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Delone lattice studies in $\mathbf{C^3}$, the space of three complex variables

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The Delone scalars are studied in $\mathbf{C^3}$, the space of three complex variables.
Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. Introduction

The scalars used by Delaunay (1932) in his formulation of Selling reduction (Selling, 1874) are (in the conventional order) $b \cdot c$, $a \cdot c$, $a \cdot b$, $a \cdot d$, $b \cdot d$, $c \cdot d$, where $d = -a - b - c$. (As a mnemonic device, observe that the first three terms use α, β, and γ, in that order, and the following terms use a, b, c, in that order.)

Andrews *et al.* (2019a) chose to represent the scalars in the space $\mathbf{S^6}$, $\{s_1, s_2, s_3, s_4, s_5, s_6\}$ (defined in the order above), as a way to create a metric space for the measurement of the distance between lattices. They also consider the representation of this space as the space of three complex dimensions, $\mathbf{C^3}$ or $\{c_1, c_2, c_3\}$. In $\mathbf{C^3}$, in terms of the Delone scalars, a vector is $\{(s_1,s_4), (s_2,s_5), (s_3,s_6)\}$, where the real and imaginary parts of each are the "opposite" scalars according to the definition of Delaunay (1932) (see Andrews *et al.* (2019b)). As a memonic device, note that the complex components involve (α, a), (β, b), and (γ, c).

Andrews *et al.* (2019a) considered the matrix representations of the reflections in $\mathbf{C^3}$ (and in $\mathbf{S^6}$). This paper will describe the boundary transformations at the edges of the fundamental unit of $\mathbf{C^3}$. In $\mathbf{S^6}$, the fundamental unit is the all negative orthant, which contains only and all of the reduced cells. In $\mathbf{S^6}$ and $\mathbf{C^3}$, the boundaries are found where any scalar (or correspondingly the real or imaginary part) is equal to zero. The rationale for this work was that it might lend insights into the topology of the space of lattices.

2. Notation

Complex numbers will be represented in Cartesian format (x, y), where x is the real part and y is the imaginary part.

We will represent a vector in $\mathbf{C^3}$ by $\{(x_1, y_1), (x_2, y_2), (x_3, y_3)\}$ as an alternative to $\{(s_1,s_4), (s_2,s_5), (s_2,s_6)\}$.

Next we define the operators in $\mathbf{C^3}$ that will be used in the matrix descriptions of the transformations at the boundaries of the fundamental unit.

Operator	Usage	Result	Name
$\mathfrak{M}_r$	$\mathfrak{M}_r(c_j)$	$(-x_j, -x_j + y_j)$	Minus real
$\mathfrak{M}_i$	$\mathfrak{M}_i(c_j)$	$(x_j - y_j, -y_j)$	Minus imag
$\mathfrak{P}_r$	$\mathfrak{P}_r(c_j)$	(x_j, x_j)	Plus real
$\mathfrak{P}_i$	$\mathfrak{P}_i(c_j)$	(y_j, y_j)	Plus imag
$\Re$	$\Re(c_j)$	x_j	Real
$\Im$	$\Im(c_j)$	y_j	Imaginary

3. Matrices of boundary transformations

For the boundary at s_1: (the real component of c_1).

$$\begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathrm{i}\Re & \Re \\ \mathfrak{P}_r & \mathrm{i}\Im & \Im \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \mathrm{i}\Im & \Im \\ \mathfrak{P}_r & \mathrm{i}\Re & \Re \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \Re & \mathrm{i}\Re \\ \mathfrak{P}_r & \Im & \mathrm{i}\Im \end{bmatrix} \begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \Im & \mathrm{i}\Im \\ \mathfrak{P}_r & \Re & \mathrm{i}\Re \end{bmatrix}$$

For the boundary at s_4: (the imaginary component of c_1).

$$\begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathrm{i}\Re & \Re \\ \mathfrak{P}_i & \mathrm{i}\Im & \Im \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \mathrm{i}\Im & \Im \\ \mathfrak{P}_i & \mathrm{i}\Re & \Re \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \Re & \mathrm{i}\Re \\ \mathfrak{P}_i & \Im & \mathrm{i}\Im \end{bmatrix} \begin{bmatrix} \mathfrak{M}_i & 0 & 0 \\ \mathfrak{P}_i & \Im & \mathrm{i}\Im \\ \mathfrak{P}_i & \Re & \mathrm{i}\Re \end{bmatrix}$$

For the boundary at s_2 (the real component of c_2):

$$\begin{bmatrix} \mathrm{i}\Re & \mathfrak{P}_r & \Re \\ 0 & \mathfrak{M}_r & 0 \\ \mathrm{i}\Im & \mathfrak{P}_r & \Im \end{bmatrix} \begin{bmatrix} \mathrm{i}\Im & \mathfrak{P}_r & \Im \\ 0 & \mathfrak{M}_r & 0 \\ \mathrm{i}\Re & \mathfrak{P}_r & \Re \end{bmatrix} \begin{bmatrix} \Re & \mathfrak{P}_r & \mathrm{i}\Re \\ 0 & \mathfrak{M}_r & 0 \\ \Im & \mathfrak{P}_r & \mathrm{i}\Im \end{bmatrix} \begin{bmatrix} \Im & \mathfrak{P}_r & \mathrm{i}\Im \\ 0 & \mathfrak{M}_r & 0 \\ \Re & \mathfrak{P}_r & \mathrm{i}\Re \end{bmatrix}$$

For the boundary at s_5: (the imaginary component of c_2).

$$\begin{bmatrix} \mathrm{i}\Re & \mathfrak{P}_i & \Re \\ 0 & \mathfrak{M}_i & 0 \\ \mathrm{i}\Im & \mathfrak{P}_i & \Im \end{bmatrix} \begin{bmatrix} \mathrm{i}\Im & \mathfrak{P}_i & \Im \\ 0 & \mathfrak{M}_i & 0 \\ \mathrm{i}\Re & \mathfrak{P}_r i & \Re \end{bmatrix} \begin{bmatrix} \Re & \mathfrak{P}_i & \mathrm{i}\Re \\ 0 & \mathfrak{M}_i & 0 \\ \Im & \mathfrak{P}_i & \mathrm{i}\Im \end{bmatrix} \begin{bmatrix} \Im & \mathfrak{P}_i & \mathrm{i}\Im \\ 0 & \mathfrak{M}_i & 0 \\ \Re & \mathfrak{P}_i & \mathrm{i}\Re \end{bmatrix}$$

For the boundary at s_3 (the real component of c_3):

$$\begin{bmatrix} \mathrm{i}\Re & \Re & \mathfrak{P}_r \\ \mathrm{i}\Im & \Im & \mathfrak{P}_r \\ 0 & 0 & \mathfrak{M}_r \end{bmatrix} \begin{bmatrix} \mathrm{i}\Im & \Im & \mathfrak{P}_r \\ \mathrm{i}\Re & \Re & \mathfrak{P}_r \\ 0 & 0 & \mathfrak{M}_r \end{bmatrix} \begin{bmatrix} \Re & \mathrm{i}\Re & \mathfrak{P}_r \\ \Im & \mathrm{i}\Im & \mathfrak{P}_r \\ 0 & 0 & \mathfrak{M}_r \end{bmatrix} \begin{bmatrix} \Im & \mathrm{i}\Im & \mathfrak{P}_r \\ \Re & \mathrm{i}\Re & \mathfrak{P}_r \\ 0 & 0 & \mathfrak{M}_r \end{bmatrix}$$

For the boundary at s_6 (the imaginary component of c_3):

$$\begin{bmatrix} i\Re & \Re & \mathfrak{P}_i \\ i\Im & \Im & \mathfrak{P}_i \\ 0 & 0 & \mathfrak{M}_i \end{bmatrix} \begin{bmatrix} i\Im & \Im & \mathfrak{P}_i \\ i\Re & \Re & \mathfrak{P}_i \\ 0 & 0 & \mathfrak{M}_i \end{bmatrix} \begin{bmatrix} \Re & i\Re & \mathfrak{P}_i \\ \Im & i\Im & \mathfrak{P}_i \\ 0 & 0 & \mathfrak{M}_i \end{bmatrix} \begin{bmatrix} \Im & i\Im & \mathfrak{P}_i \\ \Re & i\Re & \mathfrak{P}_i \\ 0 & 0 & \mathfrak{M}_i \end{bmatrix}$$

4. Basics

The standard representation of the identity operation is

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{c}$$

The identity in $\mathbf{C^3}$ can also be written:

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \Re + i\Im & 0 \\ 0 & 0 & \Re + i\Im \end{bmatrix} \mathbf{c}$$

Delaunay (1932) does not consider the boundary transformations in detail. However, he uses them to define the process of Selling reduction. For example in $\mathbf{S^6}$, he lists the following as one of the possible results for a transformation on s_1. $\{-s_1, -s_1+s_2, s_1+s_3, s_1+s_5, s_1+s_4, s_1+s_6\}$ The third matrix above (the third boundary transform for s_1) implements this operation and interchanges the real part of c_3 and the imaginary part of c_2.

$$\begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \Re & i\Re \\ \mathfrak{P}_r & \Im & i\Im \end{bmatrix}$$

In terms of $\mathbf{C^3}$, Delone's alternate transformation for the s_1 boundary would exchange the real of c_2 with the imaginary part of c_3. That is the fourth matrix in the list for s_1. The other two transformations for s_1 can be generated from the two we have just displayed by the "exchange operation" (Andrews *et al.*, 2019a) applied to the second and third $\mathbf{C^3}$ elements. Delone did not describe the latter two transformation, perhaps because even a single transformation was adequate to implement reduction. He already listed two.

5. Summary

The considerable regularity of the transformation matrices (above) highlights one of the important aspects of Selling reduction as used by Delaunay (1932) when compared to Niggli reduction (Niggli, 1928). Where all the boundaries of the fundamental orthant in $\mathbf{C^3}$ and $\mathbf{S^6}$ are basically the same (and indeed are related by reflections), the boundaries formed in Niggli reduction are of multiple types, and the fundamental unit of the space representing Niggli reduced cells ($\mathbf{G^6}$, see Andrews & Bernstein (2014)) is non-convex.

The matrices display one of the properties of $\mathbf{C^3}$ that make it a useful representation. For the scalar being transformed, it and its opposite scalar create a unique row in each matrix. Those rows contain only the minus operator and zeros, highlighting the unique relationship of that pair of scalars.

Several aspects of C3 are obvious from inspecting the matrices above. First, we see that each boundary has four possible transformations that can be applied. Because the each of the transformations at boundaries are self-inverse, they are the same transformations that would be used in the process of cell (lattice) reduction. Delaunay (1932) and Delone *et al.* (1975) give only two choices. Presumably for simplicity they did not list the transformations that used the "exchange" operator (see (Andrews *et al.*, 2019a)).

6. Availability of code

The C^{++} code for $\mathbf{C^3}$ is available in github.com, in `https://github.com/duck10/LatticeRepLib.git`.

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References

Andrews, L. C. & Bernstein, H. J. (2014). J. Appl. Cryst. **47**(1), 346 – 359.

Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019a). Acta Cryst. A**75**. Https://doi.org/10.1107/S2053273318015413.

Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019b). Acta Cryst. A**75**(3), 593–599.

Delaunay, B. N. (1932). Z. Krist. **84**, 109 – 149.

Delone, B. N., Galiulin, R. V. & Shtogrin, M. I. (1975). J. Sov. Math. **4**(1), 79 – 156.

Niggli, P., (1928). Krystallographische und Strukturtheoretische Grundbegriffe, Handbuch der Experimentalphysik, Vol. 7, part 1. Akademische Verlagsgesellschaft, Leipzig.

Selling, E. (1874). Journal für die reine und angewandte Mathematik (Crelle's Journal), **1874**(77), 143 – 229.