August 25, 2025

Niggli reduction: matrices for 3-D lattice transformations

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lattice; **reduction**; **Niggli**

Abstract

Niggli reduction finds the most compact unit cell of a 3-D lattice. Existing algorithms operate in $\mathbf{G^6}$ space, and the 3-D basis-vector changes are lost. We tabulate the $3{\times}3$ matrices for every step of the reduction, enabling direct re-indexing of reflections and full reconstruction of the reduction history.

1. Introduction

Niggli reduction (Niggli, 1928) finds the cell with the three shortest base vectors in a 3-D lattice. Gruber (1973) published a compact algorithm using scalars that were later described in the space $\mathbf{G^6}$ (Andrews & Bernstein, 2014). Although effective, the algorithm works in a six-dimensional space, losing the three-space transformations needed for changing unit cell presentation or for reindexing reflection data.

Here we tabulate the 3-D matrices for transformation of unit cell basis vectors corresponding to each step in Niggli reduction. They allow the accumulation during Niggli reduction of all of the changes in the unit cell presentation. The matrix that is finally accumulated transforms the input basis to the Niggli reduced basis.

2. Conventions

Andrews & Bernstein (2014) give the formal presentation of $\mathbf{G^6}$.

- $G^6 = (g_1, g_2, g_3, g_4, g_5, g_6)$ with

$$g_1 = a^2, \ g_2 = b^2, \ g_3 = c^2, \ g_4 = 2bc\cos\alpha, \ g_5 = 2ac\cos\beta, \ g_6 = 2ab\cos\gamma.$$

- Gruber (1973), called the process of putting the scalars into a fixed order "normalizing". We use the more descriptive term "standard presentation".
- Gruber labeled his pseudocode for standard presentation as "Algorithm N" and his pseudocode for reduction as "Algorithm B".

3. Matrices and Trigger Conditions

We list matrices to transform unit cell basis vectors during Niggli reduction in Tables 1 and 2, along with arbitrary names for the operations and also the conditions for triggering each operation during reduction. If a condition evaluates to true, then the operation should be performed. For complete Niggli reduction, the steps are repeated from the identity, SP0, to convergence.

The numbering of all the operations, both standard presentation and reduction, start from zero for the first standard presentation and continues through to R12. (Note that the matrices for operations R9, R10 and R11 are the same as those for R5, R6, and R7, respectively.)

4. Usage

1. Start with SP0.

2. Loop through SP and R tables until no trigger fires.

3. Accumulate the product of all applied matrices; the final product maps the initial basis to the Niggli-reduced basis.

Table 1. *The matrices for Standard Presentation (SP). The conditions for SP34a,b,c are patterns of (g_4, g_5, g_6). The symbols are "0" for a fixed value of zero, "+" for a positive value in that position, and "-" for negative.*

Designation	Matrix	Trigger condition on G^6
SP0	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	(identity)
SP1	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\lvert g_1 \rvert > \lvert g_2 \rvert + \delta$
SP2	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	$\lvert g_2 \rvert > \lvert g_3 \rvert + \delta$
SP34a	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$(--+)$ *or* $(+0-)$ *or* $(0+-)$
SP34b	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$(-+-)$ *or* $(+-0)$ *or* $(0-+)$
SP34c	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$(+--)$ *or* $(-+0)$ *or* $(-0+)$

Table 2: The operations for Niggli reduction

Designation	Matrix	Trigger condition on G^6 ($\delta > 0$)
R5$^+$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$	$g_4 > g_2 + \delta$, $g_4 > 0.0$
R5$^-$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$	$g_4 > g_2 + \delta$, $g_4 \leq 0.0$
R6$^+$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	$g_5 > g_1 + \delta$, $g_5 > 0$
R6$^-$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$	$g_5 > g_1 + \delta$, $g_5 <= 0$
R7$^+$	$\begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$g_6 > g_1 + \delta$, $g_6 > 0$
R7$^-$	$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$g_6 > g_1 + \delta$, $g_6 <= 0$
R8	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix}$	$g_4 + g_5 + g_6 + g1 + g_2 < -\delta$
R9$^+$	same as R5$^+$	$|g_4 - g_2| <= \delta$ and $2g_5 < g_6 + \delta$ and $g_4 > 0$
R9$^-$	same as R5$^-$	$|g_4 - g_2| <= \delta$ and $2g_5 < g_6 + \delta$ and $g_4 <= 0$
R10$^+$	same as R6$^+$	$|g_5 - g_1| <= \delta$ and $2g_4 < g_6 + \delta$ and $g_5 > 0$
R10$^-$	same as R6$^-$	$|g_5 - g_1| <= \delta$ and $2g_4 < G_6 + \delta$ and $g_5 <= 0$
R11$^+$	same as R7$^+$	$|g_6 - g_1| \leq \delta$ and $2g_4 < g_5 + \delta$ and $g_6 > 0$ or $|g_6 - g_1| < \delta$ and $2g_4 < g_5 + \delta$ and $g_6 > 0$
R11$^-$	same as R7$^-$	$|g_6 - g_1| \leq \delta$ and $2g_4 < g_5 + \delta$ and $g_6 <= 0$ or $|g_6 - g_1| < \delta$ and $2g_4 < g_5 + \delta$ and $g_6 <= 0$

Designation	Matrix	Trigger condition on G^6 ($\delta > 0$)
R12	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & -1 & 1 \end{bmatrix}$	$\lvert g_4 + g_5 + g_6 + g_1 + g_2 \rvert <= \delta$ *and* $2\lvert g_1 + g_5 \rvert + g_6 > \delta$

5. Synopsis

Niggli reduction is formulated in terms of 6 scalars that formally are the components of space $\mathbf{G^6}$. Working in a higher dimensional space loses the 3-space transformations that are needed for reindexing reflection data and for changing the orientation of atomic structure. The matrices are listed here corresponding to each of the operations of Niggli reduction.

References

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Synopsis