Novelty Assessment Report

Paper: Adaptive Canonicalization with Application to Invariant Anisotropic Geometric Networks
PDF URL: https://openreview.net/pdf?id=j2DHdrsRXI
Venue: ICLR 2026 Conference Submission
Year: 2026
Report Generated: 2026-01-04

Abstract

Canonicalization is a widely used strategy in equivariant machine learning, enforcing symmetry in neural networks by mapping each input to a standard form. Yet, it often introduces discontinuities that can affect stability during training, limit generalization, and complicate universal approximation theorems. In this paper, we address this by introducing adaptive canonicalization, a general framework in which the canonicalization depends both on the input and the network. Specifically, we present the adaptive canonicalization based on prior maximization, where the standard form of the input is chosen to maximize the predictive confidence of the network. We prove that this construction yields continuous and symmetry-respecting models that admit universal approximation properties.

We propose two applications of our setting: (i) resolving eigenbasis ambiguities in spectral graph neural networks, and (ii) handling rotational symmetries in point clouds. We empirically validate our methods on molecular and protein classification, as well as point cloud classification tasks. Our adaptive canonicalization outperforms the three other common solutions to equivariant machine learning: data augmentation, standard canonicalization, and equivariant architectures.

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Core Task Landscape

This paper addresses: **Adaptive Canonicalization for Equivariant Machine Learning**
A total of **35 papers** were analyzed and organized into a taxonomy with **14 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:
- **Canonicalization-Based Equivariance Methods**
- **Architecturally Equivariant Network Designs**
- **Symmetry-Breaking and Generative Modeling**
- **Canonical Transformations in Dynamical Systems**
- **Domain-Specific Symmetry Preservation**
- **Equivariance in Broader Machine Learning Contexts**

Complete Taxonomy Tree

- Adaptive Canonicalization for Equivariant Machine Learning Survey Taxonomy
- Canonicalization-Based Equivariance Methods
  - Adaptive and Learned Canonicalization Frameworks
  - General Adaptive Canonicalization Theory ★ (3 papers)
    - [0] Adaptive Canonicalization with Application to Invariant Anisotropic Geometric Networks (Anon et al., 2026) View paper
    - [1] Equivariance with learned canonicalization functions (Kaba, 2023) View paper
    - [22] A Canonicalization Perspective on Invariant and Equivariant Learning (Wang Yisen, 2024) View paper
  - Pretrained Model Adaptation via Canonicalization (1 papers)
    - [3] Equivariant adaptation of large pretrained models (Mondal, 2023) View paper
  - Group-Specific Canonicalization Architectures
  - SE(3) and SO(3) Canonicalization (4 papers)
    - [4] Affine steerable equivariant layer for canonicalization of neural networks (Y Li, 2025) View paper
    - [10] SE(3)-Equivariant Relational Rearrangement with Neural Descriptor Fields (Simeonov, 2022) View paper
    - [24] Shape-pose disentanglement using se (3)-equivariant vector neurons (Oren Katzir, 2022) View paper
    - [33] Equivariance by Local Canonicalization: A Matter of Representation (Lippmann, 2025) View paper
  - Lorentz and Non-Compact Group Canonicalization (2 papers)
    - [11] Lie Algebra Canonicalization: Equivariant Neural Operators under arbitrary Lie Groups (Shumaylov, 2024) View paper
    - [14] Lorentz Local Canonicalization: How to Make Any Network Lorentz-Equivariant (Spinner, 2025) View paper
  - Domain-Specific Canonicalization Applications
  - Robotics and Manipulation (3 papers)
    - [2] EqNIO: Subequivariant neural inertial odometry (Xu, 2024) View paper
    - [17] Eq.Bot: Enhance Robotic Manipulation Learning via Group Equivariant Canonicalization (Jian Deng, 2025) View paper
    - [29] Symmetric Models for Dexterous Robotic Manipulation (Colin Kohler, 2024) View paper
  - Molecular and Crystal Structure Modeling (4 papers)
    - [6] Local-Global Associative Frames for Symmetry-Preserving Crystal Structure Modeling (Lin, 2025) View paper
    - [18] Improving molecular modeling with geometric GNNs: An empirical study (Ali Ramlaoui, 2024) View paper
    - [26] Symmetry-Preserving Conformer Ensemble Networks for Molecular Representation Learning (Y Zhu, 2025) View paper
    - [35] Learning Molecular Symmetry Breaking via Symmetry-adapted Neural Networks (JM Baker, n.d.) View paper

- ○ 3D Vision and Pose Estimation (3 papers)
  - ▪ [5] Canonical Shape Reconstruction with SE (3) Equivariance Learning for Weakly-Supervised Object Pose Estimation (Jun Zhou, 2025) View paper
  - ▪ [8] Canonical fields: Self-supervised learning of pose-canonicalized neural fields (Rohith Agaram, 2023) View paper
  - ▪ [30] Local Scale Equivariance with Latent Deep Equilibrium Canonicalizer (Rahman Md. Ashiqur, 2025) View paper
- • Architecturally Equivariant Network Designs
  - ○ Frame-Based and Local Reference Equivariance (3 papers)
  - ○ [12] Frame-based Equivariant Diffusion Models for 3D Molecular Generation (Guo MoHan, 2025) View paper
  - ○ [15] se (3) equivariant convolution and transformer in ray space (Y Xu, 2023) View paper
  - ○ [31] Equivariant Light Field Convolution and Transformer (Xu, 2022) View paper
  - ○ Equivariant Convolution and Message Passing (3 papers)
  - ○ [13] Harnessing equivariance: Modeling turbulence with graph neural networks (Kurz, 2025) View paper
  - ○ [25] Equivariant Atomic and Lattice Modeling Using Geometric Deep Learning for Crystal Structure Optimization (Ziduo Yang, 2025) View paper
  - ○ [32] Convolutional Neural Networks on 3D Surfaces Using Parallel Frames (Yang, 2018) View paper
  - ○ Unsupervised and Representation Learning (2 papers)
  - ○ [19] Unsupervised learning of group invariant and equivariant representations (Winter, 2022) View paper
  - ○ [21] Group Equivariance Meets Mechanistic Interpretability: Equivariant Sparse Autoencoders (Ege Erdogan, 2025) View paper
- • Symmetry-Breaking and Generative Modeling (2 papers)
  - ○ [7] Improving Equivariant Networks with Probabilistic Symmetry Breaking (Lawrence, 2025) View paper
  - ○ [9] Symmetry-aware generative modeling through learned canonicalization (Levy, 2025) View paper
- • Canonical Transformations in Dynamical Systems (3 papers)
  - ○ [16] Deep learning for structure-preserving universal stable Koopman-inspired embeddings for nonlinear canonical Hamiltonian dynamics (Goyal, 2023) View paper
  - ○ [23] Neural canonical transformation with symplectic flows (Li Shuo-Hui, 2020) View paper
  - ○ [34] Galilean Invariance Preserving Deep Learning for Canonical Fluid Flows (C. Gonzalez, 2021) View paper
- • Domain-Specific Symmetry Preservation (2 papers)
  - ○ [27] Incorporating Cyclic Group Equivariance into Deep Learning for Reliable Reconstruction of Rotationally Symmetric Tomography Systems (Zhang Yaogong, 2025) View paper
  - ○ [28] Symmetry-preserving WENO-type reconstruction schemes in Lagrangian hydrodynamics (Xiaodong Liu, 2020) View paper
- • Equivariance in Broader Machine Learning Contexts (1 papers)
  - ○ [20] Equivariant Learning for 3D Vision and Pattern Recognition (Xu, 2025) View paper

Narrative

Core task: adaptive canonicalization for equivariant machine learning. The field addresses how to build neural networks that respect or exploit symmetries in data, with the taxonomy revealing several complementary strategies. Canonicalization-Based Equivariance Methods transform inputs into standard reference frames before processing, enabling ordinary networks to handle symmetric data; this branch includes both hand-crafted and learned canonicalization approaches such as Learned Canonicalization[1] and Canonicalization Perspective[22]. Architecturally Equivariant Network Designs instead bake symmetry constraints directly into layer operations, producing models that are equivariant by construction. Symmetry-Breaking and Generative Modeling explores how to handle settings where exact symmetry is undesirable or where generation requires controlled symmetry violation, as seen in Probabilistic Symmetry Breaking[7] and Frame-based Diffusion[12]. The remaining branches address canonical transformations in physics-inspired dynamical systems, domain-specific applications preserving particular symmetries, and broader machine learning contexts where equivariance plays a supporting role.

Recent work has intensified around the trade-off between flexibility and interpretability: architecturally equivariant designs guarantee exact symmetry but can be rigid, while canonicalization methods offer modularity at the cost of potential frame ambiguities. Adaptive Canonicalization[0] sits squarely within the learned canonicalization cluster, proposing a general theoretical framework for adapting canonical frames during training rather than fixing them a priori. This contrasts with earlier fixed-frame approaches and aligns closely with Learned Canonicalization[1], which similarly trains canonicalization mappings end-to-end. Compared to Canonicalization Perspective[22], which surveys the conceptual landscape, Adaptive Canonicalization[0] emphasizes the algorithmic and optimization aspects of making canonicalization adaptive. Meanwhile, works like Equivariant Adaptation[3] and Local Canonicalization Equivariance[33] explore related ideas of local or task-specific frame selection, highlighting ongoing questions about when and how to balance global versus local canonicalization strategies.

Related Works in Same Category

The following **2 sibling papers** share the same taxonomy leaf node with the original paper:

1. Equivariance with learned canonicalization functions

Authors: Kaba, Sékou-Oumar, Mondal, Arnab Kumar, S. Kaba, et al. (14 authors total) | **Year/Venue**: 2023 | **URL**: View paper

Abstract

Symmetry-based neural networks often constrain the architecture in order to achieve invariance or equivariance to a group of transformations. In this paper, we propose an alternative that avoids this architectural constraint by learning to produce canonical representations of the data. These canonicalization functions can readily be plugged into non-equivariant backbone architectures. We offer explicit ways to implement them for some groups of interest. We show that this approach enjoys universa...

Relationship Analysis

Both papers belong to the General Adaptive Canonicalization Theory category, focusing on foundational frameworks for adaptive canonicalization with theoretical guarantees. The original paper introduces adaptive canonicalization where the canonicalization depends on both input and network (specifically prior maximization), proving continuity and universal approximation properties. The candidate paper proposes learning canonicalization functions end-to-end rather than using predefined heuristics, but treats canonicalization as primarily input-dependent (though learned jointly with the network), representing a less general framework than the original paper's explicit input-and-network-dependent adaptive approach.

2. A Canonicalization Perspective on Invariant and Equivariant Learning

Authors: Wang Yisen, Stefanie Jegelka, George Ma, Derek Lim, Yifei Wang, et al. (6 authors total) | **Year/Venue**: 2024 | **URL**: View paper

Abstract

In many applications, we desire neural networks to exhibit invariance or equivariance to certain groups due to symmetries inherent in the data. Recently, frame-averaging methods emerged to be a unified framework for attaining symmetries efficiently by averaging over input-dependent subsets of the group, i.e., frames. What we currently lack is a principled understanding of the design of frames. In this work, we introduce a canonicalization perspective that provides an essential and complete view ...

Relationship Analysis

Both papers belong to the General Adaptive Canonicalization Theory category, focusing on foundational frameworks for adaptive canonicalization with theoretical guarantees. The candidate paper provides a canonicalization perspective on frame-averaging methods and establishes connections between frames and canonical forms, while the original paper introduces adaptive canonicalization where canonicalization depends on both input and network (specifically through prior maximization). The key difference is that the original paper proposes network-dependent adaptive canonicalization with continuity guarantees, whereas the candidate paper analyzes the design principles of frames in frame-averaging methods through a canonicalization lens.

Contributions Analysis

Overall novelty summary. The paper introduces an adaptive canonicalization framework where the canonical form depends jointly on the input and the network's predictions, specifically via prior maximization. Within the taxonomy, it resides in the 'General Adaptive Canonicalization Theory' leaf alongside two sibling papers. This leaf is part of a broader 'Adaptive and Learned Canonicalization Frameworks' branch, indicating a relatively focused but not overcrowded research direction. The taxonomy contains 35 papers across multiple branches, suggesting the paper occupies a specialized niche within the larger equivariant learning landscape.

The taxonomy reveals three main strategies for equivariance: canonicalization-based methods, architecturally constrained networks, and symmetry-breaking approaches. The paper's leaf sits within the canonicalization branch, which also includes domain-specific applications (robotics, molecular modeling, 3D vision) and group-specific methods (SE(3), Lorentz groups). Neighboring leaves address pretrained model adaptation and specialized group canonicalization, while sibling branches explore frame-based architectures and message-passing networks. The scope notes clarify that this work focuses on foundational theory with continuity and universal approximation guarantees, distinguishing it from application-driven or group-specific canonicalization methods.

Among 13 candidates examined across three contributions, no clearly refutable prior work was identified. The adaptive canonicalization framework examined 2 candidates with no refutations, prior maximization examined 10 candidates with no refutations, and anisotropic geometric network applications examined 1 candidate with no refutations. This limited search scope suggests the specific combination of adaptive canonicalization with prior maximization and theoretical guarantees appears relatively unexplored within the examined literature. However, the small candidate pool means the analysis captures only a narrow slice of potentially relevant work, particularly given the paper's position in a specialized but active research area.

Based on the top-13 semantic matches examined, the work appears to occupy a distinct position within adaptive canonicalization theory, though the limited search scope prevents definitive claims about broader novelty. The taxonomy structure indicates this is a growing subfield with established foundations but room for theoretical contributions. A more exhaustive search across the 35-paper taxonomy and beyond would be needed to fully assess overlap with related canonicalization and equivariance methods.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Adaptive canonicalization framework

Description: The authors introduce adaptive canonicalization, a general framework where the standard form of an input depends on both the input itself and the neural network. This approach resolves discontinuities inherent in standard canonicalization methods while maintaining symmetry-respecting properties and universal approximation guarantees.

This contribution was assessed against **2 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Conformal Normalization in Recurrent Neural Network of Grid Cells

URL: View paper

Brief Assessment

Conformal Grid Cells[38] focuses on conformal normalization in recurrent neural networks for grid cell modeling in neuroscience, not on adaptive canonicalization for handling symmetries in machine learning architectures.

2. Dynamically-scaled deep canonical correlation analysis

URL: View paper

Brief Assessment

Dynamically-scaled CCA[37] focuses on canonical correlation analysis with input-dependent scaling of network parameters for multi-view learning, not on general canonicalization frameworks for handling symmetries in geometric data.

Contribution 2: Prior maximization adaptive canonicalization

Description: The authors present a specific instantiation of adaptive canonicalization called prior maximization, where the canonical form is selected by maximizing the network's predictive confidence. They prove this construction yields continuous and symmetry-respecting models with universal approximation properties.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. MC Layer Normalization for calibrated uncertainty in Deep Learning

URL: View paper

Brief Assessment

MC Layer Normalization[39] focuses on uncertainty estimation through stochastic normalization in neural networks, not on canonicalization methods for handling symmetries or maximizing predictive confidence as in the original paper's contribution.

2. CP: Leveraging Geometry for Conformal Prediction via Canonicalization

URL: View paper

Brief Assessment

Conformal Prediction Canonicalization[42] focuses on conformal prediction under geometric data shifts using canonicalization for uncertainty quantification, not on adaptive canonicalization methods that maximize predictive confidence in neural networks for general machine learning tasks.

3. Mitigating neural network overconfidence with logit normalization
URL: View paper

Brief Assessment

Logit Normalization[40] focuses on mitigating neural network overconfidence for out-of-distribution detection by normalizing logit vectors during training. This is fundamentally different from the original paper's adaptive canonicalization framework that maximizes predictive confidence to select canonical forms for handling symmetries in geometric data.

4. An ensemble approach of deep CNN models with beta normalization aggregation for gastrointestinal disease detection
URL: View paper

Brief Assessment

Beta Normalization Ensemble[48] focuses on ensemble aggregation methods for gastrointestinal disease detection in medical imaging, not on canonicalization methods or neural network symmetry handling.

5. Calibration in deep learning: A survey of the state-of-the-art
URL: View paper

Brief Assessment

Calibration Survey[43] focuses on calibrating predictive confidence in classification models through post-hoc methods and regularization techniques. It does not address canonicalization methods or the construction of canonical forms by maximizing network confidence, which is the core novelty of the original paper's prior maximization approach.

6. Confidence-aware learning for deep neural networks
URL: View paper

Brief Assessment

Confidence-aware Learning[47] focuses on training neural networks to produce well-calibrated confidence estimates for classification tasks, not on canonicalization methods or symmetry-preserving transformations in equivariant machine learning.

7. Improving Calibration for Long-Tailed Recognition
URL: View paper

Brief Assessment

Long-Tailed Calibration[46] focuses on calibration methods for imbalanced classification using label smoothing techniques, not on canonicalization methods that maximize predictive confidence in neural networks for handling symmetries.

8. Uncertainty quantification and deep ensembles
URL: View paper

Brief Assessment

Deep Ensembles[41] focuses on uncertainty quantification through ensemble averaging of neural network predictions, not on canonicalization methods that maximize predictive confidence for handling symmetries in data.

9. Dynamic normalization supervised contrastive network with multiscale compound attention mechanism for gearbox imbalanced fault diagnosis
URL: View paper

Brief Assessment

Dynamic Normalization Gearbox[44] focuses on fault diagnosis in gearbox systems using normalization and attention mechanisms for imbalanced data, not on canonicalization methods that maximize predictive confidence in neural networks for symmetry-respecting models.

10. Conditional Max-preserving Normalization: an Innovative Approach to Combining Diverse Classification Models
URL: View paper

Brief Assessment

Max-preserving Normalization[45] addresses ensemble learning for combining diverse classifiers through normalization techniques, not canonicalization methods that maximize predictive confidence in neural networks for handling symmetries.

Contribution 3: Anisotropic geometric network applications

Description: The authors develop two concrete applications of their framework: anisotropic nonlinear spectral filters for resolving eigenbasis ambiguities in spectral graph neural networks, and anisotropic point cloud networks for handling rotational symmetries. These methods are shown to outperform standard canonicalization, data augmentation, and equivariant architectures.

This contribution was assessed against **1 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

1. Endowing deep 3d models with rotation invariance based on principal component analysis
URL: View paper

Brief Assessment

Rotation Invariance PCA[36] focuses on point cloud rotation invariance via PCA-based canonicalization, not on resolving eigenbasis ambiguities in spectral graph neural networks or the specific anisotropic framework proposed in the original paper.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] Adaptive Canonicalization with Application to Invariant Anisotropic Geometric Networks View paper
- [1] Equivariance with learned canonicalization functions View paper
- [2] EqNIO: Subequivariant neural inertial odometry View paper
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