

# A Theoretical Framework for Discovering Groups and Unitary Representations via Tensor Factorization

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## Motivation: Symmetry Discovery

### The Status Quo: Hard-Coded Symmetry.

Geometric Deep Learning (e.g., Equivariant NN) relies on *a priori* knowledge of symmetries to constrain the model. This guarantees generalization but limits applicability when symmetries are unknown.

### The Challenge: Automated Discovery.

Can a model *discover* the underlying symmetry group directly from data (e.g., an operation table), without hard-coding it?

**HyperCube** is a tensor factorization model that exhibits a strong inductive bias toward **Groups** and **Unitary Representations**, effectively learning symmetry from data.

## Problem Setup

$(Q, \circ)$ : a binary operation.  $|Q| = n$ .

**Cayley Tensor:**  $\delta_{abc} = \mathbb{I}_{\{a \circ b = c\}}$ .

**Quasigroup:**  $\delta$  is a Latin-square.

**Group:** A quasigroup that is associative.

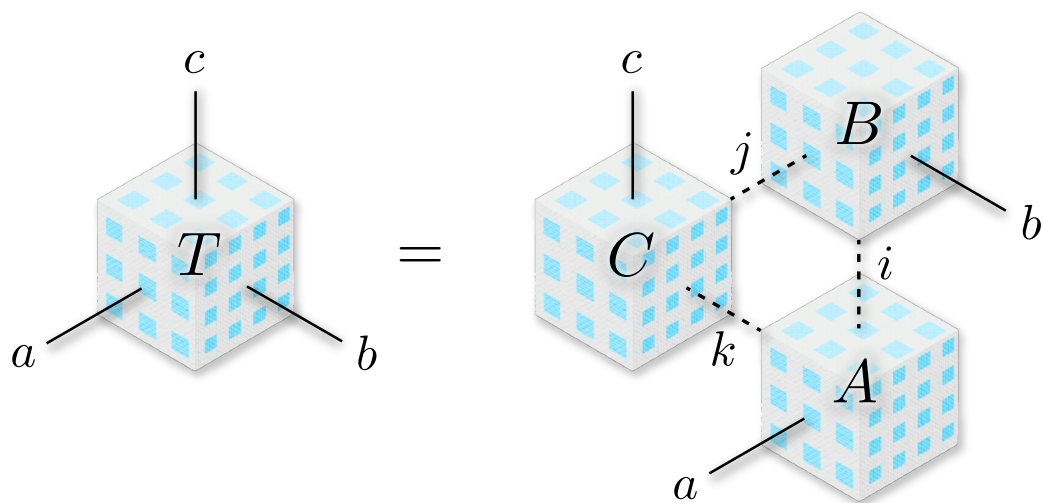
$|\delta| := \sum_{a,b,c} \delta_{abc} = n^2$ .

## HyperCube Model

Approximates  $\delta$  via a trilinear product of parameter tensors  $\Theta = (A, B, C)$ :

$$T_{abc}(\Theta) = \frac{1}{n} \text{Tr}(A_a B_b C_c) \quad (1)$$

Uses matrix product of **linear operators** ( $A_a \in \mathbb{C}^{n \times n}$ ) to capture interactions.



### Regularization Objective.

Jacobian Penalty: e.g.,  $\partial T_{abc} / \partial A_a = (B_b C_c)^\dagger$

$$\begin{aligned} \mathcal{H} &= \sum_{b,c} \|B_b C_c\|^2 + \sum_{c,a} \|C_c A_a\|^2 + \sum_{a,b} \|A_a B_b\|^2 \\ &= \sum_{a,b,c} \delta_{abc} (\|B_b C_c\|^2 + \|C_c A_a\|^2 + \|A_a B_b\|^2). \end{aligned}$$

How does this induce bias towards groups?

## Notation

Normalized inner product and norm

$$\langle X, Y \rangle := \frac{1}{n} \text{Tr}(X^\dagger Y), \quad \|X\|^2 := \langle X, X \rangle$$

so that  $\|U\|^2 = 1$  for any unitary  $U$ .

## Geometric Mechanism

### 1. C–S Lower Bound.

From Cauchy-Schwarz inequality:

$$\left\| \frac{\partial T_{abc}}{\partial A_a} \right\|^2 \geq \frac{|T_{abc}|^2}{\|A_a\|^2}$$

Derive a lower bound  $\mathcal{H} \geq \mathcal{B}$ :

$$\mathcal{B} := \sum \delta_{abc} |T_{abc}|^2 \left( \frac{1}{\|A_a\|^2} + \frac{1}{\|B_b\|^2} + \frac{1}{\|C_c\|^2} \right)$$

### 2. Orthogonal Decomposition.

$\mathcal{H}(\Theta) = \mathcal{B}(\Theta; \delta) + \mathcal{R}(\Theta; \delta)$ , where

$$\mathcal{R} := \sum \delta_{abc} \left( \|\Delta_{abc}^{(A)}\|^2 + \|\Delta_{abc}^{(B)}\|^2 + \|\Delta_{abc}^{(C)}\|^2 \right)$$

with  $\Delta_{abc}^{(A)} := \frac{T_{abc}^*}{\|A_a\|^2} A_a - (B_b C_c)^\dagger$

Orthogonality:  $\langle A_a, \Delta_{abc}^{(A)} \rangle = T_{abc}^* - T_{abc}^* = 0$ .

### 3. Collinearity Manifold.

$\mathcal{R} = 0$  iff  $A_a$  and  $(B_b C_c)^\dagger$  are collinear.

**On the Manifold ( $\mathcal{R} = 0$ ):**

### 4. Constant Gram matrix:

$$\begin{aligned} X &= \frac{A_a A_a^\dagger}{\|A_a\|^2} = \frac{C_c^\dagger C_c}{\|C_c\|^2} \\ \kappa &:= \frac{\|A_a\|^2 \|B_b\|^2 \|C_c\|^2}{|T_{abc}|^2} = \frac{\text{rank}(X)}{n} \leq 1 \end{aligned}$$

### 5. AM-GM bound within the manifold:

$$\mathcal{B} \geq 3\kappa^{-1/3} |\delta|$$

$\mathcal{B}$  forces  $\kappa \rightarrow 1$  (Full Rank)  $\implies$  **Unitarity**.

## Theoretical Results

### Regular Representation Certificate.

For any group, the *Regular Representation* ( $\rho_r$ ) defines a *unitary collinear factorization*:

$$A_g = B_g = C_g^\dagger = \rho_r(g) \implies \mathcal{H} = 3|\delta|, \mathcal{R} = 0.$$

### Uniqueness Theorem.

Any unitary collinear factorization ( $\mathcal{R} = 0$ ) is unitarily equivalent to  $\rho_r$ .

**Implication:** A quasigroup admitting  $\mathcal{R} = 0$  must be a group isotope.

### Collinearity Dominance Conjecture.

Misalignment penalty  $\mathcal{R}$  dominates  $\mathcal{B}$ . This ensures optimization stays near  $\mathcal{R} = 0$ , ruling out spurious minima.

Under the conjecture:

### Global minimum for Group isotopes.

$$\mathcal{H}_{\min}(\delta) = \mathcal{H}(\Theta^*) = 3|\delta|$$

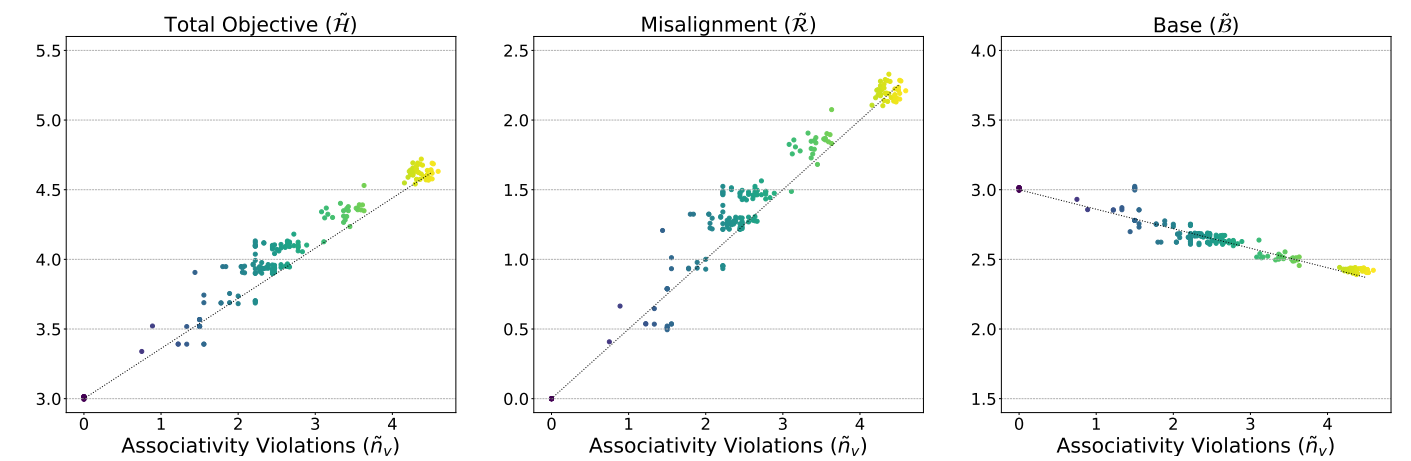
$\Theta^*$  is given by unitary collinear factors:  $\rho_r$ .

**Non-group isotopes** must incur **strictly higher loss**:

$$\mathcal{H}_{\min}(\text{Non-Group}) > \mathcal{H}_{\min}(\text{Group})$$

## Empirical Verification

We optimized  $\mathcal{H}$  for Latin-squares of orders  $n \in \{5, 6, 7, 8\}$ . We compare the minimum loss against the **Associativity Violation**  $n_v$ .



### Linear Scaling Laws.

The results reveal a precise tradeoff:

#### ► Misalignment Penalty:

$$\mathcal{R}_{\min} \approx 0.50 \cdot n_v.$$

#### ► Rank "Savings" (Right): $\mathcal{B}$ decreases

with non-associativity, but only by

$$\mathcal{B}_{\min} \approx 3|\delta| - 0.14 \cdot n_v.$$

### Collinearity Dominance.

The penalty slope (0.50) strictly dominates the savings (0.14).

$$\mathcal{H}_{\min}(\delta) \approx 3|\delta| + 0.36 \cdot n_v.$$

This confirms the global landscape forces optimization to **Group Isotopes** ( $\tilde{n}_v = 0$ ).

**Conclusion:**  $\mathcal{H}$  provides a **differentiable proxy** for groupness (associativity violation).

## Takeaways & Outlook

### 1. Novel Inductive Bias: Unitarity.

Standard DL models exhibit *Low-Rank* bias (interpolation). In contrast, HyperCube actively **maximizes rank** to achieve unitarity and enables **discrete structure discovery** beyond the limits of interpolation.

### 2. Mechanism of Discovery.

$\mathcal{H}$  decomposes into geometric forces — Collinearity + Rank Maximization — that structurally mandate Group theory.

### 3. Differentiable Associativity.

$\mathcal{H}$  serves as a differentiable proxy for associativity, allowing gradient-based discovery of discrete symmetries.

### Future Work.

Analytic proof of the Dominance Conjecture and extension to partial observation (Tensor Completion).

**NeuReps Workshop @ NeurIPS 2025**