# Welcome to a continuous world of 3-dimensional lattices

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## Abstract

A periodic 3-dimensional lattice is an infinite set of all integer linear combinations of three basis vectors in Euclidean 3-space. Any basis extends to a superbase by adding the fourth vector such that the sum of all four vectors is zero. Any lattice has an obtuse superbase whose all pairwise angles are non-acute. The recent classification of 3-dimensional lattices constructed a complete invariant consisting of up to six square roots of scalar products of four superbase vectors. The interior of the resulting 6-dimensional Lattice Isometry Space consists of all triclinic lattices. We describe the low dimensional strata representing all other Bravais classes of lattices. In each case we visualise hundreds of thousands of real crystal lattices from the Cambridge Structural Database for the first time.

## 1. Motivations, metric problem and overview of past and new results

This paper complements the recent classification of 3-dimensiobnal lattices up to isometry in the previous paper (**?**) written for mathematicians and computer scientists.

This paper for crystallographers demonstrates continuity of the Lattice Isometry Space by mapping all real crystal lattices from the Cambridge Structural Database (CSD).

Isometry is the fundamental equivalence of lattices due to rigidity of most crystals. The resulting Lattice Isometry Space (LIS) consists of infinitely many classes, where every class includes all lattices isometric to each other. Then any transition between lattices is a continuous path in the LIS. A past approach to uniquely represent any isometry class was to choose a reduced basis (Niggli's reduced cell). Any such reduction is discontinuous under perturbations, see Widdowson *et al.* (2022, Theorem 15).

## 2. Basic definitions and a review of past work on lattice classifications

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 $p$ can be drawn at any initial point. The *Euclidean* distance between points $p, q \in \mathbb{R}^n$ is $|p - q|$.

**Definition 2.1** (a lattice $\Lambda$, 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* $\Lambda$ 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 $\Lambda$. ■

**Definition 2.2** (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 $p_{ij} > 0$. ■

The indices of a conorm $p_{ij}$ are distinct and unordered, so we assume that $p_{ij} = p_{ji}$. 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.

**Theorem 2.3** (obtuse superbase existence)**.** Any lattice $\Lambda$ 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 $i \neq j$. ■

## 3. Root forms and root invariants of 3-dimensional lattices

Kurlin (2022, Lemmas 4.1-4.5) explicitly described all obtuse superbases for each of five Voronoi types of lattices. Since any obtuse superbase $B$ has only non-negative conorms, the *root products* $r_{ij} = \sqrt{p_{ij}}$ are well-defined for all distinct indices $i, j \in \{0, 1, 2, 3\}$ and have the same units as original coordinates of basis vectors, for example Angstroms: $1\mathring{A} = 10^{-10}$m. Any $r_{ij} = \sqrt{-v_i \cdot v_j}$ measures non-orthogonality of vectors $v_i, v_j$.

**Definition 3.1** (root matrices and index-permutations)**.** For any ordered obtuse superbase $B = \{v_0, v_1, v_2, v_3\}$, its six root products can written as $2 \times 3$ *root matrix* $\begin{pmatrix} r_{23} & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$. An *index-permutation* is a permutation $\sigma \in S_4$ of indices $0, 1, 2, 3$, which maps root products as follows: $r_{ij} \mapsto r_{\sigma(i)\sigma(j)}$, where $r_{ij} = r_{ji}$. ■

The group $S_4$ of all 24 index-permutations is generated by the three *index-transpositions* $0 \leftrightarrow 1$, $1 \leftrightarrow 2$, $2 \leftrightarrow 3$. To reduce the ambiguity of root matrices, Definition 3.2 introduces below a root form $\mathrm{RF}(B)$ and root invariant $\mathrm{RI}(B)$, which turns out to be a complete invariant of $\Lambda \subset \mathbb{R}^3$ up to isometry. The root invariant $\mathrm{RI}(B)$ reduces $\mathrm{RF}(B)$ to 6, 5, 4, 4, 3 root products for Voronoi types $V_1$, $V_2$, $V_3$, $V_4$, $V_5$, respectively.

**Definition 3.2** (root form $\mathrm{RF}(B)$ and root invariant $\mathrm{RI}(\Lambda)$ of a lattice $\Lambda$)**. ($V_5$)** Any obtuse superbase $B$ of a lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type $V_5$ has exactly three non-zero root products. Up to 24 index-permutations, the *root form* is $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & 0 \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$ for any odd superbase $B$ and $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & r_{01} \\ 0 & r_{02} & r_{03} \end{pmatrix}$ for any even superbase $B$, where all non-zero root products are freely permutable. The *root invariant* $\mathrm{RI}(\Lambda)$ is an ordered triple of the non-zero root products $r_{01}, r_{02}, r_{03}$.

**($V_4$)** For any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type $V_4$, any obtuse superbase $B$ has two zero root products in different columns. A *root form* is $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, where $r_{23} = 0 = r_{13}$, and the root products $r_{12}, r_{01}, r_{02}$ are freely permutable. The *root invariant* $\mathrm{RI}(\Lambda) = \{(r_{12}, r_{01}, r_{02}), r_{03}\}$ consists of $3+1$ root products, where the triple $(r_{12}, r_{01}, r_{02})$ should be written in increasing order.

**($V_3$)** For any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type $V_3$, any obtuse superbase $B$ of $\Lambda$ has exactly two zero root products in the same column. A *root form* is $\mathrm{RF}(B) = \begin{pmatrix} 0 & r_{13} & r_{12} \\ 0 & r_{02} & r_{03} \end{pmatrix}$ with $r_{23} = 0 = r_{03}$, and $r_{13}, r_{12}, r_{02}, r_{03}$ are freely permutable. The *root invariant* $\mathrm{RI}(\Lambda)$ consists of the four non-zero root products in increasing order.

**($V_2$)** For any lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type $V_2$, any obtuse superbase $B$ of $\Lambda$ has exactly one zero root product. A root form is $\mathrm{RF}(B) = \begin{pmatrix} 0 & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, where $r_{23} = 0$ and the $2 \times 2$ submatrix $\begin{pmatrix} r_{13} & r_{12} \\ r_{02} & r_{03} \end{pmatrix}$ can be changed by the symmetry group $D_4$, which can guarantee (without changing indices for simplicity) that $r_{13} = \min\{r_{13}, r_{12}, r_{02}, r_{03}\}$ and also $r_{12} \leq r_{02}$. The *root invariant* consists of $1+3+1$ root products: $\mathrm{RI}(\Lambda) = \{r_{01}, (r_{13}, r_{12}, r_{02}), r_{03}\}$, where $r_{03} \geq r_{13} \leq r_{12} \leq r_{02}$.

**($V_1$)** For any obtuse superbase $B$ of a lattice $\Lambda \subset \mathbb{R}^3$ of Voronoi type $V_1$, a *root form* $\mathrm{RF}(B)$ is the matrix $\begin{pmatrix} r_{23} & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, where root products can be rearranged by the 24 index-permutations from Definition 3.1. A permutation of indices 1, 2, 3 as in (3.1a) allows us to arrange the three columns in any order. The composition of transpositions $0 \leftrightarrow i$ and $j \leftrightarrow k$ for distinct $i, j, k \neq 0$ vertically swaps the root products in columns $j$ and $k$, for example apply the transposition $2 \leftrightarrow 3$ to the result of $0 \leftrightarrow 1$ in (3.1b). So we can put $r_{min} = \min\{r_{ij}\}$ into the top left position ($r_{23}$). Then we consider the four root products in columns 2 and 3. Keeping column 1 fixed, we can put the minimum of these four into the top middle position ($r_{13}$). Then the resulting root products in the top row should be in increasing order.

If the top left and top middle root products are equal ($r_{23} = r_{13}$), we can put their counterparts ($r_{01}$ and $r_{02}$) in the bottom row of columns 1,2 in increasing order. If the top middle and top right root products are equal ($r_{13} = r_{12}$), we can put their counterparts ($r_{02}$ and $r_{03}$) in the bottom row of columns 2 and 3 in increasing order. The resulting uniquely ordered matrix is the *root invariant* $\mathrm{RI}(\Lambda)$. ■

Scaling any lattice $\Lambda$ by a factor $s \in \mathbb{R}$ multiplies all root products in $\mathrm{RI}(\Lambda)$ by $s$.

**Theorem 3.3** (3D lattices/isometry $\leftrightarrow$ root invariants)**.** Any lattices $\Lambda, \Lambda' \subset \mathbb{R}^3$ are isometric if and only if their root invariants coincide: $\mathrm{RI}(\Lambda) = \mathrm{RI}(\Lambda')$. ▲

**Example 3.4** (root invariants of orthorhombic lattices)**.** (***oP***) The primitive orthorhombic lattice $\Lambda$ with edge-lengths $0 \leq a \leq b \leq c$ has the obtuse superbase $v_1 = (a,0,0)$, $v_2 = (0,b,0)$, $v_3 = (0,0,c)$, $v_0 = (-a,-b,-c)$, whose root form is $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & 0 \\ a & b & c \end{pmatrix}$, so the root invariant is $\mathrm{RI}(\Lambda) = (a,b,c)$. If we re-order vectors, columns of $\mathrm{RF}(B)$ are re-ordered accordingly, but $\mathrm{RI}(\Lambda)$ remains the same. Another obtuse superbase $v_1 = (a,0,0)$, $v_2 = (0,b,0)$, $v_3' = (-a,0,c)$, $v_0' = (0,-b,-c)$ has $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & a \\ 0 & b & c \end{pmatrix}$. The root invariant $\mathrm{RI}(\Lambda) = (a,b,c)$ is the same by Definition 3.2($V_5$).

(***tP***) For a primitive tetragonal lattice, set $a = b$ in the case above.

Let all orthorhombic lattices below have a base cube with sides $2a \leq 2b \leq 2c$.

(***oS***) A base-centred orthorhombic lattice $\Lambda$ has the obtuse superbase $v_1 = (2a,0,0)$, $v_2 = (-a,b,0)$, $v_3 = (0,0,c)$, $v_0 = (-a,-b,-c)$, whose root form is $\mathrm{RF}(B) = \begin{pmatrix} 0 & 0 & a\sqrt{2} \\ a\sqrt{2} & \sqrt{b^2-a^2} & c \end{pmatrix}$. The root invariant is $\mathrm{RI}(\Lambda) = \{(a\sqrt{2}, a\sqrt{2}, \sqrt{b^2-a^2}), c\}$ where the $\sqrt{b^2-a^2}$ should move to the first place if $a\sqrt{2} > \sqrt{b^2-a^2}$, $b < a\sqrt{3}$.

(***oF***) A face-centred orthorhombic lattice $\Lambda$ has the obtuse superbase $v_1 = (a,b,0)$, $v_2 = (a,-b,0)$, $v_3 = (-a,0,c)$, $v_0 = (-a,0,-c)$, whose root form is $\mathrm{RF}(B) =$

$\begin{pmatrix} \sqrt{b^2-a^2} & a & a \\ \sqrt{c^2-a^2} & a & a \end{pmatrix}$. If $b < a\sqrt{2}$, the root invariant is $\mathrm{RI}(\Lambda) = \mathrm{RF}(B)$. Otherwise, $\mathrm{RI}(\Lambda)$ is obtained from $\mathrm{RF}(B)$ above by swapping the first and last columns.

(***oI***) For a body-centred orthorhombic lattice $\Lambda$, assume that $a^2+b^2 \geq c^2$. Then $\Lambda$ has the obtuse superbase $v_1 = (a,b,-c)$, $v_2 = (a,-b,c)$, $v_3 = (-a,b,c)$, $v_0 = (-a,-b,-c)$, and $\mathrm{RF}(B) = \begin{pmatrix} \sqrt{a^2+b^2-c^2} & \sqrt{a^2-b^2+c^2} & \sqrt{-a^2+b^2+c^2} \\ \sqrt{a^2+b^2-c^2} & \sqrt{a^2-b^2+c^2} & \sqrt{-a^2+b^2+c^2} \end{pmatrix}$. If $a < b < c$, the root products are increasing in each row, so $\mathrm{RI}(\Lambda)$ coincides with $\mathrm{RF}(B)$ above.

(***tI***) For a body-centred tetragonal lattice, set $a = b$ in the case above to get $\mathrm{RI}(\Lambda) = \begin{pmatrix} \sqrt{2a^2-c^2} & c & c \\ \sqrt{2a^2-c^2} & c & c \end{pmatrix}$, where we should swap the first and last columns for $a > c$.

(***cI***) For a body-centred cubic $\Lambda$, $a = b = c$ in (***oI***) gives $\mathrm{RI}(\Lambda) = \begin{pmatrix} a & a & a \\ a & a & a \end{pmatrix}$. ■

## 4. Continuous maps of lattices by their Voronoi, Bravais and Delone types

Hahn *et al.* (2002, Table 9.1.8.1) subdivides 14 Bravais classes of lattices within each of 5 Voronoi types and lists 24 Delone's types, see the original version in Delone (1938, Fig. 36) and the latest update in Andrews *et al.* (2020, Fig. 2). These discrete splittings in 5, 14, 24 types will be extended to continuous maps below.

Examples 4.1–4.5 visualise root forms for each Voronoi type by the maps below:

• column projections $\mathrm{CP}_1, \mathrm{CP}_2, \mathrm{CP}_3$ visualise any root form as a triple of points in the quadrant $Q = \{(x,y) \in \mathbb{R}^2 \mid x, y \geq 0\}$ or as one point in the product $Q_1 \times Q_2 \times Q_3$;

• Voronoi maps $\mathrm{VM}_i : \mathrm{RIS}_i \to Q$ project root forms of type $V_i$ to the quadrant $Q$;

• Delone maps visualise strata of Bravais types of lattices within each Voronoi type.

**Example 4.1** (Voronoi map $\mathrm{VM}_1$ for lattices of type $V_1$)**.** Any root invariant $\mathrm{RI} = \begin{pmatrix} r_{23} & r_{13} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$ from Definition 3.2($V_1$) can be visualised by the three *column projections* $\mathrm{CP}_1(\mathrm{RI}) = (r_{01}, r_{23})$, $\mathrm{CP}_2(\mathrm{RI}) = (r_{02}, r_{13})$, $\mathrm{CP}_3(\mathrm{RI}) = (r_{03}, r_{12})$, where each pair lives in its own quadrant $Q_i = \{r_{0i} \geq 0,\ r_{\{1,2,3\}-i} \geq 0\}$, $i = 1, 2, 3$.

The *1st Voronoi* map is $\mathrm{VM}_1 = (\mathrm{CP}_1, \mathrm{CP}_2, \mathrm{CP}_3) : \mathrm{RIS} \to Q_1 \times Q_2 \times Q_3$. Under the 1st column projection $\mathrm{CP}_1$, the root invariants of all generic lattices of Voronoi type $V_1$ map to $\{r_{23} > 0\} \subset Q_1$ strictly above the horizontal axis $\{r_{23} = 0\}$, which represents all non-generic lattices of Voronoi types $V_2, V_3, V_4, V_5$ visualised in further examples. All lattices of Voronoi type $V_1$ split into eight Delone types below.

[***cI***] Let a body-centred cubic lattice $\Lambda$ have a base cubic cell with a side $a$. By Example 3.4(cI), $\mathrm{RI}(\Lambda) = \begin{pmatrix} a & a & a \\ a & a & a \end{pmatrix}$, which is mapped by $\mathrm{VM}_1$ to three equal diagonal points $(a, a) \in Q_i$, $i = 1, 2, 3$. The Delone map $\mathrm{DM}[cI] : \mathrm{RI}(\Lambda) \mapsto a$ projects all root invariants $\mathrm{RI}(\Lambda)$ to $\mathbb{R}$ and can be visualised as a histogram over $a \in \mathbb{R}$. Other non-primitive orthorhombic lattices will have a base cuboid with sides $2a \le 2b \le 2c$.

[$\boldsymbol{V_1 \cap tI}$] Let a body-centred tetragonal lattice $\Lambda$ of Voronoi type $V_1$ have a base cuboid cell with sides $2a, 2a, 2c$ such that $c < a\sqrt{2}$. By Example 3.4(tI), for $a \le c < a\sqrt{2}$, we have the root invariant $\mathrm{RI}(\Lambda) = \begin{pmatrix} r_{01} & r_{02} & r_{02} \\ r_{01} & r_{02} & r_{02} \end{pmatrix}$, where $r_{01} = \sqrt{2a^2 - c^2}$, $r_{02} = c$. For $a > c$, the root invariant is $\mathrm{RI}(\Lambda) = \begin{pmatrix} r_{01} & r_{01} & r_{02} \\ r_{01} & r_{01} & r_{02} \end{pmatrix}$, where $r_{01} = c$, $r_{02} = \sqrt{2a^2 - c^2}$. Then $\mathrm{VM}_1$ maps all root invariants of both types above to three diagonal points in the quadrants $Q_1, Q_2, Q_3$. The Delone map $\mathrm{DM}[V_1 \cap tI] : \mathrm{RI}(\Lambda) \mapsto (x, y)$ can be visualised as a plot in the coordinates $x = \sqrt{2a^2 - c^2}$, $y = c$.

[$\boldsymbol{V_1 \cap hR}$] A rhombohedral lattice of Voronoi type $V_1$ has $\mathrm{RI} = \begin{pmatrix} x & x & x \\ y & y & y \end{pmatrix}$, which projects under $\mathrm{VM}_1$ to three equal non-diagonal points $(x, y) \in Q_1, Q_2, Q_3$. The Delone map $\mathrm{DM}[V_1 \cap hR]$ can be plotted in the coordinates $y \ge x > 0$.

[***oF***] A face-centred orthorhombic lattice $\Lambda$ by Example 3.4(oF) has the root invariant $\mathrm{RI}(\Lambda) = \begin{pmatrix} \sqrt{b^2 - a^2} & a & a \\ \sqrt{c^2 - a^2} & a & a \end{pmatrix}$ for $b \le a\sqrt{2}$ and $\mathrm{RI}(\Lambda) = \begin{pmatrix} a & a & \sqrt{b^2 - a^2} \\ a & a & \sqrt{c^2 - a^2} \end{pmatrix}$ for $b > a\sqrt{2}$. Under the first Voronoi map $\mathrm{VM}_1$, both root invariants project to two diagonal points and one non-diagonal point in $Q_1, Q_2, Q_3$.

[$\boldsymbol{V_1 \cap oI}$] A body-centred orthorhombic lattice $\Lambda$ of type $V_1$ by Example 3.4(oI) for

$a^2+b^2>c^2$ has $\mathrm{RI}(\Lambda)=\begin{pmatrix} r_{01} & r_{02} & r_{03} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, where $r_{01}=\sqrt{a^2+b^2-c^2}$, $r_{02}=\sqrt{a^2-b^2+c^2}$, $r_{03}=\sqrt{-a^2+b^2+c^2}$. Under the first Voronoi map $\mathrm{VM}_1$, any root invariant $\mathrm{RI}(\Lambda)$ above projects to three non-equal diagonal points in $Q_1,Q_2,Q_3$.

[$\boldsymbol{V_1\cap mC}$] A centred monoclinic lattice $\Lambda$ can have two Delone types with 4 parameters: $\mathrm{RI}_1=\begin{pmatrix} r_{23} & r_{23} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$ and $\mathrm{RI}_2=\begin{pmatrix} r_{01} & r_{02} & r_{12} \\ r_{01} & r_{02} & r_{03} \end{pmatrix}$, where columns might be permuted to guarantee a top row in increasing order.

[$\boldsymbol{V_1\cap aP}$] The most generic lattices $\Lambda\subset\mathbb{R}^3$ are triclinic. Their root invariants consist of six non-zero root products and live in the interior of $Q_1\times Q_2\times Q_3$ outside all seven Delone subspaces considered above. ■

The 1st Voronoi map $\mathrm{VM}_1$ has split six root products into three pairs, which can be visualised in three quadrants. Other Voronoi maps $\mathrm{VM}_i:\mathrm{RIS}_i\to Q$ will map root invariants to one quadrant $Q$ so that higher types are represented by coordinate axes.

**Example 4.2** (Voronoi map $\mathrm{VM}_2:\mathrm{RIS}_2\to Q$)**.** Any root invariant of Voronoi type $V_2$ is $\mathrm{RI}=\{r_{01},(r_{13},r_{12},r_{02}),r_{03}\}$, where $r_{03}\geq r_{13}\leq r_{12}\leq r_{02}$, see Definition 3.2($V_3$). The *2nd Voronoi* map is $\mathrm{VM}_2(\mathrm{RI})=(r_{01},r_{13})$. The limit case of the vertical axis $\{r_{01}=0\}$ represents Voronoi types $V_3,V_5$. The limit case of the horizontal axis $\{r_{13}=0\}$ represents Voronoi types $V_4,V_5$. The origin represents Voronoi type $V_5$. ■

**Example 4.3** (Voronoi map $\mathrm{VM}_3:\mathrm{RIS}_3\to Q$)**.** Any root invariant of Voronoi type $V_3$ from Definition 3.2($V_3$) is an ordered quadruple $\mathrm{RI}=(r_{13},r_{12},r_{02},r_{03})$. The *3rd Voronoi map* is $\mathrm{VM}_3(\mathrm{RI})=(r_{03},r_{13})\in Q$. The limit case of the horizontal axis $\{r_{13}=0\}$ represents all lattices of Voronoi type $V_5$ below. ■

By Kurlin (2022, Lemma 4.4), a Voronoi domain of type $V_4$ is a hexagonal prism with strict Voronoi vectors $v_1,v_2$ generating a non-rectangular lattice in $\mathbb{R}^2$, while the 3rd vector $v_3$ is orthogonal to both $v_1,v_2$ and has the length $c=r_{03}=\sqrt{-v_0\cdot v_3}$.

**Example 4.4** (Voronoi maps $\mathrm{VM}_4 : \mathrm{RIS}_4 \to Q$)**.** Any root invariant of of Voronoi type $V_4$ is $\mathrm{RI} = \{r_{03}, (r_{12}, r_{01}, r_{02})\}$ such that $r_{12} \leq r_{01} \leq r_{02}$, see Definition 3.2($V_4$).

($\mathbf{VM}_4^{min}$) The *minimum 4th Voronoi map* is $\mathrm{VM}_4^{min}(\mathrm{RI}) = (r_{12}, r_{03})$.

[***mP***] All primitive monoclinic lattices from the Bravais class (mP) have $(x, y) = \mathrm{VM}_4^{min}(\mathrm{RI})$ in the interior of the quadrant $Q$, where $x = r_{12} > 0$ and $y = r_{03} > 0$. The limit case of the vertical axis $\{r_{12} = 0\}$ represents the lattices of Voronoi type $V_5$ when the basis vectors $v_1, v_2, v_3$ are pairwise orthogonal, see Example 4.5.

($\mathbf{VM}_4^{ort}$) Similarly to the root invariants of 2D lattices, it is convenient to scale root products in an ordered triple dividing them by the sum: $(\bar{r}_{12}, \bar{r}_{01}, \bar{r}_{02}) = \dfrac{(r_{12}, r_{01}, r_{02})}{r_{12} + r_{01} + r_{02}}$. The *orthogonal 4th Voronoi map* is $\mathrm{VM}_4^{ort}(\mathrm{RI}) = (\bar{r}_{02} - \bar{r}_{01}, 3\bar{r}_{12}) \in \mathrm{QT}$.

The above map forgets $r_{03}$ equal to the length $|v_3|$ of the 3rd basis vector $v_3$ orthogonal to $v_1, v_2$. Since $r_{0i} = -v_0 \cdot v_i = (v_1 + v_2 + v_3) \cdot v_i = (v_1 + v_2) \cdot v_i$ for $i = 1, 2$ due to $v_3 \cdot v_i = 0$, the above root products $r_{01}, r_{02}$ for the superbase in $\mathbb{R}^3$ coincide with the root products for the smaller superbase $v_1, v_2, -v_1 - v_2$ generating the 2D lattice.

[***oS***] Any base-centred orthorhombic lattice from the Bravais class (oS) includes a 2D centred-rectangular lattice $\Lambda_2$ generated by $v_1 = (2a, 0)$, $v_2 = (-a, b)$ for $0 < a \leq b$. The 2D root invariant $\mathrm{RI}(\Lambda_2)$ is an ordered triple $(a\sqrt{2}, a\sqrt{2}, \sqrt{b^2 - a^2})$, where the first and last entries should be swapped for $a \leq b < a\sqrt{3}$. The 3D root invariant is $\mathrm{RI}(\Lambda) = \{c, \mathrm{RI}(\Lambda_2)\}$. The orthogonal 4th Voronoi map shows $\Lambda$ as the point $\mathrm{VM}_4^{ort}(\mathrm{RI}(\Lambda))$ in the vertical edge or the hypotenuse (without all vertices) of QT. Any such $\Lambda$ can be represented by $(\frac{a}{b}, c)$ in a separate plot.

[***hP***] The top vertex $\mathrm{VM}_4^{ort}(\mathrm{RI}) = (0, 1) \in \mathrm{QT}$ represents all hexagonal lattices below. Any lattice $\Lambda$ from the Bravais class (hp) includes a 2D hexagonal lattice generated by vectors $v_1 = (a, 0)$ and $v_2 = (-\frac{a}{2}, \frac{\sqrt{3}}{2}a)$ of a length $a$. Then $\mathrm{RI}(\Lambda) = \{c, (\frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}}, \frac{a}{\sqrt{2}})\}$. Any 3D hexagonal lattice can represented by $(a, c)$ in a separate plot. ■

**Example 4.5** (Voronoi map $\mathrm{VM}_5 : \mathrm{RIS}_2 \to Q$)**.** Any root invariant $\mathrm{RI} = (a, b, c)$ of Voronoi type $V_5$ is an ordered triple $0 < a \leq b \leq c$ of edge-lengths of a cuboid cell.

[$\mathbf{VM_5}$] The *5th Voronoi map* is $\mathrm{VM}_5(\mathrm{RI}) = \left(\dfrac{a}{c}, \dfrac{b}{c}\right) \in \{(x, y) \in \mathbb{R}^2 \mid 0 < x \leq y \leq 1\}$.

[$\boldsymbol{cP}$] Root invariants $(a, a, a)$ of all simple cubic lattices with all three equal sides $a = b = c$ map under $\mathrm{VM}_5$ to the point $(1, 1)$. The sides $a$ of all simple cubic lattices can be shown in a histogram with vertical bars whose width is a small interval of $a$ and the height is proportional to the number of lattices with sides in this interval.

[$\boldsymbol{tP}$] Root invariants $(a, a, c)$ and $(a, b, b)$ of all simple tetragonal lattices with two equal sides $a = b$ or $b = c$, respectively, map under $\mathrm{VM}_5$ to the diagonal $\{0 < x = \frac{a}{c} = \frac{b}{c} = y < 1\}$ and the horizontal line $\{0 < x < 1, y = \frac{b}{c} = 1\}$, respectively.

[$\boldsymbol{oP}$] Root invariants $\mathrm{RI} = (a, b, c)$ of all primitive orthorhombic latices map under $\mathrm{VM}_5$ to $\left(\frac{a}{c}, \frac{b}{c}\right)$ in the open triangle $\{0 < y < x < 1\}$. ■

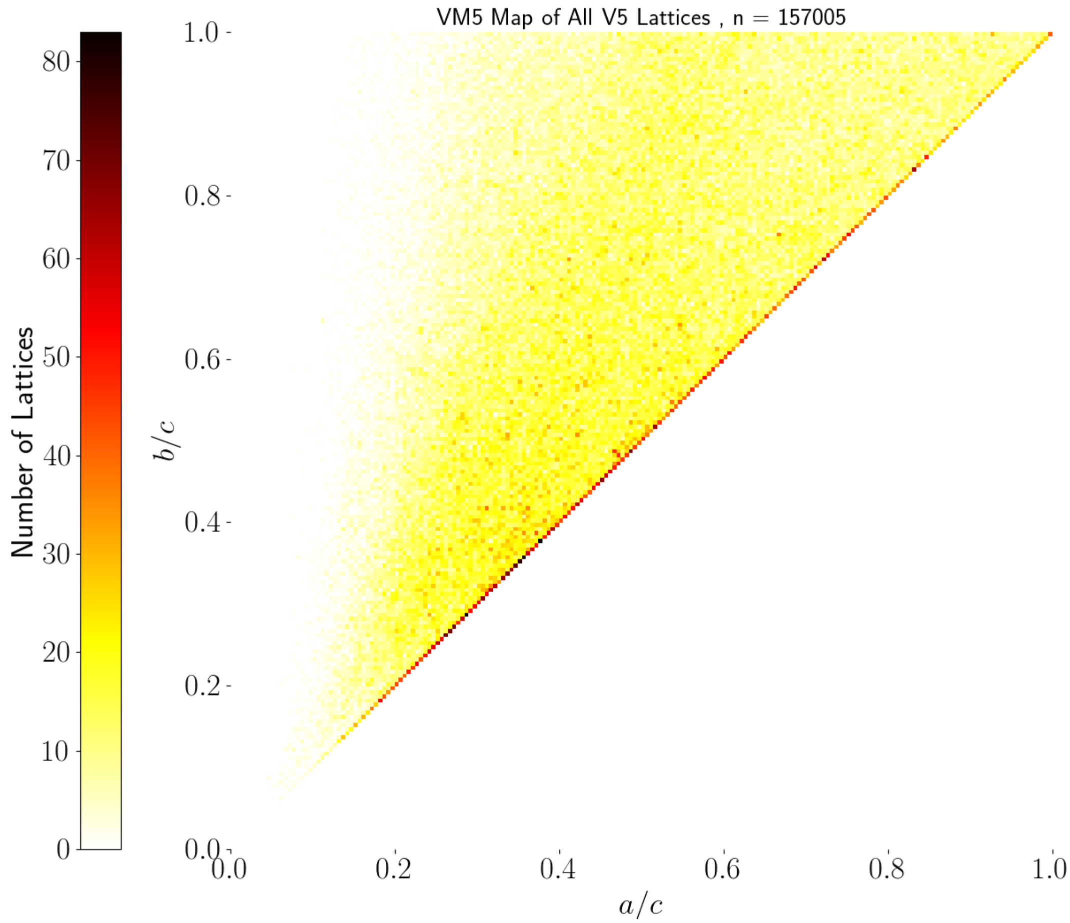


Fig. 1. The 5th Voronoi map $\mathrm{VM}_5$ for all CSD lattices of Voronoi type $V_5$ from Example 4.5. The colours of pixels indicate numbers of lattices with parameters $(\frac{a}{c}, \frac{b}{c})$.

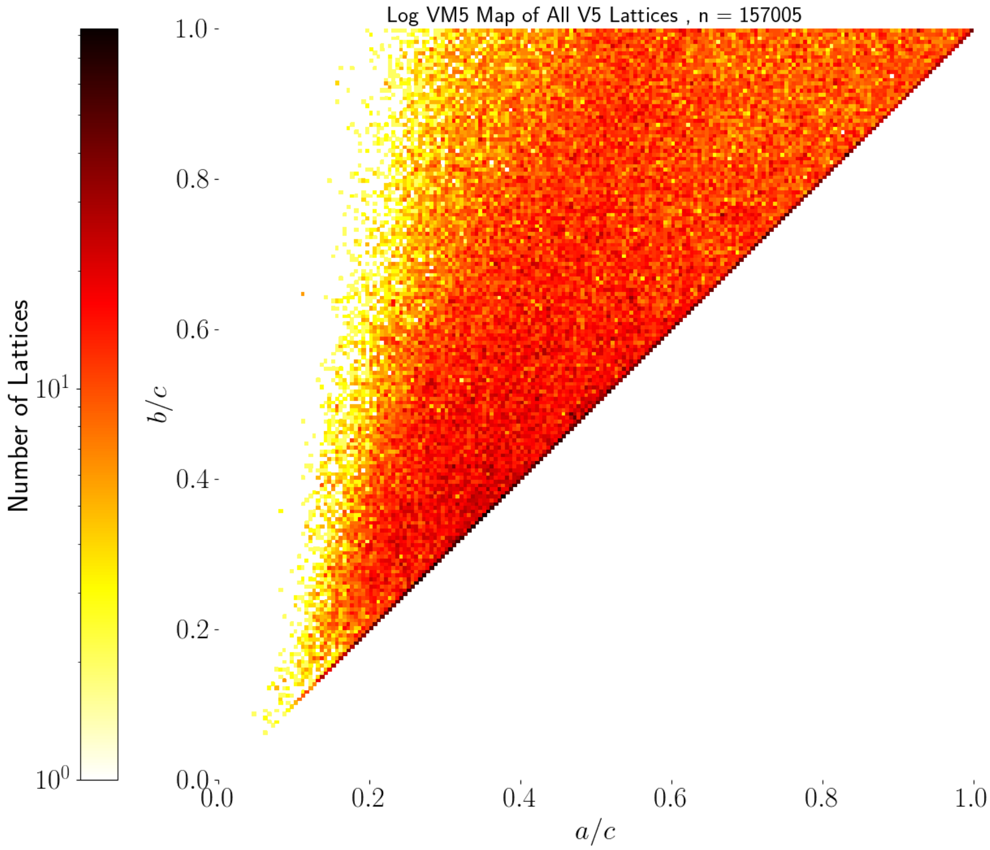


Fig. 2. The density plot of the 5th Voronoi map $VM_5$ from Fig. 1 in the logarithmic scale better visualises the interior of the triangle $0 < \frac{a}{c} < \frac{b}{c} < 1$ representing the Bravais class of all primitive orthorhombic lattices in Example 4.5[oP].

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**Synopsis**

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