Discovering Symmetry Breaking in Physical Systems with Relaxed Group Convolution

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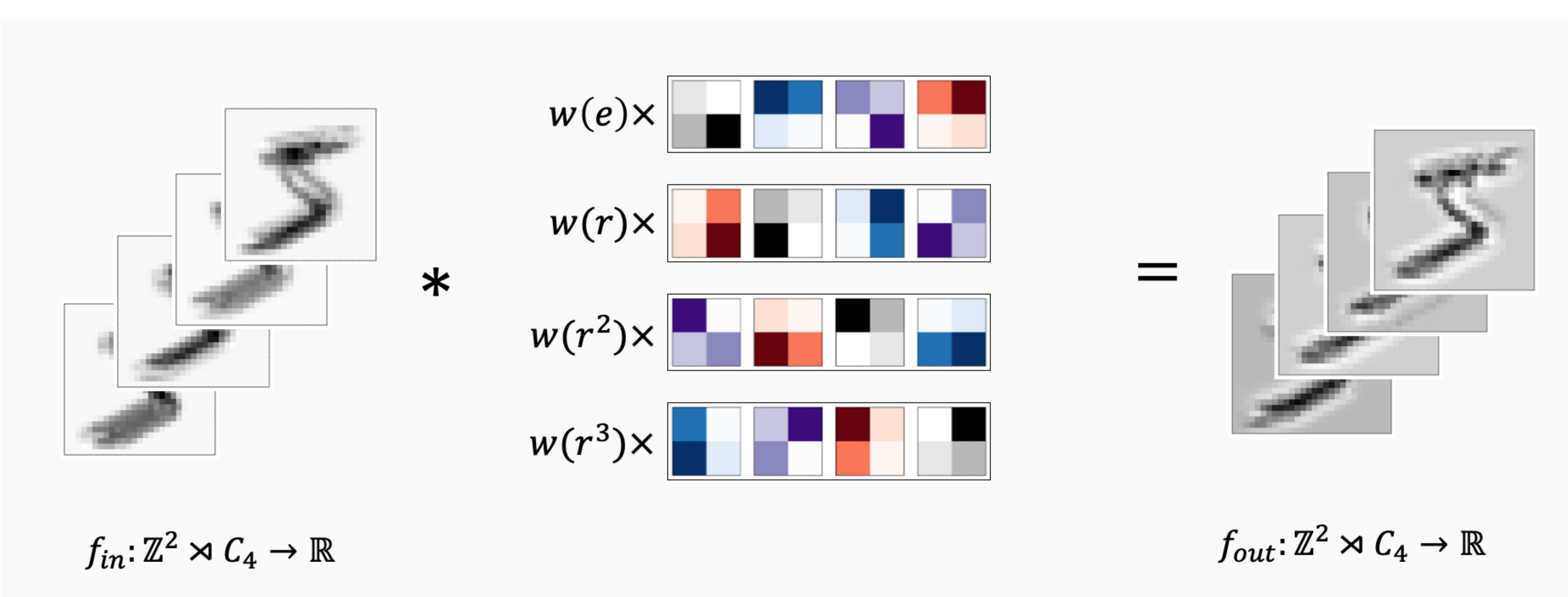
Abstract

Finding **symmetry breaking** is essential for understanding the fundamental changes in the behaviors and properties of physical systems, from microscopic particle interactions to macroscopic phenomena like fluid dynamics and cosmic structures. **Relaxed group convolution** emerges as a solution for instances when physical systems without perfect symmetries and perfectly equivariant models are restrictive. In this paper, we provide both theoretical and empirical evidence that this flexible convolution technique allows the model to **maintain the highest level of equivariance** that is consistent with data and discover the subtle symmetry-breaking factors in various physical systems. We employ various relaxed group convolution architectures to uncover symmetry-breaking factors in different physical systems, including the **phase transition of crystal structure** and the **isotropy and homogeneity breaking** in turbulence.

Relaxed Group Convolution

$$(f \tilde{\star} \Psi)(\mathbf{x}, h) = \sum_{\mathbf{y} \in \mathbb{Z}^3} \sum_{h' \in H} f(\mathbf{y}, h') \sum_{l=1}^{L} w_l(h) \Psi_l(h^{-1}(\mathbf{y} - \mathbf{x}), h^{-1}h')$$



Proposition

Consider a relaxed group convolution neural network where the relaxed weights are initialized to be identical to maintain G-equivariance. If it is trained to map an input X to the output Y, its relaxed weights will learn to be distinct across group elements in G during training in a way such that it is equivariant to $G \cap Stab(X) \cap Stab(Y)$, which is the intersection of the stabilizers of the input and the output and G.

Simple 2D Square-Rectangle Example

- The relaxed weights only deviate from being equal only when the symmetries of the input and the output are lower than that of the model.
- This suggests that by analyzing the relaxed weights post-training, we can determine which symmetries are broken.
- The group transformations with the same relaxed weights as those of the identity element stabilize both the input and the output.

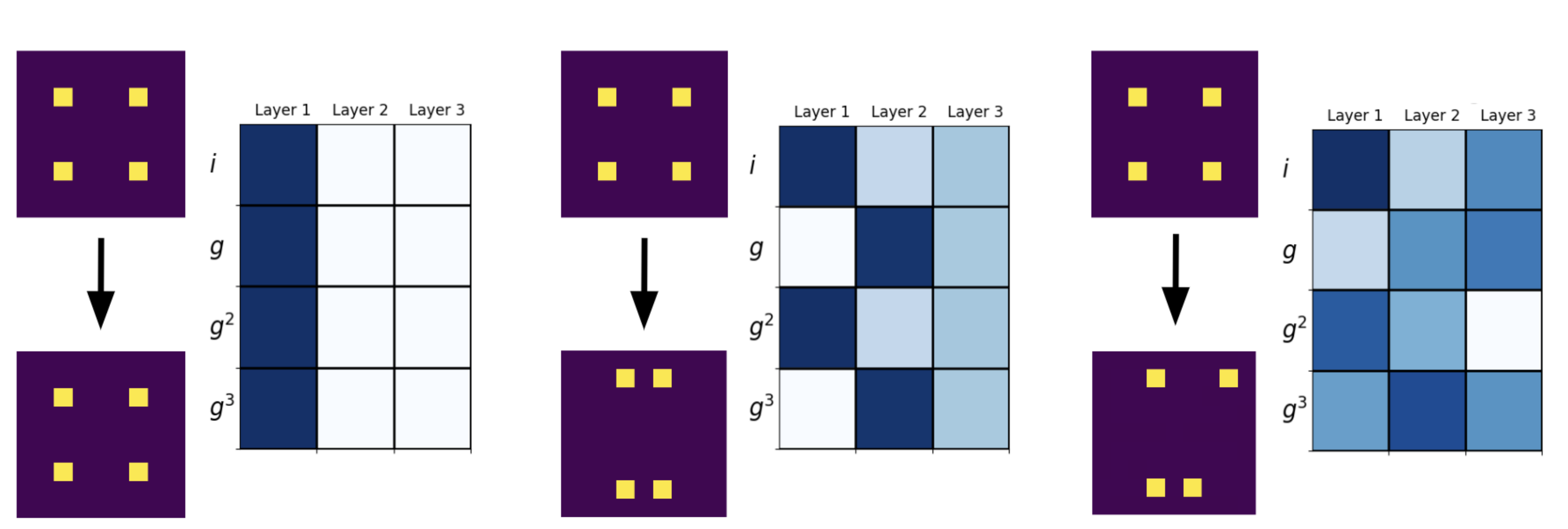


Figure: Visualization of tasks and corresponding relaxed weights after training. A 3-layer C_4-relaxed group convolution network with $L = 1$ is trained to perform the following three tasks: 1) map a square to a square; 2) deform a square into a rectangle; 3) map a square to a non-symmetric object.

Discover Symmetry Breaking Factors in Phase Transitions of Crystal Structures

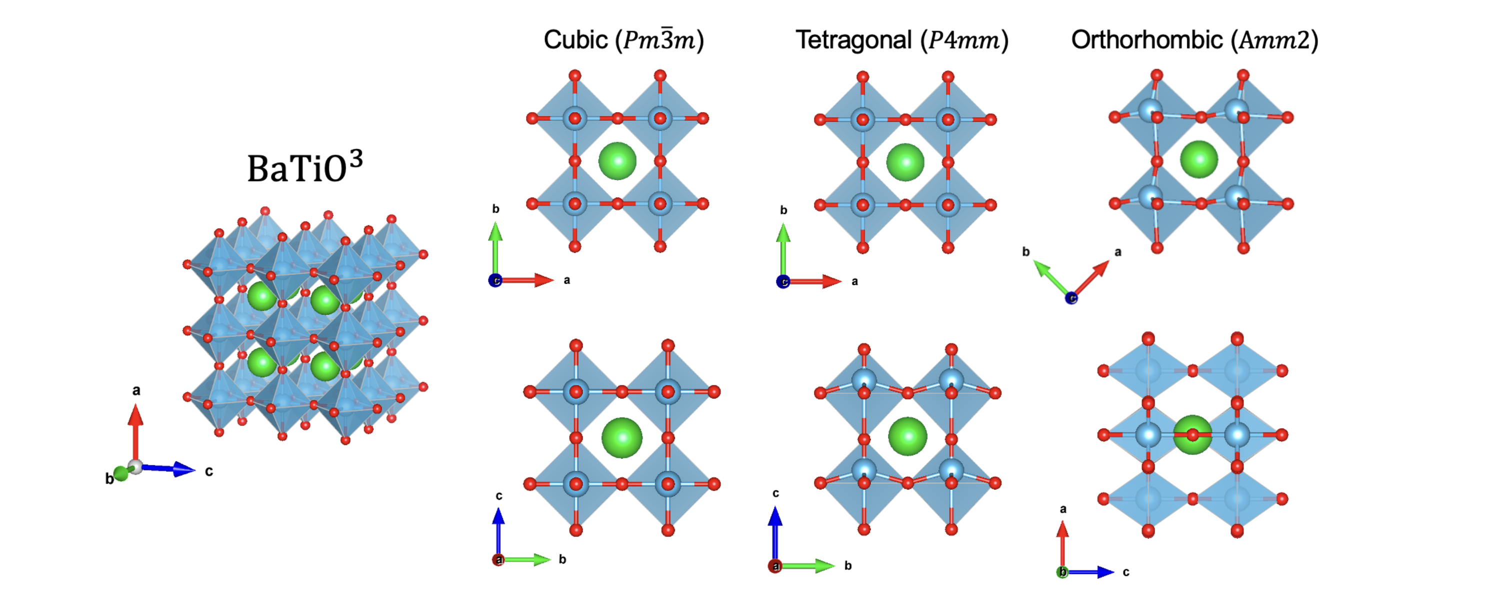


Figure: Visualization of $BaTiO_3$: As temperature decreases, it undergoes a series of symmetry-breaking phase transitions, transitioning from a cubic structure to a tetragonal phase, and eventually to an orthorhombic form.

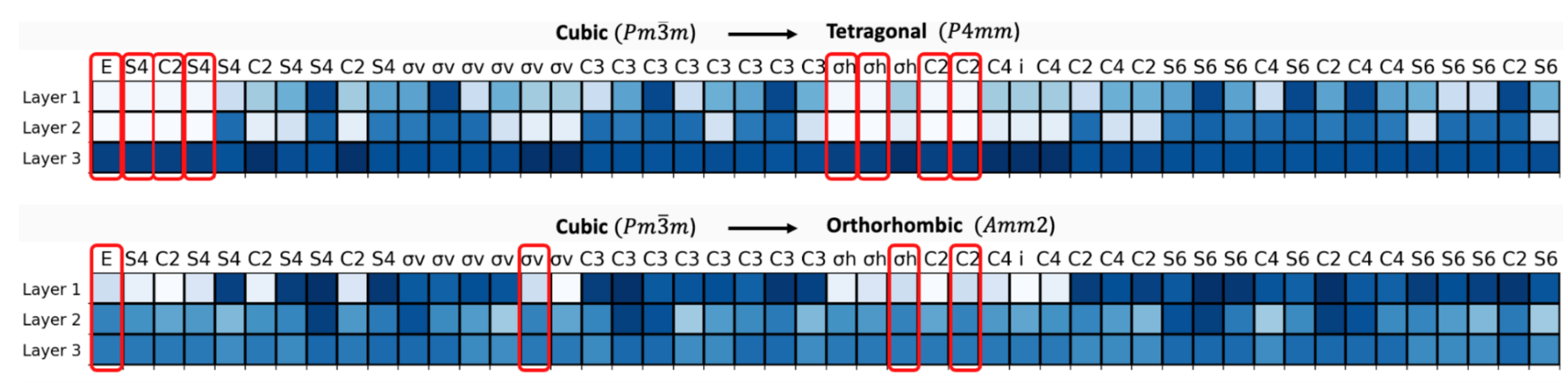


Figure: Visualization of the relaxed weights of two 3-layer relaxed octahedral group convolution networks trained to map from the cubic system to the tetragonal system and the orthorhombic system. The highlighted relaxed weights correspond to the preserved symmetry operations in these two systems that forms C_{4v} and C_{2v} group respectively.

Discover Isotropy Breaking in Turbulence

Kolmogorov's Hypothesis states that, at sufficiently high Reynolds numbers, the small-scale turbulent motions are statistically isotropic and independent of the large-scale structure.

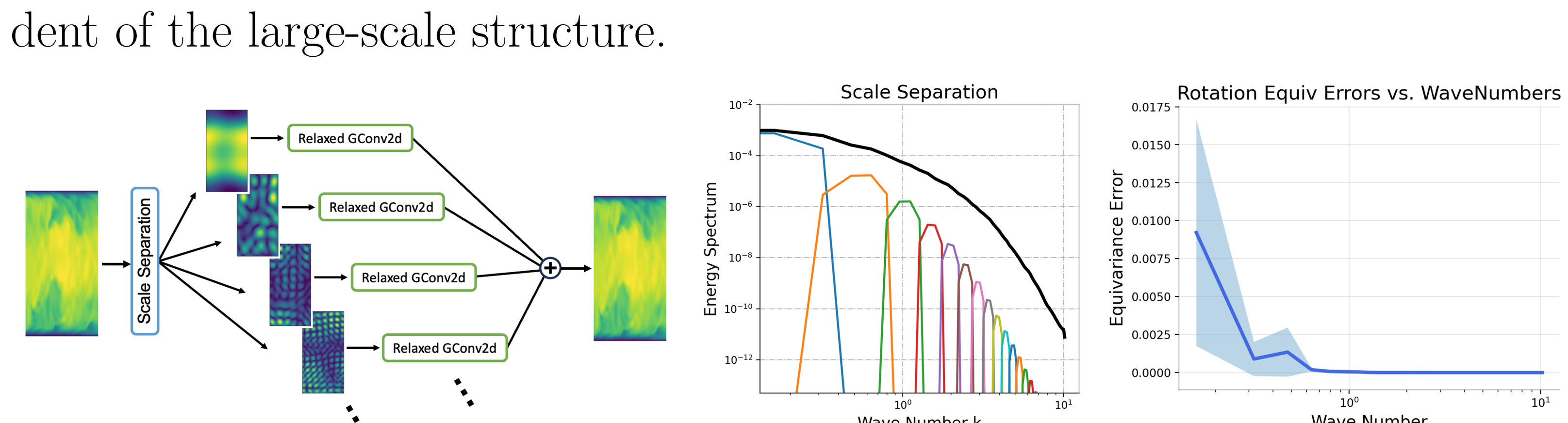


Figure: Left: Model for detecting rotational symmetry. This model breaks down the input velocity field into multiple scales using Fourier frequency cutoffs. Each scale is then processed through a distinct relaxed group convolution layer and the sum of the outputs from these layers is trained to reconstruct the input. Middle: Visualization of scale separation in energy spectrum. The black line represents the energy spectrum of the original velocity fields, while the other colored lines correspond to different scales. Right: Equivariance errors learned by the model. As the wave number gets higher (indicating smaller eddies), the equivariance error tends to decrease towards zero.

Discover Homogeneity Breaking in Turbulence

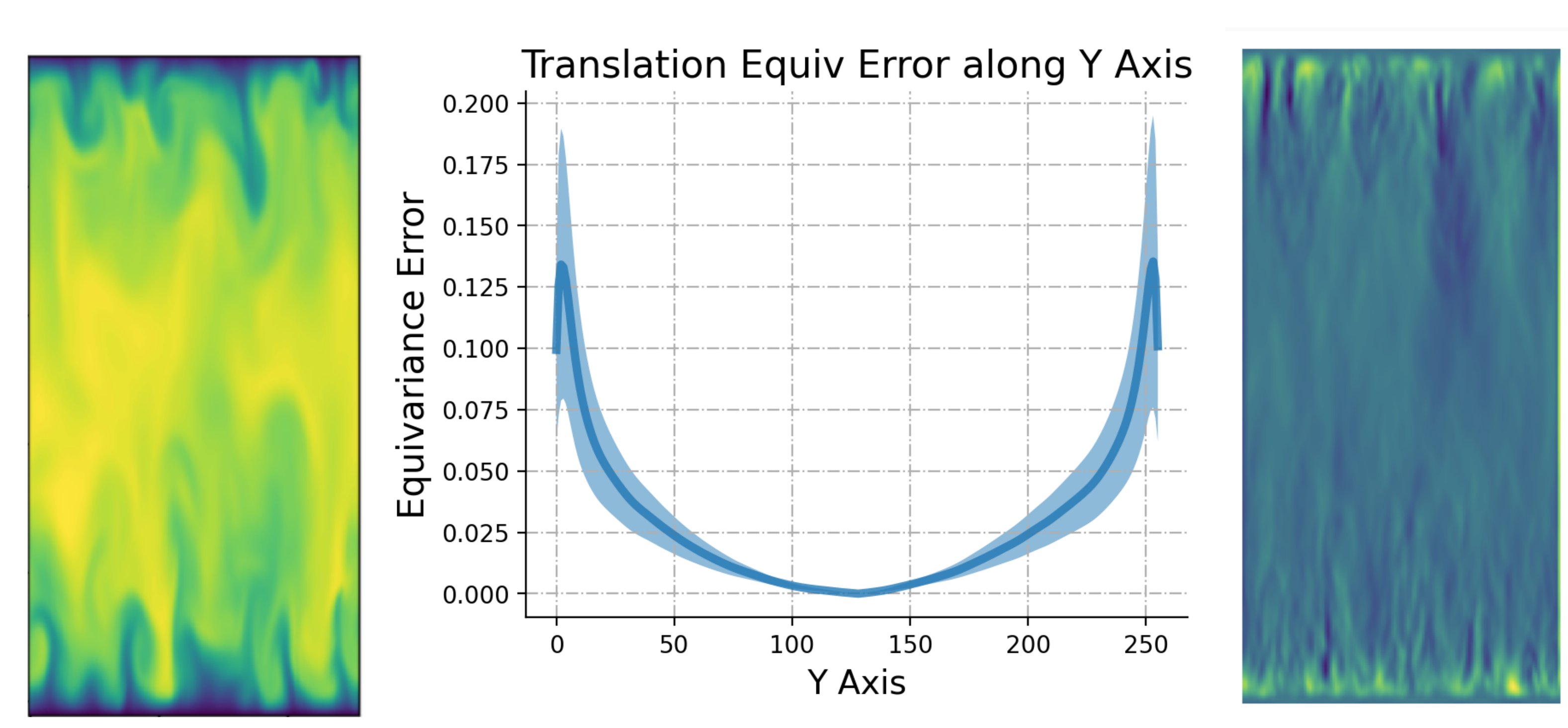


Figure: Left: Visualization of a velocity norm field. Middle: Translation equivariance error along the Y-axis. Right: The visualization of translation relaxed weights. It shows increased variation in relaxed weights as they approach the boundary areas.