A Space for Lattice Representation and Clustering

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Note Boris Delaunay in his later publications used the Russian version of his surname: Delone. We will follow that choice.

Synopsis Algorithms for defining the difference between two lattices are described. They are based on the work of Selling and Delone (Delaunay).

Abstract Algorithms for quantifying the difference between two lattices are used for Bravais lattice determination, database lookup for unit cells, and recently for clustering to group together images from serial crystallography. A space related to the reduction algorithm of Selling and to the Bravais lattice determination methods of Delone is described. Two ways of representing the space are presented and applications of its metric are discussed.

Keywords: Unit cell; reduction; Delone; Delaunay; lattice

1. Introduction

(Andrews, et al., 2018) described some of the properties of the six scalars that are treated by the Selling reduction. Considering the scalars as a definition for a metric space, rather than a simple list of numbers has advantages. We consider two representations of the space, S^6 and C^3. Although S^6 and C^3 are simply reorganizations of the same data, some operations are simpler to explain in one than the other. We will choose to show only the simpler one.

2. The Space S^6:

For a Bravais tetrahedron with defining vectors a, b, c, d (the edge vectors of the unit cell and the negative sum of them), a point in S^6 is {b.c, a.c, a.b, a.d, b.d, and c.d}. A simple example is the unit cell {10, 12, 20, 90, 90, 90}. The corresponding S^6 vector is {0, 0, 0, -100, -144, -400}. The scalars in S^6 are of a single type, unlike cell parameters (lengths and angles) and G^6 (squared lengths and dot products). (Delone et al, 1975) say, “The Selling parameters are geometrically fully homogeneous”.

Some of the properties of S^6 are simple. The six base axes are orthogonal, unlike those of G^6 (f and Bernstein, 2014). One consequence is that the projection matrices onto the axes are especially simple: 6x6 matrices of zero, with a single value one on the diagonal at the position of the axis projected to.

2.1. The Reflections in S^6:

The 24 equivalent positions in S^6 have corresponding matrices to act on S^6 vectors. They can be generated from any triple (except the identity). For convenience, they are listed here. The structure of the set is clearer in C^3 (see below).

[[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1]]

[[0,0,0,0,1,0],[0,0,0,1,0,0],[0,0,1,0,0,0],[0,1,0,0,0,0],[1,0,0,0,0,0],[0,0,0,0,0,1]]

[[1,0,0,0,0,0],[0,0,1,0,0,0],[0,1,0,0,0,0],[0,0,0,1,0,0],[0,0,0,0,0,1],[0,0,0,0,1,0]]

[[0,0,0,0,0,1],[0,0,0,1,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[1,0,0,0,0,0],[0,0,0,0,1,0]]

[[0,0,0,0,1,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,1,0,0,0,0],[0,0,0,0,0,1],[1,0,0,0,0,0]]

[[0,0,0,0,0,1],[0,1,0,0,0,0],[0,0,0,1,0,0],[0,0,1,0,0,0],[0,0,0,0,1,0],[1,0,0,0,0,0]]

[[0,1,0,0,0,0],[1,0,0,0,0,0],[0,0,1,0,0,0],[0,0,0,0,1,0],[0,0,0,1,0,0],[0,0,0,0,0,1]]

[[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,1,0,0,0],[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,0,0,0,1]]

[[0,1,0,0,0,0],[0,0,1,0,0,0],[1,0,0,0,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1],[0,0,0,1,0,0]]

[[0,0,0,0,0,1],[0,0,0,0,1,0],[1,0,0,0,0,0],[0,0,1,0,0,0],[0,1,0,0,0,0],[0,0,0,1,0,0]]

[[0,0,0,1,0,0],[0,0,1,0,0,0],[0,0,0,0,1,0],[1,0,0,0,0,0],[0,0,0,0,0,1],[0,1,0,0,0,0]]

[[0,0,0,0,0,1],[1,0,0,0,0,0],[0,0,0,0,1,0],[0,0,1,0,0,0],[0,0,0,1,0,0],[0,1,0,0,0,0]]

[[0,0,1,0,0,0],[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,0,0,0,1],[0,0,0,1,0,0],[0,0,0,0,1,0]]

[[0,0,0,1,0,0],[0,0,0,0,0,1],[0,1,0,0,0,0],[1,0,0,0,0,0],[0,0,1,0,0,0],[0,0,0,0,1,0]]

[[0,0,1,0,0,0],[0,1,0,0,0,0],[1,0,0,0,0,0],[0,0,0,0,0,1],[0,0,0,0,1,0],[0,0,0,1,0,0]]

[[0,0,0,0,1,0],[0,0,0,0,0,1],[1,0,0,0,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0],[0,0,0,1,0,0]]

[[0,0,0,1,0,0],[0,1,0,0,0,0],[0,0,0,0,0,1],[1,0,0,0,0,0],[0,0,0,0,1,0],[0,0,1,0,0,0]]

[[0,0,0,0,1,0],[1,0,0,0,0,0],[0,0,0,0,0,1],[0,1,0,0,0,0],[0,0,0,1,0,0],[0,0,1,0,0,0]]

[[0,0,1,0,0,0],[0,0,0,0,1,0],[0,0,0,1,0,0],[0,0,0,0,0,1],[0,1,0,0,0,0],[1,0,0,0,0,0]]

[[0,1,0,0,0,0],[0,0,0,0,0,1],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,1,0,0,0],[1,0,0,0,0,0]]

[[0,0,1,0,0,0],[0,0,0,1,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1],[1,0,0,0,0,0],[0,1,0,0,0,0]]

[[1,0,0,0,0,0],[0,0,0,0,0,1],[0,0,0,0,1,0],[0,0,0,1,0,0],[0,0,1,0,0,0],[0,1,0,0,0,0]]

[[0,1,0,0,0,0],[0,0,0,1,0,0],[0,0,0,0,0,1],[0,0,0,0,1,0],[1,0,0,0,0,0],[0,0,1,0,0,0]]

[[1,0,0,0,0,0],[0,0,0,0,1,0],[0,0,0,0,0,1],[0,0,0,1,0,0],[0,1,0,0,0,0],[0,0,1,0,0,0]]

The unsorted nature of Selling reduction implies that distance calculations will need to consider the effect of the reflections. Even if a usable sorting were created, at least some of the reflections would still be required.

2.2. Reduction: in S^6

Lattice reduction is quite simple in S^6 (Andrews et al., 2018), but it has a simpler structure in C^3, so it will be treated there. Due to the simple nature of S^6 the inverse operations are the same set as the reduction operations. The matrices in S^6 are unitary, so the metric is the same in the each region. However, the transformation matrices are not diagonal with the result that the boundaries are not simple mirrors.

We present the reductions as matrices; the second line for each is the alternate choice of which pair to exchange.

[[-1,0,0,0,0,0],[1,1,0,0,0,0],[1,0,0,0,1,0],[-1,0,0,1,0,0],[1,0,1,0,0,0],[1,0,0,0,0,1]]
[[-1,0,0,0,0,0],[1,0,0,0,0,1],[1,0,1,0,0,0],[-1,0,0,1,0,0],[1,0,0,0,1,0],[1,1,0,0,0,0]]

[[1,1,0,0,0,0],[0,-1,0,0,0,0],[0,1,0,1,0,0],[0,1,1,0,0,0],[0,-1,0,0,1,0],[0,1,0,0,0,1]]
[[0,1,0,0,0,1],[0,-1,0,0,0,0],[0,1,1,0,0,0],[0,1,0,1,0,0],[0,-1,0,0,1,0],[1,1,0,0,0,0]]

[[1,0,1,0,0,0],[0,0,1,1,0,0],[0,0,-1,0,0,0],[0,1,1,0,0,0],[0,0,1,0,1,0],[0,0,-1,0,0,1]]
[[0,0,1,0,1,0],[0,1,1,0,0,0],[0,0,-1,0,0,0],[0,0,1,1,0,0],[1,0,1,0,0,0],[0,0,-1,0,0,1]]

[[1,0,0,-1,0,0],[0,0,1,1,0,0],[0,1,0,1,0,0],[0,0,0,-1,0,0],[0,0,0,1,1,0],[0,0,0,1,0,1]]
[[1,0,0,-1,0,0],[0,1,0,1,0,0],[0,0,1,1,0,0],[0,0,0,-1,0,0],[0,0,0,1,0,1],[0,0,0,1,1,0]]

[[0,0,1,0,1,0],[0,1,0,0,-1,0],[1,0,0,0,1,0],[0,0,0,1,1,0],[0,0,0,0,-1,0],[0,0,0,0,1,1]]
[[1,0,0,0,1,0],[0,1,0,0,-1,0],[0,0,1,0,1,0],[0,0,0,0,1,1],[0,0,0,0,-1,0],[0,0,0,1,1,0]]

[[0,1,0,0,0,1],[1,0,0,0,0,1],[0,0,1,0,0,-1],[0,0,0,1,0,1],[0,0,0,0,1,1],[0,0,0,0,0,-1]]
[[1,0,0,0,0,1],[0,1,0,0,0,1],[0,0,1,0,0,-1],[0,0,0,0,1,1],[0,0,0,1,0,1],[0,0,0,0,0,-1]]

2.3. Boundaries in S^6:

The first boundaries in S^6 are the zeros of the axes. (Contrast this with G^6, (Andrews and Bernstein, 2014) which has 15 boundaries.) Obviously, they correspond to unit cell angles of 90 degrees. In S^6, the zeros mark the regions where the components change from negative to positive, the place where cells become not Selling-reduced. A second kind of boundary is where the "opposite" pairs of scalars are equal; more easily visualized in C^3.

The consequence for distance calculations will be that the reduction operations will be involved in the distance computations.

3. The Space C^3:

Alternatively, the space S^6 can be as C^3, a space of three complex axes. C^3 has advantages for understanding some of the properties of the space. Where we compose S^6 of the scalars s1, … S^6, the components of C^3 are the pairs of "opposite" scalars. In terms of the elements of S^6, a vector in C^3 is {(s1,s4), (s2,s5), (s3,s6)}. The C^3 presentation of the above vector is {(0,-100), (0, -144), (0, -400)}.

3.1. The Reflections in C^3:

The 24 reflections of the scalars correspond to 24 operations in C^3. First, any pc3air of C^3 coordinates may be exchanged. The other operation is the exchange of the real and imaginary parts of any pair of C^3 coordinates. For example, c1(real, imag) and c3(real, imag) can transform to c1(imag, real) and c3(imag, real).

Combining the exchange operation with the coordinate interchanges in all possible combinations gives the 24 reflections (including the identity).

Representing the operation of interchanging the real and imaginary parts of a complex number by an underline, the reflections in C^3 are:

Table 1 Reflections in C^3

$[c_1, c_2, c_3]$	$[\underline{c}_1, \underline{c}_2, c_3]$	$[\underline{c}_2, \underline{c}_1, c_3]$	$[\underline{c}_3, \underline{c}_2, c_1]$
$[c_1, c_3, c_2]$	$[\underline{c}_1, c_2, \underline{c}_3]$	$[\underline{c}_2, c_1, \underline{c}_3]$	$[\underline{c}_3, c_2, \underline{c}_1]$
$[c_2, c_1, c_3]$	$[c_1, \underline{c}_2, \underline{c}_3]$	$[c_2, \underline{c}_1, \underline{c}_3]$	$[c_3, \underline{c}_2, \underline{c}_1]$
$[c_2, c_3, c_1]$	$[\underline{c}_1, \underline{c}_3, c_2]$	$[\underline{c}_2, \underline{c}_3, c_1]$	$[\underline{c}_3, \underline{c}_1, c_2]$
$[c_3, c_1, c_2]$	$[\underline{c}_1, c_3, \underline{c}_2]$	$[\underline{c}_2, c_3, \underline{c}_1]$	$[\underline{c}_3, c_1, \underline{c}_2]$
$[c_3, c_2, c_1]$	$[c_1, \underline{c}_3, \underline{c}_2]$	$[c_2, \underline{c}_3, \underline{c}_1]$	$[c_3, \underline{c}_1, \underline{c}_2]$

Table 2 Matrix versions of reflections in C^3

$[[1,0,0],[0,1,0],[0,0,1]]$	$[[\underline{1,0,0}],[\underline{0,1,0}],[0,0,1]]$	$[[\underline{0,1,0}],[\underline{1,0,0}],[0,0,1]]$	$[[\underline{0,0,1}],[\underline{0,1,0}],[1,0,0]]$
$[[1,0,0],[0,0,1],[0,1,0]]$	$[[\underline{1,0,0}],[0,1,0],[\underline{0,0,1}]]$	$[[\underline{0,1,0}],[1,0,0],[\underline{0,0,1}]$	$[[\underline{0,0,1}],[0,1,0],[\underline{1,0,0}]]$
$[[0,1,0],[1,0,0],[0,0,1]]$	$[[1,0,0],[\underline{0,1,0}],[\underline{0,0,1}]]$	$[[0,1,0],[\underline{1,0,0}],[\underline{0,0,1}]]$	$[[0,0,1],[\underline{0,1,0}],[\underline{1,0,0}]]$
$[[0,1,0],[0,0,1],[1,0,0]]$	$[[\underline{1,0,0}],[\underline{0,1,0}],[0,0,1]]$	$[[\underline{0,1,0}],[\underline{0,0,1}],[1,0,0]]$	$[[\underline{0,0,1}],[\underline{1,0,0}],[0,1,0]]$
$[[0,0,1],[1,0,0],[0,1,0]]$	$[[\underline{1,0,0}],[0,1,0],[\underline{0,0,1}]]$	$[[\underline{0,1,0}],[0,0,1],[\underline{1,0,0}]]$	$[[\underline{0,0,1}],[1,0,0],[\underline{0,1,0}]]$
$[[0,0,1],[0,1,0],[1,0,0]]$	$[[1,0,0],[\underline{0,1,0}],[\underline{0,0,1}]]$	$[[0,1,0],[\underline{0,0,1}],[\underline{1,0,0}]]$	$[[0,0,1],[\underline{1,0,0}],[\underline{0,1,0}]]$

3.2. Reduction: in C^3

We can write a vector in S^6 as {s1, … s6} and the corresponding vector in C^3 is {(s1,s4), (s2,s5), (s3,s6)} or {c1, c2, c3}. For the case where s1 is the positive element we will reduce, the C^3 vector after that step will be:

{(-s1, s4-s1). (s2+s1, <u>s5+s1</u>), (<u>s3+s1</u>, s6+s1) or
{(-s1, s4-s1), (<u>s6+s1</u>, s3+s1), (s5+s1, <u>s2+s1</u>)},
where the underlined pairs have been exchanged. The rule (in terms of C^3) is that from the pair of C^3 coordinates that have sums, one real and one imaginary part are exchanged. Either choice is valid, and both lead toward the reduced cell.

The reduction operations do not commute, which will add complexity to distance calculations (see distance measure below).

3.3. Boundaries in C^3:

In C^3, there are two types of boundaries. Referring to S^6, any C^3 real or imaginary part that is zero marks a boundary. Also, the interchange of real and imaginary parts in reflections marks another type of boundary: where the real part equals the imaginary part. This boundary is not so easily apparent in S^6.

3.4. A Fundamental Unit in C^3:

C^3 provides the possibility to choose a particular one of the 24 reflections as the fundamental unit (similar to an asymmetric unit in a space group). The three components can be sorted by their magnitude. The second step is to interchange the real and imaginary parts of c1 such that the real part is less than or equal to the imaginary part (if necessary); that requires also interchanging c2 or c3. Finally, c2 has its real and imaginary parts interchanged (if necessary).

S^6 does not provide a comparable suggestion for a fundamental unit. It is necessary to note that the fundamental unit defined this way in C^3 is compact, but the same unit in S^6 is not compact.

4. Measuring Distance:

We require a distance metric that defines the shortest path between all the representations of two points (lattices). Common uses of a metric for lattices are finding possible Bravais lattice types, searching in databases of unit cell parameters, and, recently, clustering of the images from serial crystallography.

A simple example of the complexity of the task is that we must decide which of the 24 reflections of one point is the closest to the other. Adding the reduction operations so that other paths are examined is also required. That the reduction operations do not commute means that the order of operations is important.

The non-diagonal reduction operations in this space means that measuring the distance between point in different regions of space is not as simple as finding the Cartesian distance. Reduction of a value of zero generates a new point that is also the same boundary. We present two algorithms.

4.1. Measuring Distance: Virtual Cartesian Point

4.2. Measuring Distance: Tunneled Mirrored Boundaries

Figure 1 Virtual Cartesian Point

Figure 2 Tunnelled Mirrored Boundaries

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