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Journal: Acta Crystallographica Section A: Foundations and Advances
Paper: uv5016
Authors: Lawrence C Andrews* and Herbert J Bernstein
Title: Measuring Lattices

Review of manuscript uv5016

This submission approaches the "surprisingly complex and computationally demanding problem" (p.1), which is correctly noted in the abstract. However, some other statements require substantial corrections. The history section might be more appropriate for an appendix, especially since several quoted facts are a bit outdated. For example, the Cambridge Structural Database (p.2) now has over 1.21 million structures. A couple of references on page 3 are displayed by question marks.

The introductory section discusses the apparent simplicity of unit cells but misses the key difference between lattices and their cells. Both concepts can be most suitably defined in section 1, for example, after merging the currently very short sections 2-5.

The authors correctly emphasize that "to measure a meaningful distance between two objects, the objects need to be placed in a ”metric space”" (p.5). Hence a metric space and a distance metric satisfying the metric axioms can be explicitly defined otherwise the crystallographers might remain "convinced that unit cells are simple" (p.4).

Fig. 2 (p.6) shows a drawing of an open curve in a plane, which is surprisingly called an empty unit cell. If a unit cell was formally defined, say as a parallelepiped spanned by a linear basis, there would be no confusion. Another undefined but frequently used concept is a fundamental cell or unit, which is also called a fundamental region (p.9) in the abstract. This concept requires a clearly specified group action (see below in more detail).

The authors should be praised for attempting to use a topological (or continuous) language or approach for lattices. Since topology is a rather abstract and deep area of pure mathematics, a lot of care is needed to make correct statements. For example, "gluing" two edges of the one-dimension cell turns the cell into a circle" but does not make the problem two dimensional (p.7). Any topological circle still has dimension 1, not 2, because any local neighborhood of a point on the circle is homeomorphic to an interval in the 1-dimensional line.

The above confusion with the dimension is very common, unfortunately. Of course, we cannot draw a circle (without overlaps) within a 1-dimensional line, but the possibility of drawing a circle in the plane without self-intersections doesn't make the circle 2-dimensional.
In particular, any graph is intrinsically 1-dimensional because it can be parameterized by a single variable (using different range intervals for different edges) with appropriate identifications at vertices. In the same way, the surface of a sphere (say, of our planet Earth) is 2-dimensional, because any geographic position can be uniquely described by two coordinates (latitude and longitude), without taking the altitude into account.

Similarly, gluing opposite pairs of edges of a two-dimensional cell turns it into a 2-dimensional torus, not a 3-dimensional torus (p.7).

Since the authors start from the 1-dimensional case, the readers could be reminded that this case was completely resolved in arxiv:2205.04388, for all high-dimensional sequences of points that are periodic in one direction. Since Fig. 2-6 and their comments summarize the knowledge from the 19th century, this part might be reasonably combined with the history section in the appendix. The very short section 7 mainly consists of references to the appendix, hence, might also benefit from moving there.

Section 8 entitled "Fundamental region" (p.8) should properly define this region because the mathematical meaning (https://en.wikipedia.org/wiki/Fundamental_domain) seems to substantially differ from a region of G^6 or S^6, which is expected to uniquely represent all lattices by six parameters. Reference to a Wikipedia article does not resolve the issue of a lack of definitions as Wikipedia provides only "Hints at general definition" with the clearly stated possibility to choose between "several precisely defined ways". Without proper definitions, this choice remains a mystery in the current paper. The authors make a lot of helpful historical references and could help the reader with a key reference, where the uniqueness of Niggli's cell is formally proved as a mathematical theorem, not simply mentioned as in many papers.

On several pages, the Selling/Delone reduction is claimed to give uniquely defined negative parameters (scalar products of basis vectors a,b,c, and d=-a-b-c). Could the authors similarly provide a reference to a proper proof of this claim and also discuss if the following two bases of the simplest cubic lattice are Selling/Delone reduced in the sense that all scalar products are not positive?

a=(1,0,0), b=(0,1,0), c=(0,0,1), d=(-1,-1,-1)

a=(1,0,0), b=(0,1,0), c'=(-1,0,1), d'=-a-b-c'=(0,-1,-1)

Section 9 starts with a great correct statement that "measuring the distance between two lattices comes down to finding a geodesic between them" (p.10). Hence the authors could agree that a metric on the space of lattices needs to be formally defined. The claim that "the obvious step to find the shortest distance between two lattices is to simply compute the Euclidean distance between them in the fundamental unit" (p.10) seems to contradict the wise warning from the introduction: "the concept of the simple lattice is felt to be almost as simple as unit cells" (p.4). A lattice itself also remains undefined in the paper. When arbitrary lattices are compared, what "fundamental unit" is used in this "obvious step"?

Since all further constructions use this undefined "fundamental unit", a substantial revision of the important notations and their definitions are needed before any further steps can make sense. If Niggli's cell is considered as the fundamental unit, the authors' work from the 1980s already showed that Niggli's cell can substantially change under tiny perturbations. It seems that this paper aims to go beyond this important achievement and produce a continuous metric between lattices.

It remains to re-iterate the understanding that this "surprisingly complex and computationally demanding problem" (from the abstract, p.1) requires rigorous definitions and formal proofs, of all metric axioms and continuity under perturbations in particular. Looking forward to receiving an improved version.

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The paper deals with practically important problem of comparing two unit cells or, in other words, measuring the distance between them. The exposition of the material is clear albeit sometimes more mathematical rigour would be desirable. For example, the authors somehow managed not to use the language of quadratic forms when discussing lattices.

The problem of comparing lattices is inherent to any crystal structure determination. In particular, the primitive cell found from X-ray scattering is transformed to a reduced one, and this reduced cell is then compared to the reference list of reduced cells. In this way (the type of) Bravais lattice is determined. This procedure is included in the software that is integrated into any automatic diffractometer. It would be advantageous if the authors could give some overview of the algorithms which are used by modern diffractometers for determining the (type of) Bravais lattices from experimental data.

In Part 8 it is not clear which kind of fundamental region is meant. A fundamental region is related to the action of some group on some space (or a set of elements). In this way we can speak of a fundamental region for a point group, a space group etc. It is not clear which kind of a fundamental region is considered, particularly, it is not clear the action of which group in 6D space is assumed. So please clarify.

Finally, I would like to bring to the attention of the authors a seminal paper by Burzlaff and Zimmermann that compares Delaunay and Niggli reduction schemes (On the metrical properties of lattices. Z. Kristallogr. 170, 247-262).

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The authors present a comprehensive paper entitled “Measuring Lattices”. The paper presents comprehensive dive into measuring distances between three-dimensional lattices which is a complex topic but also gaining importance in light of emerging computation methods. The paper gives an overview of the related history (which I very much enjoyed), discusses different methods and reviews available software making.

In summary a timely paper and my only comments are concerning the figures. The paper has a large number of figures which I find illustrate the discussion text, but I am wondering if some can be combined or presented as a multi-panel figure. Fig 7 seems to be missing a proper caption.

Apart from these very minor editorial comments, I recommend the paper as is and look forward to seeing it in print.