Making DC7 Invertible

Herbert Bernstein[1], Larry Andrews[2]

[1]Ronin Institute for Independent Scholarship, c/o NSLS-II, Brookhaven National Lab, Bldg 745

[2]Ronin University

yayahjb@gmail.com

There are many metrics that can be used to estimate distances between lattices. An ideal metric should vary smoothly with small changes in the lattices, but also be uniformly sensitive to such changes, return a zero distance if and only if the lattices are identical, satisfy the triangle inequality, and be computable quickly. Many metrics are available. The V7 metric has most of the desired characteristics, but has poor sensitivity near 90 degree angles. The Niggli-reduction G6-based NCDist metric has fairly uniform sensitivity but is computationally expensive and has issues in terms of smoothness. The Selling-reduction S6-based metrics are computationally less expensive and, by restricting the space to all-obtuse cells, avoid glitches associated with the transitions between all-acute and all-obtuse cells. This leads naturally to consideration of Dirichlet cells which arise from the Voronoi decomposition of a lattice. The Dirichlet cell is fully characterized by thirteen distances derived from a Niggli reduced cell: the three edge length, the six face diagonals and the four body diagonals which form a -dimensional space called DC. If used directly as a vector space, DC is far from smooth. If we sort those elements in increasing order, the first seven sorted elements form a space called DC7 [Bernstein Andrews 2021], which is very smooth, and for lattices of known high symmetry is invertible, but which lumps together some lattices that differ in lower symmetry cases [Bright et al. 2021]. We propose an unsorted version of DC7 which is fully invertible. The DC7u space consists of the three cell edges, the three shorter face diagonals, and the shortest body diagonal.

Bernstein, H.J. and Andrews, L.C., 2021, August. DC7, A very efficient lattice comparison metric. Acta Cryst. A77, C809

Bright, M., Cooper, A.I. and Kurlin, V., 2021. A complete and continuous map of the Lattice Isometry Space for all 3-dimensional lattices. arXiv preprint arXiv:2109.11538.