Understanding Experimental Data by Identifying Symmetries with Deep Learning

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1 Abstract

Utilizing computational methods to extract actional information from scientific data is essential due to the time-consuming and inaccurate nature of the manual processes of humans. To better serve the purpose, equipping computational methods with physical rules is necessary. Integrating deep learning models with symmetry awareness has emerged as a promising approach to significantly improve symmetry detection in experimental data, with techniques such as parameter sharing and novel convolutional layers enhancing symmetry recognition.[1, 2, 3, 4, 5, 6] However, the challenge of integrating physical principles, such as symmetry, into these models persists. To address this, we have developed benchmarking datasets and training frameworks, exploring three perspectives to classify wallpaper group symmetries effectively. Our study demonstrates the limitations of deep learning models in understanding symmetry, as evidenced by benchmark results. A detailed analysis is provided with a hierarchical dataset and training outcomes, while a symmetry filter is designed aiming to improve symmetry operation recognition. This endeavor aims to push the boundaries of deep learning models in comprehending symmetry and embed physical rules within them, ultimately unlocking new possibilities at the intersection of machine learning and physical symmetry, with valuable applications in materials science and beyond.

2 Introduction

Scientific discoveries rely on extracting profound insights from experimental results; however, data collected regularly surpasses human analysis capabilities. Consequently, computational methods have become a promising solution for extracting actionable knowledge from this vast reservoir of scientific data. Nevertheless, a fundamental challenge persists within computational methodologies, as they are inherently bound by the constraints of logical rules, limiting their ability to apply generalized concepts and sentiments. Consequently, there is a pressing need to empower deep learning models with the inherent capability to seamlessly integrate the governing principles of the physical world into the complex information extraction process. In recent years, the domain of deep learning has undergone remarkable transformations, unveiling unprecedented potential in the revelation of concealed patterns within data.[1, 2, 3, 4, 5, 6, 7, 8, 9] However, it is a formidable challenge for deep learning models to extract information from experimental data following physical rules such as symmetry.

In materials physics, symmetry is one of the most pervasive predictors of structure-property relations. Symmetry is an indispensable tool for characterizing material structures and foretelling the properties of various substances, including oxides and metal materials like perovskite oxides. For instance, consider the case of perovskite oxide compounds; their unique electronic and magnetic properties are intricately linked to the underlying symmetry of their crystal structure. Symmetry is not confined solely to these materials; it plays an equally irreplaceable role in interpreting characteristic results obtained from surface morphology probing techniques. When scientists study surface features through methods such as scanning electron microscopy or atomic force microscopy, they rely on symmetry principles to decipher the intricate patterns and arrangements of atoms on the surface.

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The significance of symmetry extends further; symmetry is defined as the long-range order or periodicity of crystal structure, which is a promising indicator of a material's property. In 2D Euclidean space, symmetry is a foundational concept, encompassing a rich array of transformations, including translation, rotation, mirror reflection, and glide reflection. This diversity in symmetry operations allows researchers to describe various spatial arrangements and patterns, making symmetry an indispensable tool for materials scientists and physicists. Mathematical representations of symmetry are essential for precise description and evaluation. One notable mathematical definition of symmetry 2D space is wallpaper [10], which comprises 17 distinct symmetry classes, each denoted by symbols of p1, p2, pm, pg, pmm, pmg, pgg, cm, cmm, p4, p4m, p4g, p3, p3m1, p31m, p6, and p6m. Interpretation based on the data with a well-defined classification system will be unavoidable and critical. We develop three datasets based on the concept of wallpaper group, and design benchmarking frameworks with a specialized deep learning workflow tailored to classify wallpaper group symmetries to investigate the boundaries of the deep learning models in understanding symmetry and explore potential avenues for embedding physical rules within these models.

3 Result and Discussion

The benchmarking and identification process relies heavily on the availability of a comprehensive and large-scale dataset. To put it simply, achieving fair benchmark results necessitates a dataset that includes many image examples and accurately represents the practical scenarios encountered in research. In our pursuit of this goal, we have developed three distinct datasets: the ImageNet Symmetry dataset, the Atom Symmetry dataset, and the Noise Symmetry dataset (**Figure. 1**). These datasets consist of images that are constructed from a primitive unit cell, which encompasses various shapes such as squares, rectangles, rhombic shapes, oblique shapes, and hexagons. Initially, this primitive unit cell is subjected to different symmetry operations, including rotation, mirroring, and glide transformations, ultimately resulting in a rectangular unit cell defined as a translation unit cell. The translation unit cell is then translated and padded to attain a predetermined image size to ensure uniformity. While the three datasets differ in the content of their primitive unit cells, they all share the same construction methodology involving the 17 symmetries. It's worth noting that the area size of the unit cell is randomly distributed within a defined range. This deliberate approach ensures that the symmetry images possess an appropriate area size. Specifically, the size is not excessively small, enabling human examination for validation purposes, yet not overly large, ensuring that each symmetry image can encompass at least four translation unit cells. In total, we have amassed a substantial dataset, consisting of 10 million images in the ImageNet Symmetry dataset and 2 million images in both the Atom Symmetry dataset and the Noise Symmetry dataset. This extensive collection of images provides a robust foundation for conducting thorough benchmarking and identification tasks, allowing us to explore the boundaries of deep learning models' understanding of symmetry and their ability to embed physical rules effectively.

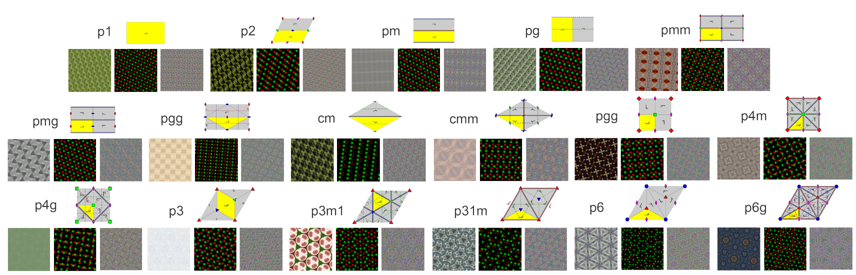

Figure 1: Wallpaper group diagram and image examples. In 17 symmetry classes, every class contains symmetry operation diagram, and three images generated with unit cells from crop region in ImageNet dataset, simulated atom and random noise.[3, 10]

In our benchmarking study, we evaluated the performance of various neural networks in identifying symmetry using three datasets: the ImageNet Symmetry dataset, the Atom Symmetry dataset, and the Noise Symmetry dataset. We deployed several deep learning models for this benchmarking task, including ResNet50[11], DeepNet161[12], the feature pyramid network with a ResNet50 backbone (FPN)[13], and cross-variance image transformers (XCiT)[14]. The results in terms of loss and accuracy are presented in **Table 1**, and further details regarding training and validation can be found in supplemental material **Figure. 4**. During the training and validation phases on the ImageNet Symmetry dataset all models achieved training and validation accuracy results exceeding 99%. While this may initially suggest that these models have learned a generalized concept of symmetry, it is important to highlight that this perception is misleading.

To shed light on the true ability of these state-of-the-art deep learning models to identify symmetry as a physical concept rather than approximating symmetry, we conducted cross-validation experiments using the Atom Symmetry dataset. The results of this cross-validation, presented in **Table 1**, reveal a significant drop in accuracy, with values lower than 55%. This marked reduction from the validation accuracy obtained on the training dataset (ImageNet Symmetry dataset) provides crucial insights. We propose the following assumption to interpret this accuracy discrepancy across the training, validation, and cross-validation phases. These models are adept at fitting themselves to a large dataset constructed according to a specific logical framework. However, the learned rules within these deep learning models do not necessarily align with physically meaningful concepts. Therefore, the observed difference in accuracy can be attributed to the models' limited capacity to grasp the fundamental physical concept of symmetry.

Model	Accuracy			Loss		
	Train	Valid	Cross-Validation	Train	Valid	Cross-Validation
ResNet50	99.96%	99.91%	54.33%	0.0011	0.0037	6.188
DenseNet161	99.94%	99.93%	58.69%	0.0012	0.0042	5.856
FPN	99.94%	99.91%	52.59%	0.0017	0.0031	4.312
XCiT	99.96%	99.90%	45.00%	0.0010	0.0061	10.116

Table 1: Training, validation, and cross-validation accuracy and loss results of models' train, validate on ImageNet Symmetry dataset and cross-validate on Atom Symmetry dataset.

The benchmarked results illustrate the deep learning model's ability to comprehend symmetry, prompting an analysis of the underlying reasons for its limited efficacy. This limitation arises from the absence of equivariance in complex symmetry operations like rotation and mirror transformations.[2, 5, 6] Consequently, the deep learning model struggles to consistently produce similar results for images subjected to the same symmetry operation during classification tasks. In pursuit of a potential solution and the development of a physically informed model, we propose three potential approaches as following. Exploring these three potential routes holds promise for enhancing the deep learning model's capacity to grasp and apply the principles of symmetry, ultimately contributing to more robust and accurate classification results.

1. **Data Preprocessing with Equivariance**: One avenue involves preprocessing the data to instill equivariance with respect to rotation, mirror, and glide operations. By incorporating these symmetries into the data before training, we aim to enhance the model's ability to recognize and classify symmetric patterns.

2. **Enabling Equivariance in Convolution Layers**: Another route involves enabling equivariance of complex symmetry operations directly within the convolutional layers of the model. This approach seeks to ensure that the model can inherently account for the intricate symmetries present in the data, potentially leading to improved performance.

3. **Novel Training Workflow**: Lastly, we consider the development of a novel Training Workflow explicitly designed to encourage the deep learning model to learn the fundamental physical concept of symmetry. This approach may involve specialized architectural elements and training methodologies tailored to symmetry recognition, with the aim of surpassing the limitations observed in current models.

In exploring the first route, we employed preprocessing techniques on the existing data, including the utilization of Fast Fourier transformation (FFT), Radon transformation, and a customized symmetry filter applied to the datasets. In the context of 2D space, FFT converted the image signal from the spatial domain to the frequency domain, while the Radon transformation accentuated angular information in the outputs. The cross-validation accuracy yielded 9% and 43% results for the FFT-processed dataset and the Radon transformation-processed dataset, respectively. Notably, these accuracies did not exhibit improvement compared to the model trained on the plain dataset. This outcome can be attributed to the inherent limitations of the pre-existing filters, which were primarily sensitive to translation operations for FFT and rotation-based operations for Radon transformation.

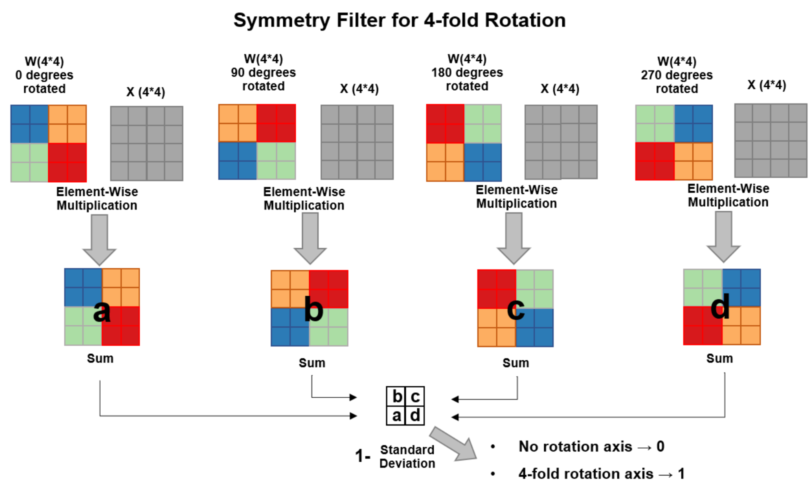

Figure 2: Graphic demonstration of custom symmetry filter for 4-fold rotation. A custom 4-fold rotation filter is defined by rotating a randomly defined matrix four times for four different kernels. Then, we perform the element-wise multiplication on the four kernels with the gray region, a sliding window from the symmetry image. The sum of the matrix is calculated as a, b, c, and d for four output matrices. Using one minus the standard deviation of the a, b, c, and d, the indicating feature value is extracted to determine the existence of a 4-fold rotation in the center of the sliding window.

To address these limitations, we introduced a customized symmetry filter designed to convert symmetry operations into unique indicators through hard-coded transformations. This filter generated distinctive feature patterns in the output images, with a detailed graphical example provided in **Figure. 2**. Feature vectors were generated by applying the filter's transformation to manually selected regions within symmetry classes, encompassing fundamental symmetry operators such as 2-fold rotation, mirror, and 4-fold rotation. For simplification, a transformed dataset comprising five classes was utilized for validation. The cross-validation accuracy notably increased, rising from 55.32% to 88.74%. This substantial improvement underscores the efficacy of the custom symmetry filter in transforming symmetry operators into unique indicators for the deep learning model. However, it is essential to acknowledge that successfully completing the classification task still requires manual selection of the center of symmetry operators. This arises from the deep learning model's limited capacity to process complex symmetry operations. Consequently, we face the challenge of devising a model architecture or convolutional layer that is intrinsically informed by physical principles, offering an enhanced ability to comprehend symmetry.

Progress has been made from various perspectives in our pursuit of enabling equivariance of symmetry operations within convolutional layers.[2, 4, 5, 6] We subjected existing layers and models to validation using our symmetry datasets, but observed limited improvements in their ability to understand symmetry compared to plain models. Following the path of designing a model architecture that actively acquires critical information to comprehend symmetry, we conducted a detailed analysis of benchmark results. The confusion matrix in **Figure. S1** revealed that the ResNet50 model often made incorrect predictions for images exhibiting the same basic symmetry operation during cross-validation with the Atom Symmetry dataset. Notably, images featuring 3-fold rotation-based symmetry posed a significant challenge for accurate predictions. Additionally, instances of images with p2 symmetry being incorrectly predicted as p6 can be attributed to both symmetry classes having a 2-fold rotation operation in common.

In response to these challenges, we dedicated our efforts to developing a model architecture that encourages the model to capture the distinguishing features used to differentiate between various symmetries. We implemented existing methods such as feature pyramid networks, spatial transformer layers, and contrastive loss functions; however, these methods yielded insignificant improvements over plain models. To delve deeper into the mystery of the low cross-validation accuracy, we constructed datasets in a hierarchical manner, as depicted in **Figure. 3**. This hierarchical approach involved classifying classes based on rotation axes in the first level and subsequently filtering based on finer conditions, such as reflection axes or higher-order rotation axes. We explore the hierarchy dataset with the same benchmark workflow – train and validate on the ImageNet Symmetry dataset, then cross-validate on the Atom Symmetry dataset. Surprisingly, the training, validation, and cross-validation accuracy is 99.98%, 96.18%, and 48.7%, respectively - even when working with a three-class dataset classification—consisting of "No rotation axis," "2-fold rotation axis," and "3-fold rotation axis"—the cross-validation accuracy remained unsatisfactory. Yet, the results are consistent with our assumption that the mechanism convolutional layer inherently lacks equivariance of complex symmetry operation. Design training workflow based on the hierarchy structure of symmetry construction could be beneficial. For example, fine-tuning models to classify one higher-order symmetry transformation and assembling models to achieve decent cross-validation accuracy. To move forward with a novel workflow on symmetry identification tasks, further investigation into the underlying reasons is inevitable and imperative to provide a thorough explanation for the observed limitations and to develop effective improvement techniques. This persistent challenge in enabling deep learning models to understand symmetry highlights the broader difficulty of achieving physically informed models in the field of material physics.

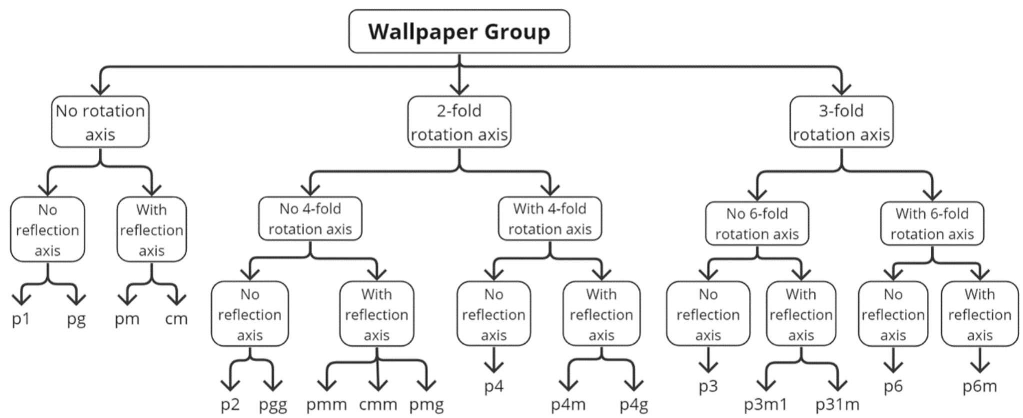

Figure 3: Hierarchy organization of wallpaper group symmetry classification. Symmetries are classified based on whether the images have a rotation or reflection axis. The determination rule of the last hierarchy is not shown because of too detailed illustration in limited space.

4 Conclusion

In conclusion, our study has underscored the critical importance of comprehensive and large-scale datasets in benchmarking and identifying symmetry using deep learning models. We have meticulously developed three distinct datasets, namely the ImageNet Symmetry dataset, the Atom Symmetry dataset, and the Noise Symmetry dataset, each constructed with a focus on preserving the integrity of symmetry in various forms. These datasets have served as the foundation for evaluating a range of neural networks, including ResNet50, DenseNet161, feature pyramid networks, and XCiT. While initial training and validation results appeared promising, demonstrating high accuracy, our cross-validation on the Atom Symmetry dataset revealed a substantial drop in accuracy, challenging the notion that these models truly grasp the underlying physical concept of symmetry. To address this limitation, we've explored multiple routes, including data preprocessing, enabling equivariance within convolutional layers, and novel training workflows. While progress has been made, further investigation is required to unlock the full potential of deep learning in understanding symmetry, particularly in the context of material physics. Our ongoing pursuit aims to bridge the gap between deep learning models and the intricate principles of symmetry, offering new insights and applications in materials science and beyond.

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