Easily computable continuous metrics on the space of isometry classes of all 2-dimensional lattices

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Abstract

A periodic lattice in Euclidean space is the infinite set of all integer linear combinations of basis vectors. Any lattice can be generated by infinitely many different bases. Motivated by rigid crystal structures, we consider lattices up to rigid motion or isometry, which preserves inter-point distances. Then all isometry classes of lattices form a continuous space. There are several parameterisations of this space in dimensions two and three, but this is the first which is not discontinuous in singular cases. We introduce new continuous coordinates (root products) on the space of lattices and new metrics between root forms satisfying all metric axioms and continuity under all perturbations. The root forms allow visualisations of hundreds of thousands of real crystal lattices from the Cambridge Structural Database for the first time.

1. Motivations, problem statement and overview of new results

A *lattice* $\Lambda \subset \mathbb{R}^n$ consists of all integer linear combinations of basis vectors $v_1, \dots, v_n$, which span a parallelepiped called a *unit cell* U. Our motivation to classify lattices comes from crystal structures that are determined in a rigid form. A lattice can be considered as crystal whose atomic motif consists of a single point. For example, graphene consists of layers of a hexagonal 2-dimensional lattice derived from a single carbon atom. Any periodic crystal is obtained from a lattice by adding finitely many copies, each shifted to the position of one of the atomic motif points in a unit cell U.

Crystallography traditionally splits crystals into finitely many classes, for instance by their symmetry groups. These finite classifications are insufficient to distinguish infinitely many classes of lattices up to *rigid motion* (a composition of rotations and translations). In this paper we consider classification up to *isometry*, which also includes reflections. However, orientation-preserving isometries in $\mathbb{R}^d$ can be distinguished by sign, hence it is simple to restrict the argument to rigid motions only.

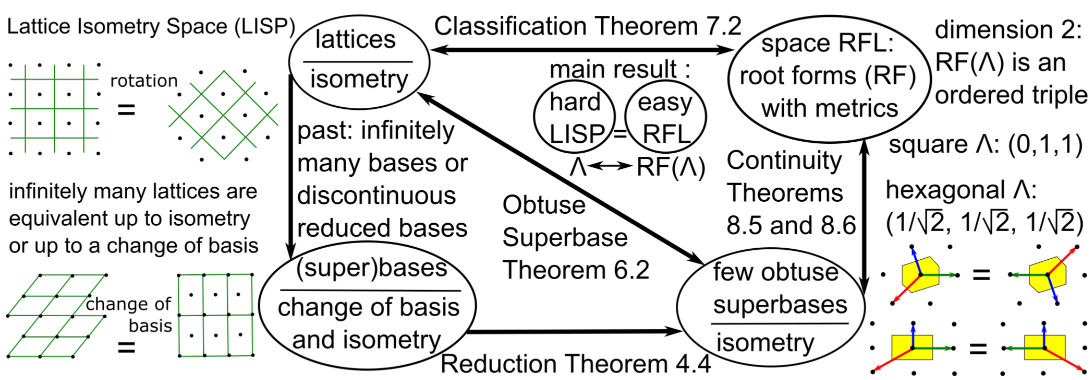

Fig. 1. The LISP is bijectively and bi-continuously mapped to root forms of lattices, which are triples of root products between vectors of an obtuse superbase in $\mathbb{R}^2$.

Since crystal structures are considered as rigid bodies, isometry is the most natural equivalence relation on lattices. The square lattices in the top left corner of Fig. 1 have different bases (related by a rotation) but belong to the same isometry class of unit square lattices. The resulting quotient space under this relation, the Lattice Isometry Space (LISP), consists of infinitely many classes, where every class includes all lattices isometric to each other. Any continuous transition between lattices is a continuous path in the LISP. Previous approaches to uniquely representing any isometry class was to choose a reduced basis (Niggli's reduced cell). Any such reduction is discontinuous under perturbations of a basis, see Widdowson *et al.* (2022, Theorem 15) in the sense that a slight change of basis vectors can lead to a very different reduced basis.

Though Niggli's reduced cell identifies a lattice up to isometry, its discontinuity under perturbations motivates Problem 1.1 to find a continuous metric on the LISP.

Problem 1.1 (metric on lattices)**.** Find a metric $d(\Lambda, \Lambda')$ on lattices in $\mathbb{R}^2$ such that

(1.1a) $d(\Lambda, \Lambda')$ is independent of given primitive bases of lattices Λ, Λ';

(1.1b) $d(\Lambda, \Lambda')$ is preserved under any isometry or rigid motion of $\mathbb{R}^2$;

(1.1c) d satisfies the metric axioms: $d(\Lambda, \Lambda') = 0$ if and only if Λ, Λ' are isometric, symmetry $d(\Lambda, \Lambda') = d(\Lambda', \Lambda)$ and triangle inequality $d(\Lambda, \Lambda') + d(\Lambda', \Lambda'') \geq d(\Lambda, \Lambda'')$;

(1.1d) $d(\Lambda, \Lambda')$ continuously changes under perturbations of primitive bases of Λ, Λ';

(1.1e) $d(\Lambda, \Lambda')$ is computed from reduced bases of Λ, Λ' in a constant time. ■

The metric problem above and most results are stated in the case of $\mathbb{R}^2$, which is already non-trivial and new. Our follow-up paper extends all conclusions to $\mathbb{R}^3$.

2. Overview of related past work and new metrics on lattices

Niggli's reduced cell (Niggli, 1928) is unique in the sense that two lattices are isometric if and only if their Niggli's reduced cells are isometric. Since cells are easy to compare (Křivỳ & Gruber, 1976), one can get the discrete metric $d(\Lambda, \Lambda')$ taking the same non-zero value (say, 1) for any non-isometric lattices Λ, Λ'. This is the simplest example of a discontinuous metric satisfying all metric axioms on a set of equivalence classes.

Discontinuity of Niggli's cell up to perturbations was practically demonstrated in the seminal work (Andrews *et al.*, 1980). More recently, the non-existence of a continuous reduction was mentioned in the introduction of Edelsbrunner *et al.* (2021) and formally proved in Widdowson *et al.* (2022, Theorem 15). Since 1980 Larry Andrews and Herbert Bernstein have made important advances for Problem 1.1 in the numerous papers (Andrews & Bernstein, 1988; Andrews & Bernstein, 2014; McGill *et al.*, 2014; Andrews *et al.*, 2019) by analysing progressively more complicated boundary cases where cell reductions can be discontinuous. Since these advances are specialised for $\mathbb{R}^3$, we defer a more detailed comparison with new metrics to the follow-up paper for 3D lattices.

The invariant-based approach is to compare crystals or lattices by their isometry *invariants*, which are descriptors or features preserved under any isometry. For example, a cell basis is not invariant, but the primitive cell volume is, though this invariant is discontinuous in the more general case of crystals, see Widdowson *et al.* (2022, Fig. 1). The Euclidean (or any other) distance between isometry invariants I of crystals or lattices can satisfy the first metric axiom only if I is a *complete* meaning that so if $I(\Lambda) = I(\Lambda')$ then Λ, Λ' are isometric. Then $d(I(\Lambda), I(\Lambda')) = 0$ implies $I(\Lambda) = I(\Lambda')$ and we need completeness of I to conclude that Λ, Λ' are isometric.

About 30 years ago John Conway and Neil Sloane published a series of seven papers on low-dimensional lattices. The most relevant for Problem 1.1 is Conway & Sloane (1992), whose main result included the continuity claim (item 1 on page 55) saying that certain lattice invariants (conorms) ‘vary continuously with the lattice’.

Unfortunately, Conway & Sloane (1992) had no further discussion of continuity, otherwise Problem 1.1 might have been solved 30 years ago. To show that an invariant $I(\Lambda)$ is continuous, we need a metric on the space of lattices (LISP) and a metric on the space of invariants. In general topology, it suffices to define open subsets on both spaces, but we are interested in metric continuity for practical measurements.

Since a lattice in $\mathbb{R}^n$ can be represented by a basis, one can define $d(\Lambda, \Lambda')$ as a distance between bases B, B' (given as $n\times n$ matrices) minimised over all permutations of vectors and orthogonal transformations from the group $\mathrm{SO}(\mathbb{R}^n)$ or $\mathrm{O}(\mathbb{R}^n)$.

Permutations were excluded from this approach by Mosca & Kurlin (2020) by taking Voronoi domains (Wigner-Seitz cells) and minimising their overlap only over rotations. However, the resulting metric can be only approximated, so computability condition (1.1e) was not satisfied. A similar approach with an approximate metric was extended from lattices to periodic point sets representing all periodic crystals (Anosova & Kurlin, 2021*b*; Anosova & Kurlin, 2021*a*). Related advances include the isometry invariants discussed in (Edelsbrunner *et al.*, 2021; Widdowson *et al.*, 2022; Widdowson & Kurlin, 2021), whose completeness was proved for crystals in general position.

Without full completeness of the above invariants or easily computable distance between complete invariant isosets, Problem 1.1 was unresolved even for lattices.

Section 3 formally defines key concepts, most importantly Voronoi domains. Following Conway & Sloane (1992), section 4 recalls an obtuse superbase consisting of vectors v_1, v_2 and $v_0 = -v_1 - v_2$ in $\mathbb{R}^2$ such that all vectors have non-acute angles, equivalently non-positive scalar products $v_i \cdot v_j \leq 0$. Section 5 introduces the root products $r_{ij} = \sqrt{-v_i \cdot v_j}$, coordinates on the space of root forms of lattices (RFL).

This 3-parameter space RFL provides a complete and continuous parameterisation of the Lattice Isometry Space (LISP) due to the following new results.

- Theorem 6.2 substantially reduces the ambiguity of lattice representations by infinitely many bases to only very few obtuse superbases, see Fig. 1.
- Theorem 7.2 proves completeness of root forms via a 1-1 map LISP $\leftrightarrow$ RFL.
- Theorems 8.5 and 8.6 prove that this 1-1 map is continuous in both directions.
- Section 9 visualises hundreds of thousands of lattices extracted from the Cambridge Structural Database (CSD) in a common space for the first time.

- Section 10 concludes with a vision that a new continuous crystallography will elucidate similarities between lattices that were incomparable in the past.

3. Key definitions and results of computational geometry for lattices

Any point p in Euclidean space $\mathbb{R}^n$ can be represented by the vector from the origin $0 \in \mathbb{R}^n$ to p. So p may also denote this vector, though an equal vector $\vec{p}$ can be drawn at any initial point. The *Euclidean* distance between points $p, q \in \mathbb{R}^n$ is $|p - q|$.

Definition 3.1 (a lattice Λ, a unit cell U)**.** Let vectors $v_1, \dots, v_n$ form a linear *basis* in $\mathbb{R}^n$ so that if $\sum\limits_{i=1}^{n} c_i v_i = 0$ for some real c_i, then all $c_i = 0$. Then a *lattice* Λ in $\mathbb{R}^n$ consists of all linear combinations $\sum\limits_{i=1}^{n} c_i v_i$ with integer coefficients $c_i \in \mathbb{Z}$. The parallelepiped $U(v_1, \dots, v_n) = \left\{ \sum\limits_{i=1}^{n} c_i v_i \, : \, c_i \in [0, 1) \right\}$ is a *primitive unit cell* of Λ. ■

The (signed) volume V of a unit cell $U(v_1, \dots, v_n)$ equals the determinant of the $n \times n$ matrix with columns $v_1, \dots, v_n$. The sign of V is used to define an *orientation*.

Definition 3.2 (isometry, orientation and rigid motion)**.** An *isometry* is any map $f : \mathbb{R}^n \to \mathbb{R}^n$ such that $|f(p) - f(q)| = |p - q|$ for any $p, q \in \mathbb{R}^n$. For any basis $v_1, \dots, v_n$ of $\mathbb{R}^n$, the volumes of $U(v_1, \dots, v_n)$ and $U(f(v_1), \dots, f(v_n))$ have the same absolute non-zero value. If these volumes are equal, the isometry f is *orientation-preserving*, otherwise f is *orientation-reversing*. Any orientation-preserving isometry f is a composition of translations and rotations, and can be included into a continuous family of isometries f_t, where $t \in [0, 1]$, f_0 is the identity map and $f_1 = f$, which is also called a *rigid motion*. Any orientation-reversing isometry is a composition of a rigid motion and a single reflection in a linear subspace of dimension $n - 1$. ■

The Voronoi domain defined below is also called the *Wigner-Seitz cell*, *Brillouin zone* or *Dirichlet cell*. We use the word *domain* to avoid a confusion with a unit cell, which is a parallelepiped spanned by a vector basis. Though the Voronoi domain can be defined for any point of a lattice, it will suffice to consider only the origin 0.

Definition 3.3 (Voronoi domain and Voronoi vectors of a lattice)**.** The *Voronoi domain* of a lattice Λ is the neighbourhood $V(\Lambda) = \{p \in \mathbb{R}^n : |p| \leq |p - v| \text{ for any } v \in \Lambda\}$ of the origin $0 \in \Lambda$ consisting of all points p that are non-strictly closer to 0 than to other points $v \in \Lambda$. A vector $v \in \Lambda$ is called a *Voronoi vector* if the bisector hyperspace $H(0, v) = \{p \in \mathbb{R}^n : p \cdot v = \frac{1}{2}v^2\}$ between 0 and v intersects $V(\Lambda)$. If $V(\Lambda) \cap H(0, v)$ is an $(n-1)$-dimensional face of $V(\Lambda)$, then v is called a *strict* Voronoi vector. ■

The Voronoi domain $V(\Lambda)$ is the intersection of the closed half-spaces $S(0, v) = \{p \in \mathbb{R}^n : p \cdot v \leq \frac{1}{2}v^2\}$ with the boundaries $H(0, v)$ for all strict Voronoi vectors $v \in \Lambda$. Any lattice is uniquely determined by its Voronoi domain in the sense below.

Lemma 3.4 (lattices $\leftrightarrow$ Voronoi domains)**.** Any lattices $\Lambda, \Lambda' \subset \mathbb{R}^n$, which share the origin $0 \in \mathbb{R}^n$, are related by a map from a subgroup $G \subset \mathrm{Iso}(\mathbb{R}^n)$ if and only if their Voronoi domains $V(\Lambda), V(\Lambda')$ are related by the same map from the subgroup G. ■

Lemma 3.4 reduces an isometry classification of infinite lattices to one of bounded polyhedra, see proofs in appendices. However, Voronoi domains are compared modulo infinitely many rotations. (Mosca & Kurlin, 2020) defined two Voronoi-based metrics on the lattice space, which were approximated by sampling over many rotations.

Lemma 3.5 shows how to find all Voronoi vectors. The doubled lattice is $2\Lambda = \{2v : v \in \Lambda\}$. Vectors $u, v \in \Lambda$ are 2Λ-equivalent if $u - v \in 2\Lambda$. Then any vector $v \in \Lambda$ generates its 2Λ-class $v + 2\Lambda = \{v + 2u : u \in \Lambda\}$, which contains the vector $-v$. All classes of 2Λ-equivalent vectors form the quotient space $\Lambda/2\Lambda$. A 1D lattice Λ generated by a vector v has the quotient $\Lambda/2\Lambda$ consisting of two classes $\Lambda, v + \Lambda$.

Lemma 3.5 (Voronoi vector criterion, Theorem 2 in (Conway & Sloane, 1992))**.** For any lattice $\Lambda \subset \mathbb{R}^n$, a non-zero vector $v \in \Lambda$ is a Voronoi vector of Λ if and only if v is a shortest vector in its 2Λ-class $v + 2\Lambda$. Also, v is a strict Voronoi vector if and only if $\pm v$ are the only shortest vectors in $v + 2\Lambda$. ■

Any lattice $\Lambda \subset \mathbb{R}^2$ generated by v_1, v_2 has the quotient $\Lambda/2\Lambda = \{v_1, v_2, v_1+v_2\}+\Lambda$. Notice that the vectors $v_1 \pm v_2$ belong to the same class modulo 2Λ. Assume that v_1, v_2 are not longer than $v_1 + v_2$, which holds if $\angle(v_1, v_2) \in [60°, 120°]$. If the vector $v_1 + v_2$ is shorter than $v_1 - v_2$ as in Fig. 2, then L has three pairs of strict Voronoi vectors $\pm v_1, \pm v_2, \pm(v_1 + v_2)$. If $v_1 \pm v_2$ have the same length, then the unit cell spanned by v_1, v_2 degenerates to a rectangle, so Λ has four non-strict Voronoi vectors $\pm v_1 \pm v_2$.

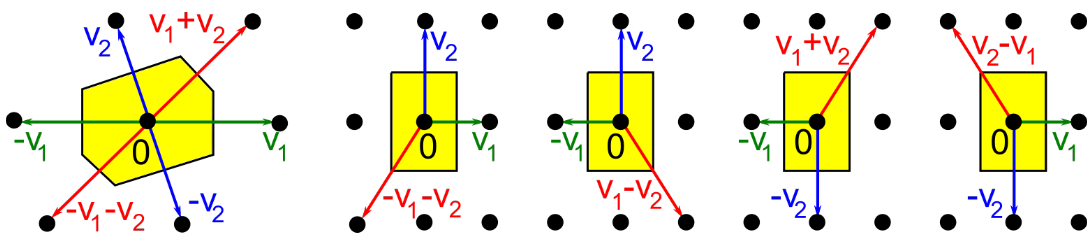

Fig. 2. **Left**: a generic 2D lattice has a hexagonal Voronoi domain with an obtuse superbase $v_1, v_2, v_0 = -v_1 - v_2$, which is unique up to permutations and central symmetry. **Other pictures**: isometric superbases for a rectangular Voronoi domain.

4. Vonorms and conorms of an (obtuse) superbase of a lattice

The triple of Voronoi vector pairs $\pm v_1, \pm v_2, \mp(v_1+v_2)$ in Fig. 2 motivates the concept of a superbase with the extra vector $v_0 = -v_1 - v_2$, which extends to any dimension n by setting $v_0 = -\sum_{i=1}^{n} v_n$. For the dimensions 2 and 3, Theorem 4.4 will prove that any lattice has an obtuse superbase of vectors whose pairwise scalar products are non-positive and are called *Selling parameters*. For any superbase in $\mathbb{R}^n$, the negated parameters $p_{ij} = -v_i \cdot v_j$ can be interpreted as conorms of lattice characters, functions $\chi : \Lambda \to \{\pm 1\}$ satisfying $\chi(u + v) = \chi(u)\chi(v))$, see Conway & Sloane (1992, Theorem 6). So p_{ij} will be defined as *conorms* only for an obtuse superbase below.

Definition 4.1 (obtuse superbase and its conorms p_{ij})**.** For any basis $v_1,\dots,v_n$ in $\mathbb{R}^n$, the *superbase* $v_0,v_1,\dots,v_n$ includes the vector $v_0=-\sum\limits_{i=1}^{n} v_i$. The *conorms* $p_{ij}=-v_i\cdot v_j$ are equal to the negative scalar products of the vectors above. The superbase is called *obtuse* if all conorms $p_{ij}\geq 0$, so all angles between vectors v_i,v_j are non-acute for distinct indices $i,j\in\{0,1,\dots,n\}$. The superbase is called *strict* if all $p_{ij}>0$. ■

Conway & Sloane (1992, formula (1)) has a typo initially defining p_{ij} as exact Selling parameters, but their Theorems 3,7,8 explicitly use non-negative $p_{ij}=-v_i\cdot v_j\geq 0$.

The indices of a conorm p_{ij} are distinct and unordered. We always set $p_{ij}=p_{ji}$ for all $i,j,$. A 1D lattice generated by a vector v_1 has the obtuse superbase of $v_0=-v_1$ and v_1, so the only conorm $p_{01}=-v_0\cdot v_1=v_1^2$ is the squared norm of v_1. Any basis of $\mathbb{R}^n$ has $\dfrac{n(n+1)}{2}$ conorms p_{ij}, for example three conorms p_{01},p_{02},p_{12} in dimension 2.

Lemma 4.2 (squared norm formula)**.** For any basis $v_1,\dots,v_n$ in $\mathbb{R}^n$, let $p_{ij}=-v_i\cdot v_j$ be the conorms of the superbase $v_0,v_1,\dots,v_n$ with $v_0=-\sum\limits_{i=1}^{n} v_i$. The squared norm $v^2=v\cdot v$ of any vector $v=\sum\limits_{i=1}^{n} c_iv_i$ equals $N(v)=\sum\limits_{i=1}^{n} c_i^2p_{0i}+\sum\limits_{1\leq i<j\leq n}(c_i-c_j)^2p_{ij}$. ■

Proof. In the right hand side of the required formula we substitute the conorms in terms of scalar products of basis vectors as follows: $p_{ij}=-v_i\cdot v_j$ for $i,j\in\{1,\dots,n\}$. Then $p_{0i}=-v_0\cdot v_i=v_i\cdot\sum\limits_{j=1}^{n} v_j=v_i^2+\sum\limits_{j\neq i}^{n} v_i\cdot v_j$ and

$$\sum_{i=1}^{n} c_i^2p_{0i}+\sum_{1\leq i<j\leq n}(c_i-c_j)^2p_{ij}=\sum_{i=1}^{n} c_i^2(v_i^2+\sum_{j\neq i}^{n} v_i\cdot v_j)-\sum_{1\leq i<j\leq n}(c_i^2-2c_ic_j+c_j^2)v_i\cdot v_j=$$

$$=\sum_{i=1}^{n} c_i^2v_i^2+\sum_{i=1}^{n} c_i^2\sum_{j\neq i}^{n} v_i\cdot v_j-\sum_{1\leq i<j\leq n}(c_i^2+c_j^2)(v_i\cdot v_j)+\sum_{1\leq i<j\leq n}2c_ic_j(v_i\cdot v_j)=$$

$$=\sum_{i=1}^{n} c_i^2v_i^2+2\sum_{1\leq i<j\leq n}c_ic_j(v_i\cdot v_j)=\left(\sum_{i=1}^{n} c_iv_i\right)^2=N(v)\text{ as required.}$$ □

Definition 4.3 introduces partial sums v_S for any superbase $\{v_i\}_{i=0}^{n}$ of a lattice Λ.

Definition 4.3 (partial sums v_S and their vonorms)**.** Let a lattice $\Lambda \subset \mathbb{R}^n$ have any superbase $v_0, v_1, \dots, v_n$ with $v_0 = -\sum\limits_{i=1}^{n} v_i$. For any proper subset $S \subset \{0, 1, \dots, n\}$ of indices, consider its complement $\bar{S} = \{0, 1, \dots, n\} - S$ and the *partial sum* $v_S = \sum\limits_{i \in S} v_i$ whose squared lengths v_S^2 are called *vonorms* of the superbase $\{v_i\}_{i=0}^n$. The *vonorms* can be expressed as $v_S^2 = (\sum\limits_{i \in S} v_i)(-\sum\limits_{j \in \bar{S}} v_j) = -\sum\limits_{i \in S, j \in \bar{S}} v_j \cdot v_j = \sum\limits_{i \in S, j \in \bar{S}} p_{ij}$. ■

(Conway & Sloane, 1992) call lattices $\Lambda \subset \mathbb{R}^n$ that have an obtuse superbase *lattices of Voronoi's first kind*, which are all lattices in dimensions 2 and 3 by Theorem 4.4.

Theorem 4.4 (obtuse superbase existence)**.** Any lattice Λ in dimensions $n = 2, 3$ has an obtuse superbase $v_0, v_1, \dots, v_n$ so that $p_{ij} = -v_i \cdot v_j \geq 0$ for any $i \neq j$. ■

Conway & Sloane (1992, section 7) attempts to prove Theorem 4.4 for $n = 3$ by example and sketches an analogous idea for a proof for $n = 2$. We provide a compete proof for Theorem 4.4 for $n = 2$ in section 5, including a method for obtaining the obtuse superbase from any initial lattice basis. The follow-up paper will give a similar proof in $n = 3$, correcting key details from Conway & Sloane (1992, section 7).

Lemma 4.5 will later help to prove that a lattice is uniquely determined up to isometry by an obtuse superbase, hence by its vonorms or, equivalently, conorms.

Lemma 4.5 (Voronoi vectors v_S, Theorem 3 in (Conway & Sloane, 1992))**.** For any obtuse superbase $v_0, v_1, \dots, v_n$ of a lattice, all partial sums v_S from Definition 4.3 split into $2^n - 1$ symmetric pairs $v_S = -v_{\bar{S}}$, which are Voronoi vectors representing distinct 2Λ-classes in $\Lambda/2\Lambda$. All Voronoi vectors v_S are strict if and only if all $p_{ij} > 0$. ■

5. Voforms and coforms are isometry invariants of lattices in dimension 2

Definition 5.1 introduces voforms and coforms, which are triangular cycles whose three nodes are marked by vonorms and conorms, respectively. Though we start from any obtuse superbase B of a lattice Λ to define a voform VF, a coform CF and root form RF, Lemma 5.4 will justify that they are independent of B up to isomorphism.

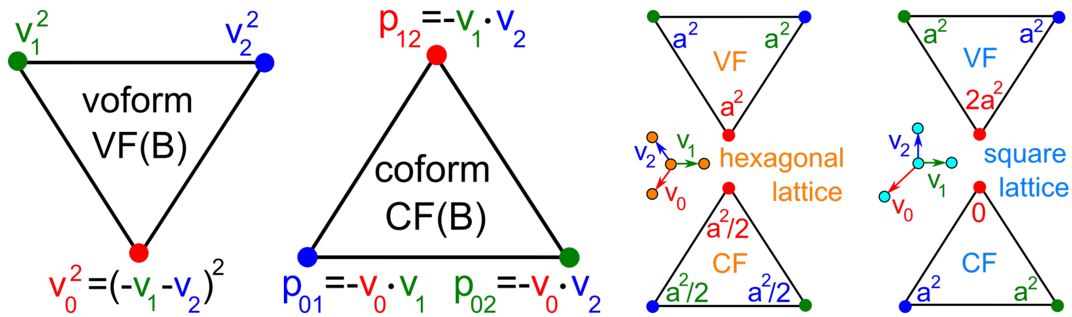

Fig. 3. **1st**: a voform VF(B) of a 2D lattice with an obtuse superbase $B = (v_0, v_1, v_2)$. **2nd**: nodes of a coform CF(B) are marked by conorms p_{ij}. **3rd and 4th**: VF and CF of the hexagonal and square lattice base with a minimum vector length a.

Definition 5.1 (2D *voforms*, *coforms*, *root forms* and *isomorphisms*)**.** Any obtuse superbase $B = (v_0, v_1, v_2)$ of a lattice $\Lambda \subset \mathbb{R}^2$ has three pairs of partial sums $\pm v_0 = \mp(v_1 + v_2)$, $\pm v_1$, $\pm v_2$. The formula $v_S^2 = \sum\limits_{i \in S, j \in \bar{S}} p_{ij}$ in Definition 4.3 implies that

$$(5.1a) \qquad v_0^2 = p_{01} + p_{02}, \qquad v_1^2 = p_{01} + p_{12}, \qquad v_2^2 = p_{02} + p_{12}.$$

The conorms are conversely expressed from the above formulae as

$$(5.1b) \quad p_{12} = \frac{1}{2}(v_1^2 + v_2^2 - v_0^2), \quad p_{01} = \frac{1}{2}(v_0^2 + v_1^2 - v_2^2), \quad p_{02} = \frac{1}{2}(v_0^2 + v_2^2 - v_1^2).$$

Briefly, $p_{ij} = \dfrac{1}{2}(v_i^2 + v_j^2 - v_k^2)$ for any distinct $i, j \in \{0, 1, 2\}$ and $k = \{0, 1, 2\} - \{i, j\}$.

The *voform* VF(B) is the cycle on three nodes marked by the vonorms v_0^2, v_1^2, v_2^2, see Fig. 3. The *coform* CF(B) is the cycle on three nodes marked by the conorms p_{12}, p_{02}, p_{01}. An *isomorphism* (denoted by $\sim$) of voforms (coforms, respectively) is any permutation σ of the three vonorms (conorms, respectively) from the permutation group S_3 on the indices 0,1,2. This isomorphism is *orientation-preserving* (denoted by $\overset{+}{\sim}$) if σ is one of even permutations that form the alternating subgroup $A_3 \subset S_3$.

Since all conorms p_{ij} are non-negative, we can define the *root products* $r_{ij} = \sqrt{p_{ij}}$, which have the same units as original coordinates, for example in Angstroms: $1\mathring{A} = 10^{-10}$m. Up to isomorphism of coforms, these root products can be ordered: $r_{12} \leq r_{01} \leq r_{02}$, which is equivalent to $v_1^2 \leq v_2^2 \leq v_0^2$ by formulae (5.1a). This unique ordered triple (r_{12}, r_{01}, r_{02}) is called the *root form* RF(B). If we consider only orientation-preserving isomorphisms (even permutations), the last two entries may be swapped, then the triple is called the *orientation-preserving root form* RF$^+(B)$. ■

Lemma 5.2 (equivalence of VF, CF, RF)**.** For any obtuse superbase B in $\mathbb{R}^2$, its voform VF(B), coform CF(B) and unique RF(B) are reconstructible from each other.

Proof. The conorms p_{12}, p_{02}, p_{01} are uniquely expressed via the vonorms v_0^2, v_1^2, v_2^2 by formulae (5.1ab) and vice versa. If we apply a permutation of indices $0, 1, 2$ to the conorms, the same permutation applies to the vonorms. Hence we have a 1-1 bijection CF$(\Lambda) \leftrightarrow$ VF(Λ) up to (orientation-preserving) isomorphism. The root form RF(Λ) is uniquely defined by ordering root products without any need for isomorphisms. □

Lemma 5.3 (isometry→isomorphism)**.** Any (orientation-preserving) isometry of obtuse superbases $B \to B'$ induces an (orientation-preserving) isomorphism of voforms VF$(B) \sim$ VF(B'), coforms CF$(B) \sim$ CF(B') and keeps RF$(B) =$ RF(B'). ■

Proof. Any isometry preserves lengths and scalar products of vectors. □

Proof of Theorem 4.4 for $n = 2$. For any lattice $\Lambda \subset \mathbb{R}^2$, permuting vectors of a superbase $B = (v_0, v_1, v_2)$ allows us to order the conorms: $p_{12} \leq p_{01} \leq p_{02}$. Our aim is to reduce B so that all conorms non-negative. Assuming that $p_{12} = -v_1 \cdot v_2 = -\varepsilon < 0$, we change the superbase: $u_1 = -v_1$, $u_2 = v_2$, $u_0 = v_1 - v_2$ so that $u_0 + u_1 + u_2 = 0$.

Two vonorms remain the same: $u_1^2 = v_1^2$ and $u_2^2 = v_2^2$. The third vonorm decreases by $4\varepsilon > 0$ as follows: $u_0^2 = (v_1 - v_2)^2 = (v_1 + v_2)^2 - 4v_1v_2 = v_0^2 - 4\varepsilon$. One conorm changes its sign: $q_{12} = -u_1 \cdot u_2 = -p_{12} = \varepsilon > 0$. The two other conorms decrease:

$$q_{01} = -u_0 \cdot u_1 = -(v_1 - v_2) \cdot (-v_1) = -(-v_1 - v_2)v_1 - 2v_1 \cdot v_2 = p_{01} - 2\varepsilon,$$

$$q_{02} = -u_0 \cdot u_2 = -(v_1 - v_2) \cdot v_2 = -(-v_1 - v_2)v_2 - 2v_1 \cdot v_2 = p_{02} - 2\varepsilon.$$

If one of the new conorms becomes negative, we apply the above reduction again. To prove that all conorms become non-negative in finitely many steps, notice that every reduction can make superbase vectors only shorter, but not shorter than a minimum distance between points of Λ. The angle between v_i, v_j can have only finitely many values when lengths of v_i, v_j are bounded. Hence the scalar product $\varepsilon = v_i \cdot v_j > 0$ cannot converge to 0. Since every reduction makes one of the superbase vectors shorter by a positive constant, the reductions should finish in finitely many steps. □

By Theorem 4.4 any lattice $\Lambda \subset \mathbb{R}^2$ has an obtuse superbase with all $p_{ij} \geq 0$. At least two conorms p_{ij} should be positive, otherwise one vonorm vanishes, but there are no other restrictions on values of conorms. The vonorms $v_0^2, v_1^2, v_2^2 > 0$ should satisfy three triangle inequalities such as $v_0^2 \leq v_1^2 + v_2^2$, only one of them can be an equality.

Lemma 5.4. All obtuse superbases of any lattice $\Lambda \subset \mathbb{R}^2$ are isometric. Hence VF(Λ), CF(Λ), RF(Λ) are independent of a superbase (well-defined up to isomorphism). ■

Proof. By Lemma 4.5 for $n = 2$, if a lattice Λ has a strict obtuse superbase v_0, v_1, v_2, then the Voronoi vectors of Λ are the three pairs of symmetric partial sums $\pm v_0, \pm v_1, \pm v_2$. Hence the superbase is uniquely determined by the strict Voronoi vectors up to a sign. So Λ has symmetric obtuse superbases $\{v_0, v_1, v_2\}$ and $\{-v_0, -v_1, -v_2\}$, see Fig. 2.

If a superbase of Λ is non-strict, one conorm vanishes, say $p_{12} = 0$. Then v_1, v_2 span a rectangular cell and Λ has four non-strict Voronoi vectors $\pm v_1 \pm v_2$ with all combinations of signs. Hence Λ has four obtuse superbases $\{v_1, v_2, -v_1 - v_2\}$, $\{-v_1, v_2, v_1 - v_2\}$, $\{v_1, -v_2, v_2 - v_1\}$, $\{-v_1, -v_2, v_1 + v_2\}$, which are related by reflections, see Fig. 2.

Any (even) permutation of vectors v_0, v_1, v_2 induces an (orientation-preserving) isomorphism of voforms and coforms and keeps the root form invariant. Lemma 5.3 implies that $\mathrm{VF}(\Lambda)$, $\mathrm{CF}(\Lambda)$, $\mathrm{RF}(\Lambda)$ do not depend on an obtuse superbase B of Λ. $\square$

6. The simpler space of obtuse superbases up to isometry in dimension 2

Definition 6.1 (space OSI of obtuse superbases up to isometry)**.** Let $B = \{v_0, v_1, v_2\}$ and $B' = \{u_0, u_1, u_2\}$ be any obtuse superbases in $\mathbb{R}^2$. The maximum Euclidean length of vector differences $L_\infty(B, B') = \min\limits_{R \in \mathrm{O}(\mathbb{R}^2)} \max\limits_{i=0,1,2} |R(u_i) - v_i|$ is minimised over all orthogonal maps from the compact group $\mathrm{O}(\mathbb{R}^2)$. Let OSI denote the space of all *obtuse superbases up to isometry*, which we endow by the metric L_∞. For orientation-preserving isometries, we similarly introduce the space OSI^+ with the metric L_∞^+ defined by minimising the distances over all rotations around the origin 0 in $\mathbb{R}^2$. ■

Theorem 6.2 substantially reduces the representation ambiguity for the lattice isometry space by the 1-1 map LISP $\to$ OSI. Indeed, any fixed lattice $\Lambda \subset \mathbb{R}^2$ has infinitely many (super)bases but only a few obtuse superbases, maximum four as shown in Fig. 2.

Theorem 6.2 (lattices up to isometry $\leftrightarrow$ obtuse superbases up to isometry)**.** Lattices in $\mathbb{R}^2$ are isometric if and only if any of their obtuse superbases are isometric. ■

Proof. Part *only if* ($\Rightarrow$): any isometry f between lattices Λ, Λ' maps any obtuse superbase B of Λ to the obtuse superbase $f(B)$ of Λ', which should be isometric to any other obtuse superbase of Λ' by Lemma 5.4. Part *if* ($\Leftarrow$): any isometry between obtuse superbases of Λ, Λ' linearly extends to an isometry between the lattices Λ, Λ'. $\square$

Definition 6.3 (sign of a lattice)**.** A lattice $\Lambda \subset \mathbb{R}^2$ is called *neutral* (or *achiral*) if two of its three vonorms are equal, so Λ maps to itself under a mirror reflection: if $v_1^2 = v_2^2$, then map $v_1 \leftrightarrow v_2$, $v_0 \mapsto v_0$. A non-neutral lattice Λ is called *positive* if its root form $\mathrm{RF}(\Lambda)$ has its root products in increasing order starting from the smallest. If the last two root products are not in increasing order, then Λ is called *negative*. ■

Example 6.4. (a) The square lattice $S \subset \mathbb{R}^2$ with side length a has four obtuse superbases in Fig. 2, for example $v_1 = (a, 0)$, $v_2 = (0, a)$, $v_0 = (-a, -a)$ and $u_1 = (a, a)$, $u_2 = (0, -a)$, $u_0 = (-a, 0)$. These superbases have the vonorms $v_0^2 = 2a^2$, $v_1^2 = a^2$, $v_2^2 = a^2$ and ${u_0}^2 = a^2$, ${u_1}^2 = 2a^2$, ${u_2}^2 = a^2$. The conorms are $p_{12} = 0$, $p_{01} = a^2 = p_{02}$ and $q_{12} = a^2 = q_{01}$, $q_{02} = 0$. Both superbases have the same root form $\mathrm{RF}(S) = (0, a, a)$ of ordered root products, because the coforms $(0, a^2, a^2)$ and $(a^2, a^2, 0)$ are isomorphic by a cyclic permutation, so any square lattice S is neutral.

(b) The hexagonal lattice $H \subset \mathbb{R}^2$ with side length a has two obtuse superbases in Fig. 2, which are symmetric with respect to the origin: $v_1 = (a, 0) = -u_1$, $v_2 = (-\frac{a}{2}, \frac{\sqrt{3}}{2}a) = -u_2$, $v_0 = (-\frac{a}{2}, -\frac{\sqrt{3}}{2}a) = -u_0$. These superbases have the same vonorms $v_i^2 = a^2 = u_i^2$ and the same conorms $p_{jk} = \frac{a^2}{2} = q_{jk}$ for any $i, j \neq k$. Both superbases have the same root form $\mathrm{RF}(H) = (\frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}})$, so any hexagonal lattice is neutral.

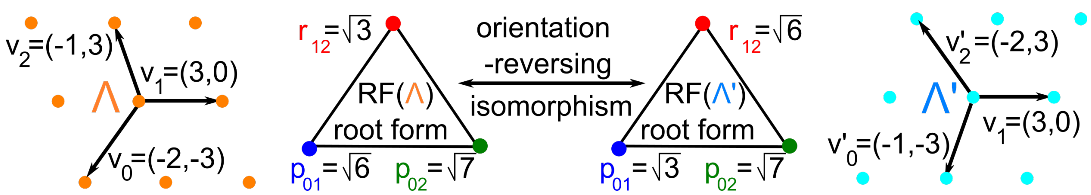

Fig. 4. Root forms of the lattices Λ, Λ', which differ by a reflection in Example 6.4(c).

(c) At first sight the lattice Λ with basis $v_1 = (3, 0)$, $v_2 = (-1, 3)$ looks non-isometric to the lattice Λ' with basis $v_1, v_2' = (-2, 3)$. However, they have extra superbase vectors $v_0 = (-2, -3)$, $v_0' = (-1, -3)$ leading to the coforms $\mathrm{CF}(\Lambda) = (3, 6, 7)$ and $\mathrm{CF}(\Lambda') = (6, 3, 7)$ written as (p_{12}, p_{01}, p_{02}). Up to isomorphism, we can shift 3 to the first place, so $\mathrm{CF}(\Lambda) \sim \mathrm{CF}(\Lambda')$ and $\mathrm{RF}^+(\Lambda) = (\sqrt{3}, \sqrt{6}, \sqrt{7}) = \mathrm{RF}^+(\Lambda')$. If we aim to preserve orientation, the orientation-preserving root forms are $\mathrm{RF}^+(\Lambda) = (\sqrt{3}, \sqrt{6}, \sqrt{7})$ and

$\mathrm{RF}^+(\Lambda') = (\sqrt{3}, \sqrt{7}, \sqrt{6})$, which differ up to orientation-preserving isomorphism. The lattices Λ, Λ' are related by the mirror reflection $x \leftrightarrow -x$, see Fig. 4. By Definition 6.3 the lattice Λ is positive, while its mirror image Λ' is negative. ■

7. Unique root forms classify all lattices up to isometry in dimension 2

Lemma 7.1 (superbase reconstruction)**.** For any lattice $\Lambda \subset \mathbb{R}^2$, an obtuse superbase B of Λ can be reconstructed up to isometry from $\mathrm{VF}(\Lambda)$ or $\mathrm{CF}(\Lambda)$ or $\mathrm{RF}(\Lambda)$. ■

Proof. Since $\mathrm{VF}(\Lambda), \mathrm{CF}(\Lambda), \mathrm{RF}(\Lambda)$ are expressible via each other by Lemma 5.2, it suffices to consider $\mathrm{VF}(\Lambda)$. Choosing any two vonorms from $\mathrm{VF}(\Lambda) = (v_0^2, v_1^2, v_2^2)$, say v_1^2, v_2^2, we can find the lengths $|v_1|, |v_2|$ and the angle $\alpha = \arccos \dfrac{v_1 \cdot v_2}{|v_1| \cdot |v_2|} \in [0, \pi)$ between the basis vectors v_1, v_2 from $v_1 \cdot v_2 = -p_{12} = \dfrac{1}{2}(v_0^2 - v_1^2 - v_2^2)$. Hence an obtuse superbase (v_0, v_1, v_2) of Λ is reconstructed and will be unique up to isometry by Lemma 5.4. If a cyclic order of vonorms is fixed, say v_0^2 goes after the ordered pair v_1^2, v_2^2, we draw the angle α from v_1 to v_2 counterclockwise, otherwise clockwise. □

Theorem 7.2 (isometry classification: 2D lattices $\leftrightarrow$ root forms)**.** Lattices $\Lambda, \Lambda' \subset \mathbb{R}^2$ are isometric if and only if their root forms coincide: $\mathrm{RF}(\Lambda) = \mathrm{RF}(\Lambda')$ or, equivalently, their coforms and voforms are isomorphic: $\mathrm{CF}(\Lambda) \sim \mathrm{CF}(\Lambda')$, $\mathrm{VF}(\Lambda) \sim \mathrm{VF}(\Lambda')$. The existence of orientation-preserving isometry is equivalent to $\mathrm{RF}^+(\Lambda) = \mathrm{RF}^+(\Lambda')$. ■

Proof. The part *only if* ($\Rightarrow$) means that any isometric lattices Λ, Λ' have $\mathrm{RF}(\Lambda) = \mathrm{RF}(\Lambda')$. Lemma 5.3 implies that the root form $\mathrm{RF}(B)$ of an obtuse superbase B is invariant under isometry. Theorem 5.4 implies $\mathrm{RF}(\Lambda)$ is independent of B.

The part *if* ($\Leftarrow$) follows from Lemma 7.1 by reconstructing a superbase of Λ. □

Though both vonorms and conorms are complete continuous invariants, we use the unique root form RF based on conorms, because formulae (5.1a) are easier than (5.1b).

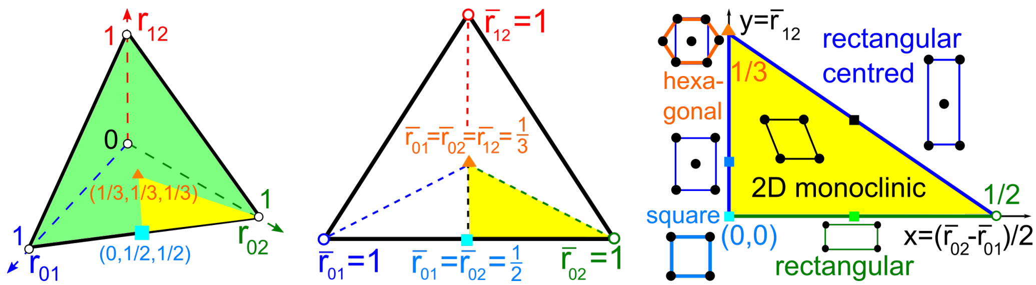

Fig. 5. **Left**: the *octant* $\mathrm{Oct} = \{(r_{12}, r_{01}, r_{02}) \in \mathbb{R}^3 \mid \text{ all } r_{ij} \geq 0, \text{ only one can be } 0\}$. **Middle**: under the scaling (projection from the origin) $r_{ij} \mapsto \bar{r}_{ij} = r_{ij}(r_{12} + r_{01} + r_{02})^{-1}$, the octant Oct projects to the *full triangle* $\mathrm{FT} = \mathrm{Oct} \cap \{r_{12} + r_{01} + r_{02} = 1\}$. **Right**: the quotient triangle $\mathrm{QT} = \mathrm{FT}/S_3$ consists of ordered triples $\bar{r}_{12} \leq \bar{r}_{01} \leq \bar{r}_{02}$ and can be parameterised by $x = \frac{1}{2}(\bar{r}_{02} - \bar{r}_{01}) \in [0, \frac{1}{2}]$ and $y = \bar{r}_{12} \in [0, \frac{1}{3}]$.

Definition 7.3 (full triangle FT and quotient triangle QT)**.** All isometry classes of lattices $\Lambda \subset \mathbb{R}^2$ with root forms $\mathrm{RF}(\Lambda) = (r_{12}, r_{01}, r_{02})$ are in a 1-1 correspondence with all ordered triples $r_{12} \leq r_{01} \leq r_{02}$. If we allow any permutations (all isomorphisms of coforms), these triples fill the octant $\mathrm{Oct} = [0, +\infty)^3$ excluding the axes. Project any point $(r_{12}, r_{01}, r_{02}) \in \mathrm{Oct}$ from the origin $(0, 0, 0)$ to a point in the plane $r_{12}+r_{01}+r_{02} = 1$ using the scaling factor $(r_{12} + r_{01} + r_{02})^{-1}$. The image of Oct is the *full triangle* $\mathrm{FT} = \mathrm{Oct} \cap \{r_{12} + r_{01} + r_{02} = 1, r_{ij} \geq 0\}$ without the three vertices. The scaled products $\bar{r}_{ij} = r_{ij}(r_{12} + r_{01} + r_{02})^{-1}$ are barycentric coordinates on FT. Take the quotient of FT by the permutation group S_3 to get the smaller *quotient triangle* QT with the extra conditions $\bar{r}_{12} \leq \bar{r}_{01} \leq \bar{r}_{02}$ (as in the root form RF). Then QT is parameterised by $x = \frac{1}{2}(\bar{r}_{02} - \bar{r}_{01}) \in [0, \frac{1}{2}]$ and $y = \bar{r}_{12} \in [0, \frac{1}{3}]$. A mirror image of a lattice Λ considered up to rigid motion (orientation-preserving isometry) is represented by the point $(-x, y)$ in the reflection of FT by $x \mapsto -x$, so FT/A_3 is the quotient of the full triangle FT by rotations through $\pm\frac{2\pi}{3}$ around the centre $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. ■

Example 7.4 (Bravais lattices)**. (a)** Any square lattice S with a side length a in Fig. 3 has the root form $(0, a, a)$ projected to $(0, \frac{1}{2}, \frac{1}{2})$ in the full triangle FT and represented by $(0, 0)$ in the quotient triangle QT. Any hexagonal lattice H has the root form $(\frac{a^2}{2}, \frac{a^2}{2}, \frac{a^2}{2})$ projected to $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) \in \text{FT}$ and represented by $(0, \frac{1}{3}) \in \text{QT}$.

(b) The vertical side of the quotient triangle has $x = 0$, $y \in [0, \frac{1}{3}]$ and represents all lattices with $r_{12} \leq r_{01} = r_{02}$. Choosing $v_0 = (a, 0)$, we get $v_1 = (-\frac{a}{2}, b)$, $v_2 = (-\frac{a}{2}, -b)$ with $0 \leq p_{12} = b^2 - \frac{a^2}{4} \leq p_{01} = \frac{a^2}{2}$, so $\frac{a}{2} \leq b \leq a\frac{\sqrt{3}}{2}$. In the lower case $b = \frac{a}{2}$, the point $(x, y) = (0, 0)$ represents all square lattices with $p_{12} = 0$. In the upper case $b = a\frac{\sqrt{3}}{2}$, the point $(x, y) = (0, \frac{1}{3})$ represents all hexagonal lattices with $p_{12} = p_{01} = p_{02}$. The vertical side of the quotient triangle QT represents lattices whose centred rectangular cells have a short side $2a$ and a longer side $2b$ within the interval $(a, a\sqrt{3})$.

(c) The hypotenuse of QT has $p_{12} = p_{01} \leq p_{02}$ and represents lattices whose centred rectangular cells have a short side $2a$ and a longer side $2b \geq a\sqrt{3}$. Indeed, for the superbase $v_1 = (a, 0)$, $v_2 = (-\frac{a}{2}, b)$, $v_0 = (-\frac{a}{2}, -b)$, we get $p_{01} = \frac{a^2}{2} \leq p_{02} = b^2 - \frac{a^2}{4}$, so $b \geq a\frac{\sqrt{3}}{2}$. The vertex of QT at $(0, 5, 0)$ represents the limit case $b \to +\infty$.

(d) The horizontal side of QT has $p_{12} = 0$, $p_{01} \leq p_{02}$ and represents all lattices with rectangular cells with sides $a \leq b$. We approach the vertex $(0.5, 0)$ as $b \to +\infty$. ■

8. Easily computable continuous metrics on root forms in dimension 2

Definition 8.1 (space RFL with root metrics $\text{RM}_d(\Lambda, \Lambda')$)**.** Let S_3 be the group of all six permutations of three conorms of a lattice $\Lambda \subset \mathbb{R}^2$, A_3 be its subgroup of three even permutations. For any metric d on $\mathbb{R}^3$, the *root metric* is $\text{RM}_d(\Lambda, \Lambda') = \min\limits_{\sigma \in S_3} d(\text{RF}(\Lambda), \sigma(\text{RF}(\Lambda')))$, where a permutation σ applies to $\text{RF}(\Lambda')$ as a vector in $\mathbb{R}^3$. The *orientation-preserving* root metric $\text{RM}_d^+(\Lambda, \Lambda') = \min\limits_{\sigma \in A_3} d(\text{RF}(\Lambda), \sigma(\text{RF}(\Lambda')))$ is minimised over even permutations. If we use the Minkowski L_q-norm $||v||_q = (\sum\limits_{i=1}^{n} |x_i|^q)^{1/q}$ of a vector $v = (x_1, \ldots, x_n) \in \mathbb{R}^n$ for any real parameter $q \in [1, +\infty]$, the root metric is denoted by $\text{RM}_q(\Lambda, \Lambda')$. The limit case $q = +\infty$ means that $||v||_{+\infty} = \max\limits_{i=1,\ldots,n} |x_i|$. Let RFL denote the space of *Root Forms of Lattices* $\Lambda \subset \mathbb{R}^2$, where we can use any of the above metrics satisfying all necessary axioms by Lemma 8.3. ■

The quotient triangle QT from the last picture in Fig. 5 appeared in Zhilinskii (2016, Fig. 8.1) as a fundamental domain of the action of $\mathrm{GL}_2(\mathbb{Z})$ on the cone of positive quadratic forms, but no metric was considered on this domain. The key novel concept is the root metric RM_d, which is minimised over permutations of root products and differs from a standard distance on the positive octant or the quotient triangle QT.

Example 8.2. **(a)** The lattices Λ, Λ' from Example 6.4(c) with root forms $\mathrm{RF}(\Lambda) = (\sqrt{3}, \sqrt{6}, \sqrt{7})$ and $\mathrm{RF}(\Lambda') = (\sqrt{3}, \sqrt{7}, \sqrt{6})$ differ by a reflection, so $\mathrm{RM}_d(\Lambda, \Lambda') = 0$ for any metric d on $\mathbb{R}^3$, but the orientation-preserving metric gives $\mathrm{RM}_q^+(\Lambda, \Lambda') = 2^{1/q}(\sqrt{7} - \sqrt{6})$ for $q \in [1, +\infty)$ and $\mathrm{RM}_{+\infty}^+(\Lambda, \Lambda') = \sqrt{7} - \sqrt{6}$ for the L_q-norm.

(b) The square lattice S with $\mathrm{RF}(S) = (0, \frac{1}{2}, \frac{1}{2})$ is represented by the right-angled vertex $(x, y) = (0, 0) \in$ QT. The centred rectangular lattice Λ with $\mathrm{RF}(\Lambda) = (\frac{1}{6}, \frac{1}{6}, \frac{2}{3})$ is represented by the mid-point $(x, y) = (\frac{1}{4}, \frac{1}{6})$ in the hypotenuse of QT. The root metric between these lattices is $\mathrm{RM}_q(S, \Lambda) = (2(\frac{1}{6})^q + (\frac{1}{3})^q)^{1/q}$, while the Minkowski metric between the points $(0, 0)$ and $(\frac{1}{2}, \frac{1}{6})$ in QT is $L_q = ((\frac{1}{4})^q + (\frac{1}{6})^q)^{1/q}$. ■

Lemma 8.3 (metric axioms for RM_d)**.** For any metric d on $\mathbb{R}^3$, the root metrics RM_d, RM_d^+ from Definition 8.1 satisfy the metric axioms in Problem 1.1c. ■

Proof. We prove the metric axioms for RM_d, the orientation-preserving case is similar. The first axiom requires that $\mathrm{RM}_d(\Lambda, \Lambda') = 0$ if and only if Λ, Λ' are isometric. By Definition 8.1 the equality $\mathrm{RM}_d(\Lambda, \Lambda') = 0$ means that there is a permutation $\sigma \in S_3$ such that $d(\mathrm{RF}(\Lambda), \sigma(\mathrm{RF}(\Lambda'))) = 0$, equivalently $\mathrm{RF}(\Lambda) = \sigma(\mathrm{RF}(\Lambda'))$ since the metric d on $\mathbb{R}^3$ satisfies the first axiom. The last equality implies that $\mathrm{RF}(\Lambda) = \mathrm{RF}(\Lambda')$, because any root form is an ordered triple. Then Λ, Λ' are isometric by Theorem 7.2.

Since d is symmetric, the symmetry follows by taking the inverse permutation:

$$\mathrm{RM}_d(\Lambda, \Lambda') = \min_{\sigma \in S_3} d(\mathrm{RF}(\Lambda), \sigma(\mathrm{RF}(\Lambda'))) = \min_{\sigma^{-1} \in S_3} d(\sigma^{-1}(\mathrm{RF}(\Lambda)), \mathrm{RF}(\Lambda')) = \mathrm{RM}_d(\Lambda', \Lambda).$$

To prove the triangle inequality, let permutations $\sigma, \tau \in S_3$ minimise the distances: $\mathrm{RM}_d(\Lambda, \Lambda') = d(\mathrm{RF}(\Lambda), \sigma(\mathrm{RF}(\Lambda')))$ and $\mathrm{RM}_d(\Lambda', \Lambda'') = d(\mathrm{RF}(\Lambda'), \tau(\mathrm{RF}(\Lambda'')))$. The triangle inequality for the auxiliary metric d implies that

$$d(\mathrm{RF}(\Lambda), \tau \circ \sigma(\mathrm{RF}(\Lambda''))) \leq d(\mathrm{RF}(\Lambda), \sigma(\mathrm{RF}(\Lambda'))) + d(\sigma(\mathrm{RF}(\Lambda')), \tau \circ \sigma(\mathrm{RF}(\Lambda''))).$$

In the final term the common permutation σ can be dropped, because σ identically permutes both root forms $\mathrm{RF}(\Lambda')$ and $\mathrm{RF}(\Lambda'')$. Hence $d(\mathrm{RF}(\Lambda), \tau \circ \sigma(\mathrm{RF}(\Lambda''))) \leq \mathrm{RM}_d(\Lambda, \Lambda') + \mathrm{RM}_d(\Lambda', \Lambda'')$. The left hand side contains one permutation $\tau \circ \sigma \in S_3$ and can only become smaller after minimising over all permutations from S_3. So the triangle inequality is proved: $\mathrm{RM}_d(\Lambda, \Lambda'') \leq \mathrm{RM}_d(\Lambda, \Lambda') + \mathrm{RM}_d(\Lambda', \Lambda'')$. □

Lemma 8.4 (continuity of products)**.** Let vectors $u_1, u_2, v_1, v_2 \in \mathbb{R}^n$ have a maximum Euclidean length l, scalar products $u_1 \cdot u_2, v_1 \cdot v_2 \leq 0$ and be δ-close in terms of Euclidean distance: $|u_i - v_i| \leq \delta$, $i = 1, 2$. Then $|\sqrt{-u_1 \cdot u_2} - \sqrt{-v_1 \cdot v_2}| \leq \sqrt{2l\delta}$. ■

Proof. If $\sqrt{-u_1 \cdot u_2} + \sqrt{-v_1 \cdot v_2} \leq \sqrt{2l\delta}$, the difference of square roots is at most $\sqrt{2l\delta}$ as required. Assuming that $\sqrt{-u_1 \cdot u_2} + \sqrt{-v_1 \cdot v_2} \geq \sqrt{2l\delta}$, it suffices to estimate the difference $|u_1 \cdot u_2 - v_1 \cdot v_2| = |\sqrt{-u_1 \cdot u_2} - \sqrt{-v_1 \cdot v_2}|(\sqrt{-u_1 \cdot u_2} + \sqrt{-v_1 \cdot v_2}) \leq 2l\delta$.

We estimate the scalar product $|u \cdot v| \leq |u| \cdot |v|$ by using Euclidean lengths. Then we apply the triangle inequality for scalars and replace vector lengths by l as follows: $|u_1 \cdot u_2 - v_1 \cdot v_2| = |(u_1 - v_1) \cdot u_2 + v_1 \cdot (u_2 - v_2)| \leq |(u_1 - v_1) \cdot u_2| + |v_1 \cdot (u_2 - v_2)| \leq$ $\leq |u_1 - v_1| \cdot |u_2| + |v_1| \cdot |u_2 - v_2| \leq \delta(|u_2| + |v_1|) \leq 2l\delta$ as required. □

Theorems 8.5 and 8.6 show that the 1-1 map OSI $\leftrightarrow$ LISP $\leftrightarrow$ RFL established by Theorems 6.2 and 7.2 is continuous in both directions.

Theorem 8.5 (continuity of OSI $\to$ RFL)**.** Let lattices $\Lambda, \Lambda' \subset \mathbb{R}^2$ have obtuse superbases $B = (v_0, v_1, v_2)$, $B' = (u_0, u_1, u_2)$ whose vectors have a maximum length l and $|u_i - v_i| \leq \delta$ for some $\delta > 0$, $i = 0, 1, 2$. Then $\mathrm{RM}_q(\mathrm{RF}(\Lambda), \mathrm{RF}(\Lambda')) \leq 3^{1/q}\sqrt{2l\delta}$ for any $q \in [1, +\infty]$, where $3^{1/q}$ is interpreted for $q = +\infty$ as $\lim\limits_{q \to +\infty} 3^{1/q} = 1$. The same upper bound holds for the orientation-preserving metric RM_q^+. ■

Proof. Lemma 8.4 implies that the root products $r_{ij} = \sqrt{-v_i \cdot v_j}$ and $\sqrt{-u_i \cdot u_j}$ of the superbases B, B' differ by at most $2l\delta$ for any pair (i, j) of indices. Then the L_q-norm of the vector difference in $\mathbb{R}^3$ is $\mathrm{RM}_q(\mathrm{RF}(\Lambda), \mathrm{RF}(\Lambda')) \le 3^{1/q}\sqrt{2l\delta}$ for any $q \in [1, +\infty]$. By Definition 8.1, the root metric RM_q is minimised over permutations of S_3 (or A_3 for the orientation-preserving metric RM_q^+), so the upper bound still holds. □

Theorem 8.5 is proved for the L_q norm only to give the explicit upper bound for RM_q. A similar argument proves continuity for RM_d with any metric d on $\mathbb{R}^3$ satisfying $d(u, v) \to 0$ when $u \to v$ coordinate-wise. Theorem 8.6 is stated for the maximum norm with $q = +\infty$ only for simplicity, because all Minkowski norms in $\mathbb{R}^n$ are topologically equivalent due to $||v||_q \le ||v||_r \le n^{\frac{1}{q} - \frac{1}{r}} ||v||_q$ for any $1 \le q \le r$ (nor, 2021).

Theorem 8.6 (continuity of RFL → OSI)**.** Let lattices $\Lambda, \Lambda' \subset \mathbb{R}^2$ have δ-close root forms, so $\mathrm{RM}_\infty(\mathrm{RF}(\Lambda), \mathrm{RF}(\Lambda')) \le \delta$. Then Λ, Λ' have obtuse superbases B, B' that are close in the L_∞ metric on the space OSI so that $L_\infty(B, B') \to 0$ as $\delta \to 0$. The same conclusion holds for the orientation-preserving metrics RM_∞^+ and L_∞^+. ■

Proof. Superbases $B = (v_0, v_1, v_2), B' = (u_0, u_1, u_2)$ can be reconstructed from the root forms $\mathrm{RF}(\Lambda), \mathrm{RF}(\Lambda')$ by Lemma 7.1. By applying a suitable isometry of $\mathbb{R}^2$, one can assume that Λ, Λ' share the origin and the first vectors v_0, u_0 lie in the positive horizontal axis. Let r_{ij}, s_{ij} be the root products of B, B' respectively. Formulae (5.1a) imply that $v_i^2 = r_{ij}^2 + r_{ik}^2$ and $u_i^2 = s_{ij}^2 + s_{ik}^2$ for distinct indices $i, j, k \in \{0, 1, 2\}$, for example if $i = 0$ then $j = 1$, $k = 2$. For any continuous transformation from $\mathrm{RF}(\Lambda)$ to $\mathrm{RF}(\Lambda')$, all root products have a finite upper bound M, which is used below:

$$|v_i^2 - u_i^2| = |(r_{ij}^2 + r_{ik}^2) - (s_{ij}^2 + s_{ik}^2)| \le |r_{ij}^2 - s_{ij}^2| + |r_{ik}^2 - s_{ik}^2| \le$$

$$(r_{ij} + s_{ij})|r_{ij} - s_{ij}| + (r_{ik} + s_{ik})|r_{ik} - s_{ik}| \le (r_{ij} + s_{ij})\delta + (r_{ik} + s_{ik})\delta \le 4M\delta.$$

Since at least two continuously changing conorms should be strictly positive to guarantee positive lengths of basis vectors by formula (5.1a), there is a minimum length $a > 0$ of all basis vectors during a transformation $\Lambda' \to \Lambda$. Then $||v_i| - |u_i|| \leq \dfrac{4M\delta}{|v_i| + |u_i|} \leq \dfrac{2M}{a}\delta$. Since the first basis vectors v_0, u_0 lie in the positive horizontal axis, the lengths can be replaced by vectors: $|v_0 - u_0| \leq \dfrac{2M}{a}\delta$, so $|v_0 - u_0| \to 0$ as $\delta \to 0$.

For other indices $i = 1, 2$, the basis vectors v_i, u_i can have a non-zero angle equal to the difference $\alpha_i - \beta_i$ of the angles from the positive horizontal axis to v_i, u_i, respectively. These angles are expressed via the root products as follows:

$$\alpha_i = \arccos \frac{v_0 \cdot v_i}{|v_0| \cdot |v_i|} = \arccos \frac{-r_{0i}^2}{\sqrt{r_{01}^2 + r_{02}^2}\sqrt{r_{ij}^2 + r_{ik}^2}},$$

$$\beta_i = \arccos \frac{u_0 \cdot u_i}{|u_0| \cdot |u_i|} = \arccos \frac{-s_{0i}^2}{\sqrt{s_{01}^2 + s_{02}^2}\sqrt{s_{ij}^2 + s_{ik}^2}},$$

where $j \neq k$ differ from $i = 1, 2$. If $\delta \to 0$, then $s_{ij} \to r_{ij}$ and $\alpha_i - \beta_i \to 0$ for all indices, because all the above functions are continuous for $|u_j|, |v_j| \geq a$, $j = 0, 1, 2$.

Then we estimate the squared length of the difference by using the scalar product:

$$|v_i - u_i|^2 = v_i^2 + u_i^2 - 2u_i v_i = (|v_i|^2 - 2|u_i| \cdot |v_i| + |u_i|^2) + 2|u_i| \cdot |v_i| - 2|u_i| \cdot |v_i| \cos(\alpha_i - \beta_i) =$$

$$= (|v_i| - |u_i|)^2 + 2|u_i| \cdot |v_i|(1 - \cos(\alpha_i - \beta_i)) = (|v_i| - |u_i|)^2 + |u_i| \cdot |v_i| 4 \sin^2 \frac{\alpha_i - \beta_i}{2} \leq$$

$$\leq (|v_i| - |u_i|)^2 + |u_i| \cdot |v_i| 4 \left(\frac{\alpha_i - \beta_i}{2}\right)^2 = (|v_i| - |u_i|)^2 + |u_i| \cdot |v_i|(\alpha_i - \beta_i)^2,$$

where we have used that $|\sin x| \leq |x|$ for any real x. The upper bound M of all root products guarantees a fixed upper bound for lengths $|u_i|, |v_i|$. If $\delta \to 0$, then $|v_i| - |u_i| \to 0$ and $\alpha_i - \beta_i \to 0$ as proved above, so $v_i - u_i \to 0$ and $L_\infty(B, B') \to 0$. □

9. Large families of 2D lattices from the Cambridge Structural Database

The Cambridge Structural Database (CSD) has about 145K crystals whose lattices are primitive orthorhombic. By orthogonally projecting such a lattice to $\mathbb{R}^2$ along their longest sides, we get a rectangular lattice with root products $r_{12} = 0$ and $r_{01} \leq r_{02}$.

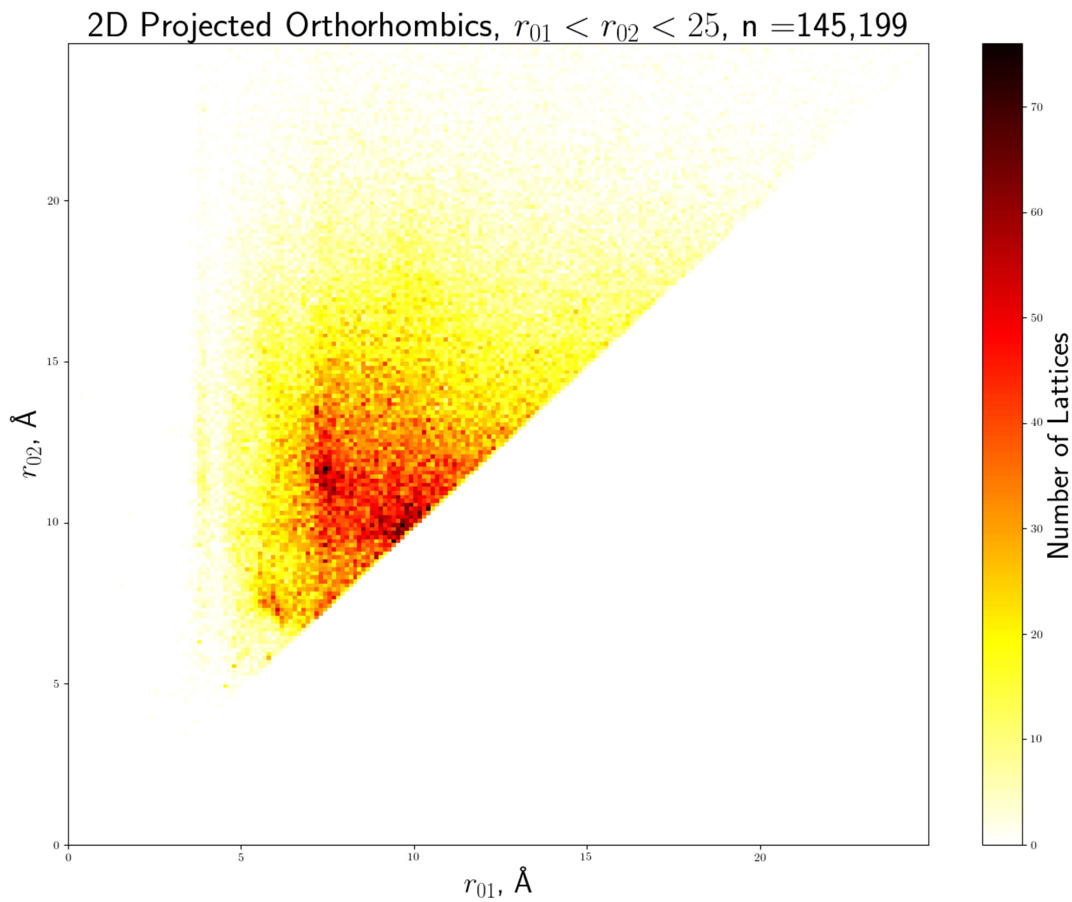

Fig. 6. Density plot of rectangular 2D lattices extracted from primitive orthorhombic crystals in the CSD and represented by the two non-zero root products $r_{01} \leq r_{02}$.

To represent such a large number of known lattices, we subdivide the triangle $\{0 < r_{01} \leq r_{02} < 25\mathring{A}\}$) into a 200×200 grid and count lattices whose root products (r_{01}, r_{02}) fall into each pixel. These counts (from 0 to 75) are represented the colour bar on the right hand side of Fig. 6. The resulting plot shows a high density cluster close to the diagonal, where the projected lattice is nearly square, and also another less expected cluster with root products $r_{01}, r_{02} \approx (7, 12)\mathring{A}$. To make these clusters more visible, we removed about 1% of outliers with large root products $r_{02} > 25\mathring{A}$.

Any monoclinic 3D lattice can be orthogonally projected to a generic 2D lattice. The CSD contains about 374K monoclinic lattices, whose projected 2D lattices have generic root forms $r_{12} \le r_{01} \le r_{02}$. Any such a triple is projected to the quotient triangle QT from Definition 7.3. The projection of a triple has the coordinates $x = \frac{1}{2}(\bar{r}_{02} - \bar{r}_{01})$ and $y = \bar{r}_{12}$, which becomes unitless after scaling by $r_{12} + r_{02} + r_{01}$.

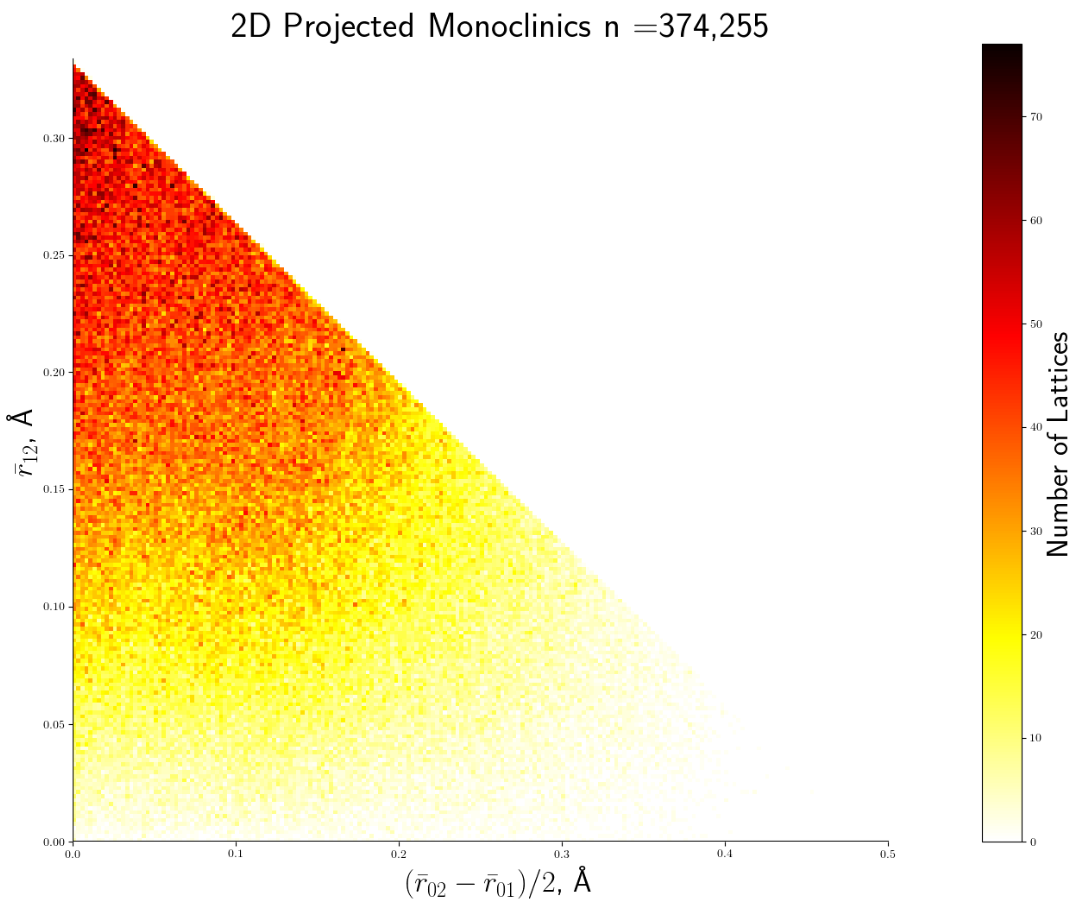

Fig. 7. Density plot of all monoclinic 2D lattices extracted from primitive monoclinic crystals in the CSD and represented in the quotient triangle QT.

The density plot in Fig. 7 shows that projected monoclinic lattices fill the quotient triangle QT almost completely with white spots only for small $\bar{r}_{12} < 0.01$ and near the vertex $(x, y) = (\frac{1}{2}, 0)$ representing infinitely long cells. The high density pixels are close to (but not exactly at) the vertex $(0, \frac{1}{3})$ representing hexagonal lattices.

10. Main conclusions and motivations for a continuous crystallography

This paper finally resolves Metric Problem 1.1 for 2D lattices, whose continuity and computability conditions remained unfulfilled despite years of persistent attempts. The follow-up paper will extend the presented tools to 3D lattices whose space will be bijectively and bi-continuously parameterised by root forms of six root products.

The density plot in Fig. 7 shows that all reasonable primitive monoclinic 2D lattices appear in known crystals from the CSD. In other words, real crystal lattices fill a continuous space, which should be studied by continuous invariants and metrics that only slightly change under small perturbations, such as the thermal vibrations of atoms. Using a geographic analogue, the proposed solution to Problem 1.1 creates a complete and continuous map for efficient navigation on the space of all 2D lattices.

Using a biological analogue, classical crystallography has taken a similar approach to the classical taxonomists, dividing lattices into an increasingly complex sequence of discrete categories based on symmetries as they divided organisms according to observed physical characteristics. Continuous crystallography allows us to use the fundamental geometric properties of the lattice itself to completely classify an individual in as granular a manner as we like, in a manner akin to the modern use of genetic sequences and markers to classify organisms. Indeed, since the proposed root form of a lattice is a complete isometry invariant, this invariant could be said to represent the DNA of a lattice. In addition, any lattice can be explicitly built up from this DNA.

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Synopsis
