1. Introduction

This is an analysis of Niggli Reduction.

2. *

Historical Evolution of Lattice Reduction: Selling, Niggli, and Krivy–Gruber

Selling's Trace Minimization (Late 19th Century)

Selling's reduction aimed to simplify lattice bases by minimizing the trace of the metric tensor:

$$\mathrm{Tr}(\mathbf{G}) = g_1 + g_2 + g_3 = a^2 + b^2 + c^2$$

This corresponds to minimizing the sum of squared edge lengths, favoring compact and symmetric cells. Selling worked geometrically in an inner product space, seeking convex minimal representations. His approach did not enforce uniqueness—multiple minimal cells could exist.

Niggli's Canonical Reduction (1928)

Niggli adopted Selling's trace minimization as a first-order goal but introduced additional conditions to select a unique reduced cell. These include:

- **Edge Ordering:** $g_1 \le g_2 \le g_3$
- **Angle Constraints:** $|g_4| \le g_2$, $|g_5| \le g_1$, $|g_6| \le g_1$
- **Sign Consistency:** All off-diagonal terms (g_4, g_5, g_6) must be either strictly positive or strictly non-positive
- **Tie-Breaking Equalities:** When equalities occur (e.g., $g_1 = g_2$), apply axis permutations, sign flips, and secondary inequalities to resolve symmetry

These conditions define a canonical region in metric tensor space (G^6), ensuring uniqueness, symmetry, and minimal trace.

- Tolerance bands for floating-point stability
- Fallback logic for near-degenerate cases
- Classifier overrides for boundary intersections and instability zones

These enhancements extend Niggli's reduction to practical, reproducible classification pipelines.

2.1. Summary Comparison

Feature	**Selling Reduction**	**Niggli Reduction**
Goal	Minimize trace (compact cell)	Minimize trace + enforce canonical form
Space	Inner product space	Metric tensor space (G^6)
Conditions	Convex minimization	Inequalities + sign rules + tie-breakers
Output	One of many minimal cells	Unique reduced cell

Table 1: Complete catalog of 45 boundary polytopes of the Niggli-reduced region in G^6, extended with symbolic triggers. The final column encodes reduction-relevant features: **E** (Edge degeneracy), **A** (Angle saturation), **O** (Orthogonality), **C** (Compound intersection), **N** (Near-degeneracy). These tags support classifier overrides, adjacency logic, and parametric instability detection.

Label	**Condition**	**Geometric Interpretation**	**Reduction Behavior**	**Instabili**
A1	$g_1 = g_2$	Edge degeneracy between a and b	Soft	S
A2	$g_2 = g_3$	Edge degeneracy between b and c	Soft	S
A3	$g_1 = g_3$	Edge degeneracy between a and c	Soft	S
A4	$g_1 = g_2 = g_3$	Triple edge equality; cubic candidate	Hard	U
A5	$g_1 \approx g_2$	Near-degeneracy; axis ambiguity	Conditionally Hard	C
A6	$g_2 \approx g_3$	Near-degeneracy; axis ambiguity	Conditionally Hard	C
A7	$g_1 = g_2$, $g_3 \approx g_1$	Double degeneracy; ambiguous sorting	Hard	U
A8	$g_1 = g_2$, $g_4 = 0$	Edge equality with orthogonality	Conditionally Hard	C

Label	Condition	Geometric Interpretation	Reduction Behavior	Instabili
A9	$g_1 = g_3,\ g_5 = 0$	Edge equality with orthogonality	Conditionally Hard	C
A10	$g_2 = g_3,\ g_6 = 0$	Edge equality with orthogonality	Conditionally Hard	C
A11	$g_1 = g_2,\ g_5 = g_6$	Degenerate manifold with angle coupling	Hard	U
A12	$g_1 = g_2,\ g_4 = g_5$	Degenerate manifold with angle coupling	Hard	U
A13	$g_1 = g_2,\ g_4 = g_6$	Degenerate manifold with angle coupling	Hard	U
A14	$g_1 = g_2,\ g_4 = g_5 = g_6$	Fully coupled degeneracy	Hard	U
A15	$g_1 = g_2,\ g_4 = g_5 = g_6 = 0$	Orthogonality with edge degeneracy	Conditionally Hard	C
B1	$\lvert g_4\rvert = g_2$	Saturation of α cosine	Conditionally Hard	C
B2	$\lvert g_5\rvert = g_1$	Saturation of β cosine	Conditionally Hard	C
B3	$\lvert g_6\rvert = g_1$	Saturation of γ cosine	Conditionally Hard	C
B4	$\lvert g_4\rvert = g_3$	Alternate saturation for α	Conditionally Hard	C
B5	$\lvert g_5\rvert = g_3$	Alternate saturation for β	Conditionally Hard	C
B6	$\lvert g_6\rvert = g_2$	Alternate saturation for γ	Conditionally Hard	C
B7	$\lvert g_4\rvert = \lvert g_5\rvert$	Coupled angle saturation	Hard	U
B8	$\lvert g_5\rvert = \lvert g_6\rvert$	Coupled angle saturation	Hard	U
B9	$\lvert g_4\rvert = \lvert g_6\rvert$	Coupled angle saturation	Hard	U
B10	$\lvert g_4\rvert = g_2,\ \lvert g_5\rvert = g_1$	Dual saturation	Hard	U
B11	$\lvert g_4\rvert = g_2,\ g_1 \approx g_2$	Saturation with edge degeneracy	Hard	U
B12	$\lvert g_5\rvert = g_1,\ g_1 \approx g_3$	Saturation with edge degeneracy	Hard	U
B13	$\lvert g_6\rvert = g_1,\ g_2 \approx g_3$	Saturation with edge degeneracy	Hard	U
B14	$\lvert g_4\rvert = g_2,\ g_4 = 0$	Saturation and orthogonality	Conditionally Hard	C
B15	$\lvert g_5\rvert = g_1,\ g_5 = 0$	Saturation and orthogonality	Conditionally Hard	C
C1	$g_4 = 0$	$\alpha = 90°$	Soft	S
C2	$g_5 = 0$	$\beta = 90°$	Soft	S
C3	$g_6 = 0$	$\gamma = 90°$	Soft	S
C4	$g_4 = g_5 = 0$	$\alpha = \beta = 90°$	Soft	S
C5	$g_5 = g_6 = 0$	$\beta = \gamma = 90°$	Soft	S
C6	$g_4 = g_6 = 0$	$\alpha = \gamma = 90°$	Soft	S
E1	$g_1 = g_5 = g_6$	Edge and angle coupling	Hard	U
E2	$g_1 = g_2,\ g_6 = 0$	Tetragonal–orthorhombic transition	Hard	U
E3	$g_4 = g_5 = g_6 = 0$	Full orthogonality; unstable with edge degeneracy	Conditionally Hard	C
E4	$g_1 = g_2,\ \lvert g_4\rvert = g_2$	Edge degeneracy with angle saturation	Hard	U

Label	Condition	Geometric Interpretation	Reduction Behavior	Instabili
E5	$g_1 = g_3,\ g_5 = 0$	Axis ambiguity with orthogonality	Conditionally Hard	C
E6	$g_2 = g_3,\ \|g_6\| = g_1$	Coupled degeneracy and saturation	Hard	U
E7	$g_1 = g_2 = g_3,\ g_4 = g_5 = g_6 = 0$	Fully cubic cell; multiple reduction paths	Hard	U
E8	$g_1 = g_2,\ g_4 = g_5,\ g_6 = 0$	Compound degeneracy with orthogonality; ambiguous sorting	Hard	U
E9	$g_4 = g_5 = g_6 = 0,\ g_1 \approx g_2$	Orthogonality with edge near-degeneracy; classifier override may be needed	Conditionally Hard	C

3. *

Saturations in Niggli Reduction

In the context of Niggli reduction and the geometry of the reduced region in G^6, a **saturation** refers to a condition where one of the Niggli inequalities becomes an exact equality. That is, the metric tensor lies precisely on a boundary of the Niggli-reduced region.

4. *

Definitions: Reduction Behavior Categories

Each boundary polytope in the Niggli-reduced region of G^6 is classified by its reduction behavior. These categories reflect the stability, uniqueness, and reproducibility of the reduced cell under Krivy–Gruber reduction and guide classifier overrides.

Hard

A boundary is classified as **Hard** if it exhibits intrinsic instability under reduction. This includes:

- **Non-uniqueness:** Multiple unimodular transformations yield distinct but valid reduced cells.
- **Perturbation sensitivity:** Infinitesimal changes in the metric tensor cause discontinuous shifts in the reduced cell.
- **Oscillatory behavior:** Reduction may cycle or fail to converge near the boundary.
- **Classifier override required:** Reduction alone cannot guarantee correct Bravais assignment.

Hard boundaries typically involve compound degeneracies, saturated inequalities, or cubic manifolds.

Conditionally Hard

A boundary is classified as **Conditionally Hard** if it is stable in isolation but may become unstable when intersected with other boundaries. These cases include:

- **Single saturations:** Exact equality in one Niggli condition (e.g., $|g_4| = g_2$)
- **Edge equalities with orthogonality:** Stable unless combined with near-degeneracy
- **Ambiguous sorting:** Near-equalities that may flip axis order under perturbation

Classifier pipelines must monitor adjacency and apply parametric triggers when multiple such conditions co-occur.

Soft

A boundary is classified as **Soft** if it is stable, reproducible, and reduction-consistent. These boundaries:

- Yield a unique reduced cell under Krivy–Gruber reduction

- Are insensitive to small perturbations
- Do not require classifier intervention

Soft boundaries include orthogonality conditions (e.g., $g_4 = 0$) and simple edge equalities (e.g., $g_1 = g_2$) that do not intersect with other instability zones.

Usage in Classifier Pipeline

These categories are encoded in the **Reduction Behavior** column of the boundary table and inform:

- Instability tagging (S, C, U)
- Symbolic trigger logic
- Override and fallback mechanisms

They ensure that classification remains robust across the full geometry of the Niggli cone in G^6.

Definition

Each Niggli condition imposes a constraint on the components of the metric tensor:

- Edge ordering: $g_1 \leq g_2 \leq g_3$
- Angle constraints: $|g_4| \leq g_2$, $|g_5| \leq g_1$, $|g_6| \leq g_1$
- Sign consistency: all of g_4, g_5, g_6 are either strictly positive or non-positive

A **saturation** occurs when one of these inequalities becomes an equality, such as:

- $g_1 = g_2$ (edge length equality)
- $|g_4| = g_2$ (angle cosine saturation)
- $g_4 = 0$ (orthogonality boundary)

These equalities define the **boundary polytopes** of the Niggli cone in G^6.

Geometric and Algorithmic Significance

Saturations mark the transition zones between different lattice types or symmetry classes. They often correspond to Bravais lattice boundaries, such as transitions between orthorhombic and tetragonal cells.

While a single saturation may not destabilize the reduction process, multiple simultaneous saturations can lead to:

- Degeneracy in the metric tensor
- Ambiguity in the choice of reduced cell
- Oscillatory or non-convergent behavior in Krivy–Gruber reduction

These cases define **instability zones**, where classifier pipelines may need to override reduction logic or apply stabilizing transformations.

5. *

Classifier Integration: Symbolic Adjacency Logic and Parametric Triggers

To support robust Bravais classification near boundary polytopes in G^6, we define a symbolic tagging and trigger system that encodes adjacency, degeneracy, and reduction instability. This system enables classifier pipelines to override ambiguous reductions, detect compound zones, and apply parametric logic consistently.

Symbolic Tags

Each boundary polytope is assigned a symbolic tag based on its defining condition:

Symbol	**Meaning**
E	Edge degeneracy (e.g., $g_1 = g_2$, $g_1 \approx g_2$)
A	Angle saturation (e.g., $\lvert g_4 \rvert = g_2$)
O	Orthogonality (e.g., $g_4 = 0$)
C	Compound intersection (multiple conditions active)
N	Near-degeneracy (e.g., $g_1 \approx g_2$, not exact)

Each boundary in the table may be tagged with one or more symbols (e.g., EA, EO, C) to indicate its reduction behavior and adjacency to other boundaries.

Adjacency Logic

Let B_i and B_j be boundary polytopes. Define the adjacency function:

$$\mathrm{Adj}(B_i, B_j) = \begin{cases} 1 & \text{if } B_i \text{ and } B_j \text{ share a variable or saturate adjacent conditions} \\ 0 & \text{otherwise} \end{cases}$$

This adjacency matrix enables the classifier to:

- Detect compound instability zones
- Weight instability scores based on proximity
- Trigger override logic when multiple adjacent boundaries are active

Parametric Triggers

Classifier logic may be activated by parametric thresholds or symbolic conditions. Examples include:

Edge Degeneracy Trigger

$$\text{If } |g_1 - g_2| < \epsilon_1 \Rightarrow \text{trigger axis ambiguity}$$

Angle Saturation Trigger

$$\text{If } ||g_4| - g_2| < \epsilon_2 \Rightarrow \text{trigger cosine saturation}$$

Compound Zone Trigger

$$\text{If } g_1 \approx g_2 \text{ and } g_4 = 0 \Rightarrow \text{trigger compound override}$$

These triggers may be encoded as symbolic rules or embedded directly into classifier logic. Thresholds ϵ_1, ϵ_2 should be tuned based on numerical stability and benchmarking.

Classifier Strategy

- Extend the boundary table with a **Symbolic Trigger** column (e.g., E, EA, EO, C)
- Build a lookup dictionary: boundary label $\rightarrow$ trigger set
- Use adjacency matrix to detect compound zones
- Apply parametric thresholds to activate override logic
- Tag unstable zones for fallback or signature-based classification

This system ensures that classifier pipelines remain reduction-aware, reproducible, and robust near degenerate or ambiguous regions of G^6.

Examples

Consider the condition $|g_4| = g_2$. This implies:

$$|2bc\cos\alpha| = b^2 \quad \Rightarrow \quad |\cos\alpha| = \frac{b}{2c}$$

This is the maximum allowable cosine for angle α given the edge lengths b and c. The cell lies exactly on the boundary of the reduced region for that angle.

Zone	**Typical Conditions**	**Classifier Implication**
Soft	$g_1 = g_2$, $g_4 = 0$	Stable reduction; no override needed
Conditionally Hard	$\lvert g_4\rvert = g_2$, $g_1 \approx g_2$, $g_1 = g_2$, $g_4 = 0$	Stable unless intersected; monitor adjacency and apply parametric triggers
Hard	$g_1 = g_2 = g_3$, $g_4 = g_5 = g_6 = 0$, $g_1 = g_5 = g_6$	Intrinsically unstable; classifier override required

5.1. 10130

testCase(np, ”case 10130”, G6(78.145, 6.409, 1.485, -6.169, -4.536, 8.971), true);

5.1.1. t estCase(np, ”acute”, G6(0.825, 1.000, 65.850, 0.611, 0.051, 0.825), true); converged at 100, but wandered a lot Iteration 99: 0.011 0.295 51.361 0.282 0.015 0.009 Output: 0.011 0.295 51.357 -0.273 -0.007 -0.009 Converged: YES Is Niggli reduced: YES Standard Niggli: 0.011 0.295 51.357 -0.273 -0.007 -0.009 Max difference: 6.39488e-14 ? MATCH

Iteration 100: 0.011 0.295 51.357 -0.273 -0.007 -0.009 Checking all boundaries: IsNiggli true g 0.011 0.295 51.357 -0.273 -0.007 -0.009

Checking boundaries: Checking boundaries: 8 (0.022) Checking boundaries: D’ (0) 7’ (0) A’ (0) 8’ (0.0179722) B’ (0.00943398) E’ (0.00714143) CONVERGED

Output: 0.011 0.295 51.357 -0.273 -0.007 -0.009 Converged: YES Is Niggli reduced: YES Standard Niggli: 0.011 0.295 51.357 -0.273 -0.007 -0.009

5.2. acute

testCase(np, ”acute”, G6(0.825, 1.000, 65.850, 0.611, 0.051, 0.825), true);

5.3. acute

Output: 0.825 1.000 65.850 -0.560 -0.051 -0.825 Converged: YES Is Niggli reduced: YES Standard Niggli: 0.825 1.000 65.850 0.611 0.051 0.825 Max difference: 1.65 ?

5.4. testCase(np, ”obtuse”, G6(78.145, 6.409, 1.485, -6.169, -4.536, 8.971), true);

5.5. =

==

Test: obtuse Input: 78.145 6.409 1.485 0.000 0.000 0.000

==

Test: Debug test Input: 78.145 6.409 1.485 0.000 0.000 0.000

Initial Phase 1: Phase1: Pattern 111, applying M2, M1 Phase1: Pattern 010, applying M2 Phase1 complete after 3 iterations Phase1 complete after 2 iterations

Iteration 0: 1.485 6.409 78.145 0.000 0.000 0.000 Checking all boundaries: IsNiggli true g 1.485 6.409 78.145 0.000 0.000 0.000 3 (6.409) 4 (0) 5 (0) Checking boundaries: 6/7 (6.409) 9/A (1.485) C/D (1.485) Checking boundaries: 8 (6.409) Checking boundaries: D' (0) 7' (0) A' (0) 8' (0) B' (0) E' (0) CONVERGED

Output: 1.485 6.409 78.145 0.000 0.000 0.000 Converged: YES Is Niggli reduced: YES Standard Niggli: 1.485 6.409 78.145 0.000 0.000 0.000 Max difference: 0 ? MATCH