Generative Adversarial Symmetry Discovery

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Equivariance has always been an important inductive bias in deep learning. Symmetry-aware equivariant networks have led to significant improvement in generalization, sample efficiency and scientific validity (1; 2; 3; 4). Interest has surged in both theoretical analysis and practical techniques for building general group equivariant neural networks (5; 6; 7; 8).

However, a key limitation of equivariant neural networks is that they require explicit knowledge of the task symmetry before a model can be constructed. In practice, it is sometimes difficult to identify the true symmetries of the task, and constraining the model by the exact mathematical symmetry might not be optimal in real-world datasets (9). These challenges call for approaches that enable deep learning methods to automatically discover the underlying symmetry of the tasks.

Neural networks that discover unknown symmetry may play the role of AI scientists, not only by making data-driven predictions, but also by describing physical systems through their symmetries and generating new scientific insights through the close relationship between symmetry, conservation laws and underlying governing equations. Most existing works in symmetry discovery can only address a small fraction of symmetry types, such as finite groups (10), subsets of a given group (11) or individual group elements (12). L-conv (13) can discover continuous symmetries without discretizing the groups, but is limited in computational efficiency. A more general framework is needed for discovering various real-world symmetries.

In our work (14), we propose a novel framework, LieGAN, to *automatically discover equivariances* from a dataset using a paradigm akin to generative adversarial training. Our method trains a symmetry generator that transforms the training data and outputs a similar distribution to the original dataset, which suggests equivariance or invariance to the learned tranformations.

Making use of the theory of Lie groups and Lie algebras, LieGAN is able to discover continuous symmetries as matrix groups, such as rotation group $\mathrm{SO}(n)$ and restricted Lorentz group $\mathrm{SO}(1,3)^+$ in trajectory prediction and top quark tagging tasks. Moreover, through different parameterization strategies, it can also deal with other types of symmetries, such as discrete group transformation, as well as the subset of a group. LieGAN displays symmetry as a matrix representation of the Lie algebra basis. With proper regularization on the symmetry generator, it can decouple high-dimensional group structure to an interpretable, approximately orthogonal basis.

We also develop pipelines for utilizing the discovered symmetry in downstream prediction tasks through equivariant model and data augmentation. Specifically, we propose an arbitrary Lie group equivariant graph neural network, LieGNN, which incorporates symmetries learned by LieGAN by introducing group invariant metric tensors. We show that the discovered symmetry can be readily used as an inductive bias to improve accuracy and generalization in prediction experiments.

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