrt{3}}{\sqrt{2}} \text{ at distances } \sqrt{2}, \sqrt{3} \text{ from } 0.$$

It might look that the second minimum is smaller. However, for the angle $\gamma = 30^\circ$, another vertex $(-1,1)$ rotated through $\gamma - 45^\circ = -15^\circ$ has distance $\sqrt{2} - 1$ to its closest neighbor $(-\frac{1}{2}, \frac{\sqrt{3}}{2}) \in C(\Lambda_6, 0; 2)$. For any angle $\gamma \in [45^\circ, 60^\circ]$, the second function has the minimum $s_2(45^\circ) = 2 - \sqrt{3} = d^2_H$, in the 1st picture of Fig. 7. Hence the vertex $(1,1)$ has the minimum distance $\sqrt{2} - 1 \approx 0.41 < \sqrt{2} - \sqrt{3} \approx 0.52$ in the 3rd picture of Fig. 7. All other points of the square cluster $C(\Lambda_4, 0; 2)$ are even closer to their neighbors in $C(\Lambda_6, 0; 2)$. For example, the point $(1,0)$ rotated by $15^\circ$ has the distance to $(1,0)$ equal to $\sqrt{(\cos 15^\circ - 1)^2 + \sin^2 15^\circ} \approx 0.26$. The final picture in Fig. 7 confirms that all points of the hexagonal cluster $C(\Lambda_6, 0; 2)$ are covered by the $(\sqrt{2} - 1)$-offset of $C(\Lambda_4, 0; 2)$ and the boundary circle. So $BT = \sqrt{2} - 1 \approx 0.41$. ■

Lemma A.6 (re-ordering $\varepsilon$-close numbers). For any $\varepsilon \geq 0$, let $\{c_{(1)}, \ldots, c_{(k)}\}$ and $\{d_{(1)}, \ldots, d_{(k)}\}$ be unordered numbers so that $|c_{(i)} - d_{(i)}| \leq \varepsilon$, $i = 1, \ldots, k$. Write both lists in increasing order: $c_1 \leq \ldots \leq c_k$ and $d_1 \leq \ldots \leq d_k$. The numbers with the same indices are $\varepsilon$-close, so $|c_i - d_i| \leq \varepsilon$ for all $i = 1, \ldots, k$. ■

Proof. We prove by induction on $k$, where the base $k = 1$ is trivial. The inductive step will reduce $k$ to $k - 1$. Without loss of generality assume that $c_1 \leq d_1$. Let these numbers have $\varepsilon$-neighbors $d_{(1)} = d_i$ and $c_{(1)} = c_j$, respectively in the original unordered lists so that $|c_{(i)} - d_{(i)}| \leq \varepsilon$ and $|d_{(i)} - c_{(j)}| \leq \varepsilon$. Due to $c_1 \leq d_1$, the former inequality above implies that $\varepsilon \geq |c_1 - d_1| = d_i - c_i \geq d_1 - c_1 \geq 0$, so the minimum numbers are $\varepsilon$-close: $|c_1 - d_i| \leq \varepsilon$. The same inequality similarly implies that $\varepsilon \geq d_i - c_i \geq d_i - c_j$. If $d_i - c_j \geq 0$, the last inequality means that $d_i, c_j$ are $\varepsilon$-close, so $|d_i - c_j| \leq \varepsilon$. If $d_i < c_j$, the latter
inequality above implies that \( \varepsilon \geq |d_1 - c_j| = c_j - d_1 \geq c_j - d_i > 0 \), so \( |d_i - c_j| \leq \varepsilon \) also in this case. Hence by changing the pairs of \( \varepsilon \)-close numbers \( (c_1, d_i) \) and \( (d_1, c_j) \) to the new pairs of \( \varepsilon \)-close numbers \( (c_1, d_1) \) and \( (c_j, d_i) \), we can apply the inductive assumption to the \( k - 1 \) pairs excluding the first pair \( (c_1, d_1) \) of minimum numbers. The induction is complete. \( \square \)

**Proof of Lemma 5.3.** To find all points in \( C(S, p; \alpha) \), we will extend \( U \) by adding adjacent cells in ‘spherical’ shells around \( U \). After considering the initial cell \( U \) with a basis \( v_1, \ldots, v_n \), we take \( 3^n - 1 \) cells \( U + v \) for vectors \( v = \sum_{i=1}^{n} c_i v_i \in \Lambda - \{0\} \) with integer coordinates \( c_i \in \{-1, 0, 1\} \). The next ‘spherical’ shell consists of \( 5^n - 3^n \) cells \( U + v \) and so on. For any shifted cell \( U + v \) with \( v \in \Lambda \), if all vertices have distances more than \( \alpha \) to \( p \), this cell is discarded. Otherwise, we check if any translated points \( M + v \) are within the closed ball \( B(p; \alpha) \) of radius \( \alpha \). The upper union \( \bar{U} = \bigcup \{ \{ U + v \} : v \in \Lambda, (U + v) \cap B(p; \alpha) \neq \emptyset \} \) consists of \( \frac{\text{vol}[U]}{\text{vol}[U]} \) cells and is contained in the larger ball \( B(p; \alpha + d) \), because any shifted cell \( U + v \) within \( \bar{U} \) has the longest diagonal \( d \) and intersects \( B(p; \alpha) \). Since each \( U + v \) contains \( m \) points of \( S \), we check at most \( m \frac{\text{vol}[U]}{\text{vol}[U]} \) points. So

\[
|C(S, p; \alpha)| \leq m \frac{\text{vol}[\bar{U}]}{\text{vol}[U]} \leq m \frac{\text{vol}[B(p; \alpha + d)]}{\text{vol}[U]} = m \frac{(\alpha + d)^n V_n}{\text{vol}[U]} = \nu(U, \alpha, n) m,
\]

where \( \nu(U, \alpha, n) = \frac{(\alpha + d)^n V_n}{\text{vol}[U]} \). We will estimate \( \nu(U, \alpha, n) \) using the upper bound \( \alpha \leq (L + m + 1)2R(S) \) from Lemma 3.7(c). Since the longest diagonal has the upper bound \( 2R(S) \geq d \) because the closed balls with the radius \( \frac{d}{2} \) and centers at the vertex of a unit cell \( U \) cover \( \bar{U} \), so \( \alpha + d \leq (L + m + 2)2R(S) \).

Since \( \Gamma \left( \frac{n}{2} + 1 \right) = \sqrt{\pi} \frac{(2n-1)(2n-3)\ldots 1}{2^n} = \sqrt{\pi} \frac{(2n-2)(2n-4)\ldots 2}{2^n(2n-2)\ldots 2} = \frac{\sqrt{\pi} (2n)!}{2^{2n} n!} \)

the volume of the unit ball becomes \( V_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} = (\sqrt{\pi})^{n-1} \frac{2^n n!}{(2n)!} \). The bounds \( \sqrt{2\pi n} \left( \frac{\pi}{e} \right)^n \exp(\frac{12n+1}{24n+1}) < n! < \sqrt{2\pi n} \left( \frac{\pi}{e} \right)^n \exp(\frac{1}{12n}) \) imply that \( V_n \leq \left( \frac{\pi}{e} \right)^n \frac{2^n n!}{(2n)!} \leq \left( \frac{\sqrt{\pi}}{2} \right)^{n-1} \frac{2^n n!}{(2n)!} \exp(\frac{1}{12n} - \frac{1}{24n+1}) \leq \frac{\exp(\frac{1}{2n})}{\sqrt{\pi} n} \left( \frac{e}{\sqrt{\pi}} \right)^n \)

because \( \frac{1}{12n} - \frac{1}{24n+1} \leq \frac{1}{24n} \) for \( n \geq 1 \). Then \( V_n \leq \frac{\exp(\frac{1}{2n})}{\sqrt{\pi} n} \left( \frac{e}{\sqrt{\pi}} \right)^n \) implies that \( \nu(U, \alpha, n) = \frac{(\alpha + d)^n V_n}{\text{vol}[U]} \leq \frac{(L + m + 2)2R(S)^n V_n}{\text{vol}[U]} \leq \frac{\exp(\frac{1}{2n})}{\sqrt{\pi} n} \left( \frac{e}{\sqrt{\pi}} \right)^n \leq \frac{10(L + m + 2)^n R(S)^n}{2\text{vol}[U]} = \text{GC}(S) \) as required. \( \square \)
Proof of Lemma 5.6. The directed distance \( d_R(C \cup \partial \bar{B}(0; \alpha), D \cup \partial \bar{B}(0; \alpha)) \) is the minimum \( \varepsilon \in [0, \alpha] \) such that, for some \( f \in O(\mathbb{R}^n) \), all points of \( f(C) \cap B(0; \alpha - \varepsilon) \) are covered by \( D + \bar{B}(0; \varepsilon) \) as all points of \( f(C) - B(0; \alpha - \varepsilon) \) are \( \varepsilon \)-close to the boundary \( \partial \bar{B}(0; \alpha) \). Let \( j \in \{1, \ldots, k\} \) be the largest index so that \( |p_j| < \alpha - \varepsilon \). Then \( C \cap B(0; \alpha - \varepsilon) = \{p_1, \ldots, p_j\} \) and \( d_R(\{p_1, \ldots, p_i\}, D) \leq d_R(C \cap B(0; \alpha - \varepsilon), D) \leq \varepsilon \) for all \( i = 1, \ldots, j \). By the above choice of \( j \), if \( j < i \leq k \) then \( \alpha - |p_i| \leq \varepsilon \). Hence, for all \( i = 1, \ldots, k \), both terms in

\[
\min\{\alpha - |p_i|, d_R(\{p_1, \ldots, p_i\}, D)\}
\]

are at most \( \varepsilon \). Then \( d_M(C, D) \leq \varepsilon \).

Using the brief notation \( d_M = d_M(C, D) \), the converse inequality \( \varepsilon \leq d_M \) follows from \( d_R(C \cap \bar{B}(0; \alpha - \alpha_M), D) \leq d_M \), which is proved below. Let \( j \in \{1, \ldots, k\} \) be the largest index so that \( |p_j| \leq \alpha - \alpha_M \). Since \( \alpha - |p_j| \geq d_M \) and

\[
\min\{\alpha - |p_j|, d_R(\{p_1, \ldots, p_j\}, D)\} \leq d_M \]

in the minimum above is at most \( d_M \). Due to \( C \cap \bar{B}(0; \alpha - d_M) = \{p_1, \ldots, p_j\} \), we get \( d_R(C \cap \bar{B}(0; \alpha - d_M), D) \leq d_M \), which proves the required equality.

Proof of Lemma 6.4. Definition 4.1 of \( \varepsilon = \text{BT}([C(S, p; \alpha), |C(Q, q; \alpha)|]) \) implies that, for a suitable isometry \( f \in O(\mathbb{R}^n) \), the image \( f(C(S, p; \alpha - \varepsilon) - \bar{p}) \) is covered by the \( \varepsilon \)-offset of \( C(Q, q; \alpha) - \bar{q} \) shifted by \( q \) to the origin. Since \( \varepsilon \) is smaller than a minimum half-distance between points of \( S, Q \), the above covering establishes a bijection \( g \) with all (at least \( k \)) neighbors of \( p \) and \( q \) in their \((\alpha - \varepsilon)\)-clusters. The covering condition above means that the corresponding neighbors are at a maximum distance \( \varepsilon \) from each other. The triangle inequality implies that the distances from corresponding neighbors to their centers \( p, q \) differ by at most \( \varepsilon \). The ordered distances from \( p, q \) to their \( k \) neighbors in the \((\alpha - \varepsilon)\)-clusters form the rows of \( p, q \) in PDD(\( S; k \), PDD(\( Q; k \). The bijection \( g \) may not respect their order. By Lemma 3.6, the ordered distances with the same indices are \( \varepsilon \)-close. So the \( L_\infty \) distance between the rows of \( p, q \) is at most \( \varepsilon \).

Example A.7 (Earth Mover’s Distance for lattices with bottleneck distance \( d_B = +\infty \)). The 1D lattices \( S = \mathbb{Z} \) and \( Q = (1 + \delta)\mathbb{Z} \) with the bottleneck distance \( d_B(S, Q) = +\infty \) have PDD consisting of a single row (as for any lattice). For instance, PDD(\( S; 4 \)) = (1, 1, 2, 2) and PDD(\( Q; 4 \)) = (1 + \delta, 1 + \delta, 2 +
For the common stable radius $\alpha = 2 + 2\delta$, Example 4.6 computed $\text{EMD}(I(S; \alpha), I(Q; \alpha)) = 2\delta$. Theorem 6.5 considers the maximum number $k$ of points in clusters of $S, Q$ with the radius $\alpha - 2\delta = 2$, so $k = 2$.

Then $\text{EMD}(\text{PDD}(S; 2), \text{PDD}(Q; 2))$ equals the $L_\infty$ distance $\delta$ between the short rows $(1, 1)$ and $(1 + \delta, 1 + \delta)$. The above computations illustrate the lower bound $\text{EMD}(\text{PDD}(S; 2), \text{PDD}(Q; 2)) = \delta \leq \text{EMD}(I(S; \alpha), I(Q; \alpha)) = 2\delta$. This inequality becomes equality for the larger stable radius $\alpha = 2 + 4\delta$, because the clusters of $S, Q$ with the radius $\alpha - 2\delta = 2 + 2\delta$ contain $k = 4$ points. The $L_\infty$ distance between $(1, 1; 2, 2)$ and $(1 + \delta, 1 + \delta, 2 + 2\delta, 2 + 2\delta)$ is $2\delta$ for $\delta < \frac{1}{5}$, so $\text{EMD}(\text{PDD}(S; 4), \text{PDD}(Q; 4)) = 2\delta = \text{EMD}(I(S; 2 + 4\delta), I(Q; 2 + 4\delta))$. ■

**Example A.8** (lower bound for a distance between square and hexagonal lattices). The square lattice $\Lambda_4$ and hexagonal lattice $\Lambda_6$ with minimum inter-point distance 1 have a common stable radius $\alpha = 2$ as shown in Fig. 7. The maximum number of points in the stable 2-clusters is $k = 12$. The rows $\text{PDD}(\Lambda_4; 12) = (1, 1, 1, \sqrt{2}, \sqrt{2}, \sqrt{2}, 2, 2, 2, 2)$ and $\text{PDD}(\Lambda_6; 12) = (1, 1, 1, 1, \sqrt{3}, \sqrt{3}, \sqrt{3}, \sqrt{3}, \sqrt{3})$ have the $L_\infty$ distance $\max\{\sqrt{2} - 1, 2 - \sqrt{3}\} = \sqrt{2} - 1$, which coincides with $\text{EMD}(I(\Lambda_4; 2), I(\Lambda_6; 2))$ in Example 4.3. ■