MS32-2-2 Mapping the Space of Two-Dimensional Lattices
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M. Bright [1], V. Kurlin [1], A. Cooper [1]
[1]University of Liverpool - Liverpool (United Kingdom)

Abstract
Crystallographic unit cells are traditionally classified discretely (for example, into Bravais classes). We are interested in finding a continuous classification. By this we mean the derivation of some quantity from the geometric parameters of a unit cell, which does not vary under transformations giving rise to the same lattice (for example, rotation and translation), and a real number associated with pairs of these quantities which defines a 'distance' between them (for example, it is zero between two identical lattices), that takes small values between two unit cells that differ only by a small geometric perturbation.

One can use such a metric to associate the precise position of a structure in the resulting space of, and continuously measured physical properties such as conductivity or opacity.

A barrier to this approach is that the same lattice can be described by an infinite number of different basis vectors. We can impose a list of inequalities on the geometric parameters of a lattice which gives a provably unique selection – Niggli's reduced cell [1] being the most well known. However, it is proved in [2] that any such selection will be discontinuous - a small perturbation of the lattice can lead to a large change in the geometry of the unit cell.

Building on work in [3], we prove in [4] that a unique invariant can be derived for 2 dimensional lattices, and in [5] we use this invariant to develop a measure of 'chirality distance' – the closeness of a lattice to its nearest neighbour with higher symmetry – and from this a distance between any two lattices that satisfies the desired conditions, giving the first representation to our knowledge of all 2D lattices as points in a metric space. In Figure 1 we represent this space as a square with opposite edges identified where each point represents (up to scaling) a unique lattice, and show the density of millions of lattices derived from the Cambridge Crystallographic Structural Database [6].

A practical application is to look at the growing number of materials which could potentially be crystallised as monolayers. To date the most extensive database of such materials be found in [7], a subset of which have had their theoretical monolayer lattice structures computed. Figure 2 shows a plot of this data in the same square as Figure 1, which suggests that monolayer structures cluster strongly in areas of high symmetry.

References
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Density Map of Lattices in the Metric Space

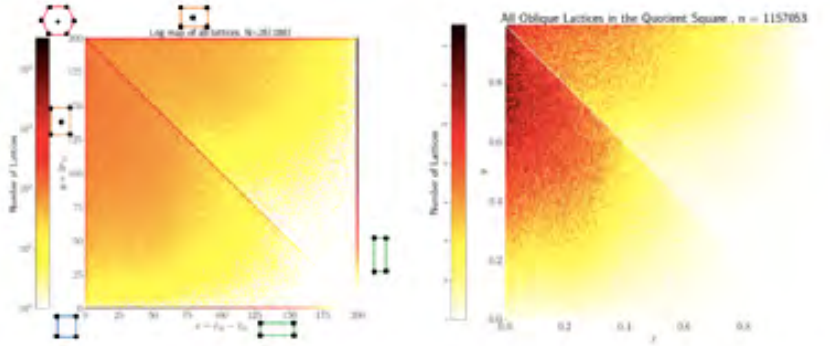

Figure 1: Density plot of all 2D unit cells derived from the Cambridge Crystallographic Structural Database in a metric space defined by geometric invariants. **Left**: All cells - position of cells with particular symmetries in the space are marked. **Right**: Cells with no reflection/rotation symmetries only.

Position of Lattices from [7] in the Metric Space

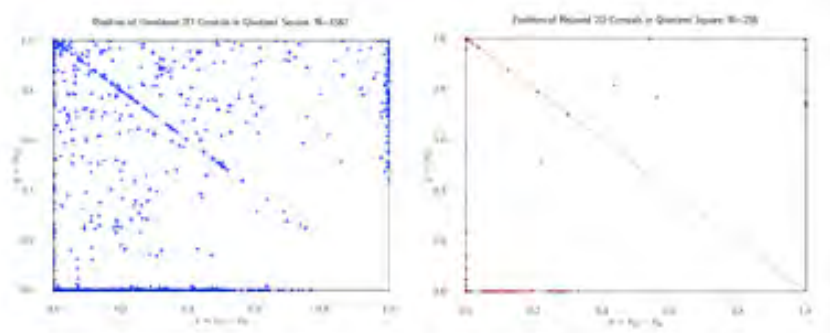

Figure 2: Plot of 2D unit cells from monolayer structures in [7], in the representation of the metric space shown in Figure 1. **Left** 'Unrelaxed' lattices, whose 2 dimensional unit cell is derived from the parent 3 dimensional lattice. **Right** 'Relaxed' lattices, where the structure of the 2 dimensional cell in isolation from its parent structure has been simulated.