Generative Adversarial Symmetry Discovery

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Problem

How to design a data-driven approach to automatically discover symmetries, i.e. invariances and equivariances, in a predictive task?

Our Contributions

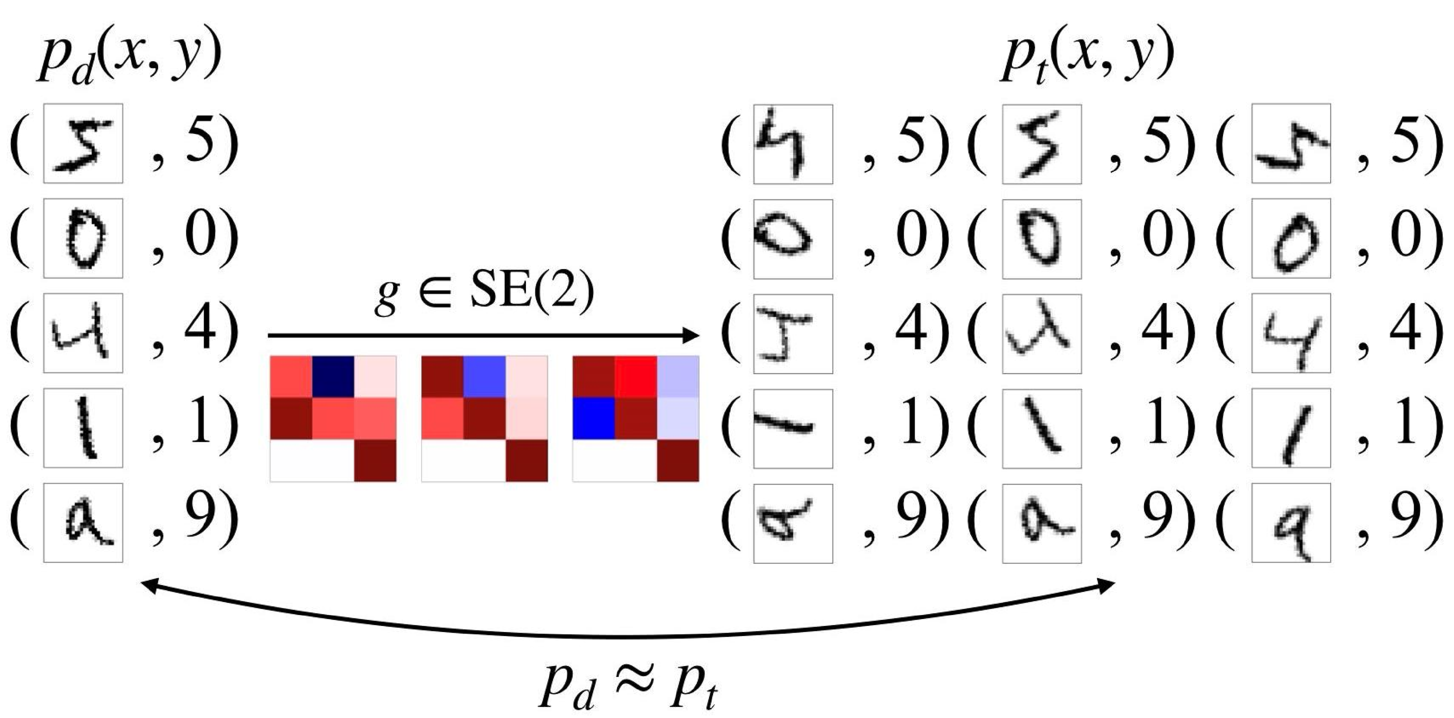
We propose the framework of Lie algebra Generative Adversarial Network (LieGAN). Combining generative adversarial training and the theory of Lie groups, our model:

- Learns a distribution over symmetry transformations and produce a transformed data distribution that is indistinguishable from original distribution.
- Discovers various general linear symmetries in datasets, including the rotation group $\mathrm{SO}(n)$ and the restricted Lorentz group $\mathrm{SO}(1,3)^+$.
- Can be combined with customized equivariant neural networks to construct arbitrary group equivariant models and achieve excellent performance in predictive tasks.

Our full paper is available at: `https://arxiv.org/abs/2302.00236`

Invariance, Equivariance and Data Distribution

Invariance and equivariance have become an important inductive bias in deep learning architectures. A function $f : \mathcal{X} \to \mathcal{Y}$ is invariant to a group G if $f(gx) = f(x), \forall g \in G, x \in \mathcal{X}$. It is G-equivariant if $f(gx) = gf(x), \forall g \in G, x \in \mathcal{X}$. From another perspective, invariant or equivariant transformations preserve the data distribution:



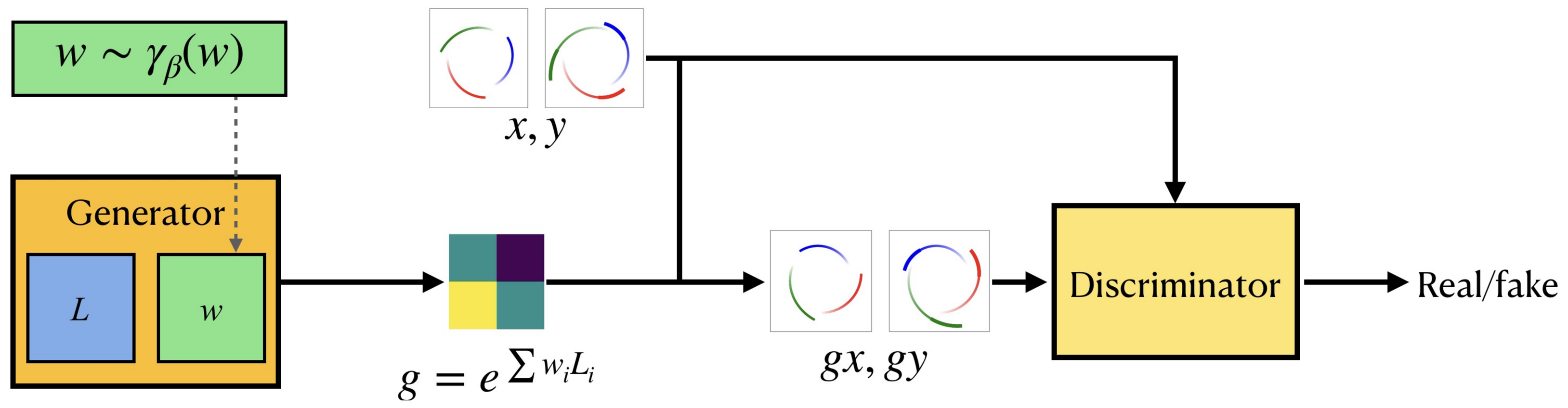
Comparison of Symmetry Discovery Methods

Symmetry	MSR [5]	Augerino [1]	LieGAN
Discrete group	✓	✗	✓
Continuous group	✗	✗	✓
Subset of given group	✗	✓	✓
Subset of unknown group	✗	✗	✓

Different approaches with deep learning have been developed to discover symmetries from data. Our approach (LieGAN) is the *first* to address the discovery of such a variety of symmetries including discrete group, continuous group, and subset of given or unknown group.

Generative Adversarial Training Architecture

Existing equivariant neural networks rely on explicit knowledge about symmetry, which is sometimes unavailable. Our work aims to discover unknown symmetry directly from data.



LieGAN Structure: The transformation generator learns a distribution of transformations acting on the data that preserves the original joint distribution. The symmetry transformations can either be a continuous Lie group or a subset of a group, depending on how we parameterize the distribution γ_β over Lie algebra basis coefficients. The discriminator learns towards an adversarial objective: to distinguish between the original data distribution and the transformed distribution.

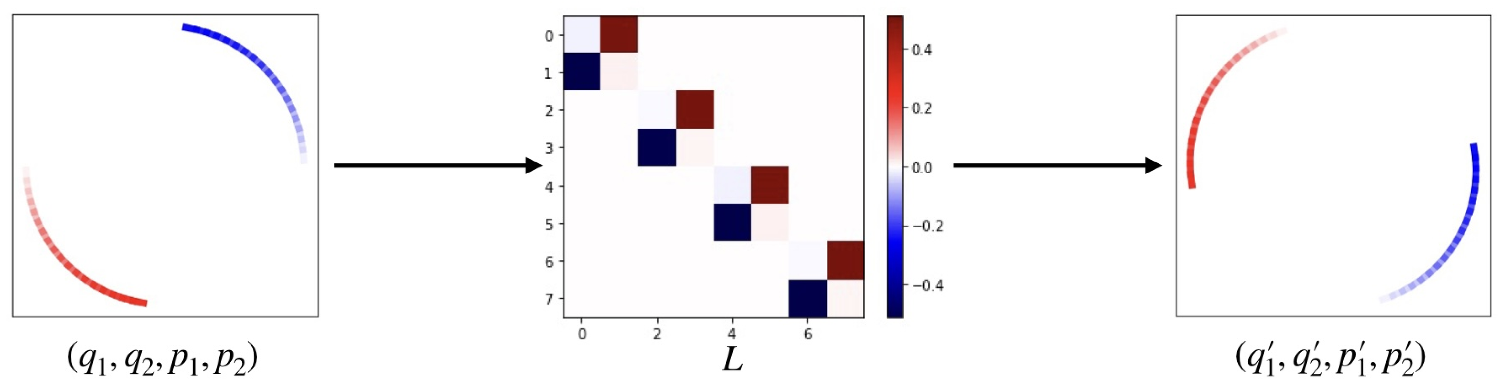
Learning Distributions over Lie Group: Our model learns Lie algebra basis $\{L_i \in \mathbb{R}^{k\times k}\}_{i=1}^c$ and samples the coefficients $w_i \in \mathbb{R}$ for their linear combination from either a fixed or a learnable distribution:

$$w \sim \gamma_\beta(w), \quad g = \exp\left[\sum_i w_i L_i\right]$$

Task #1: Two-Body Trajectory Prediction

Task: Predict the positions and momenta of future planar 2-body movements based on past observations.

Discovery: LieGAN can discover SO(2) symmetry that simultaneously rotates the positions and momenta of the two masses.



Prediction: We use different ways to use the discovered Lie algebra representation for prediction.

Data Augmentation. The training data can be augmented with LieGAN generator. To perform data augmentation for equivariance, we transform the input with group element g and transform the output with its inverse: $\hat{y} = g^{-1} f_{\text{model}}(gx)$.

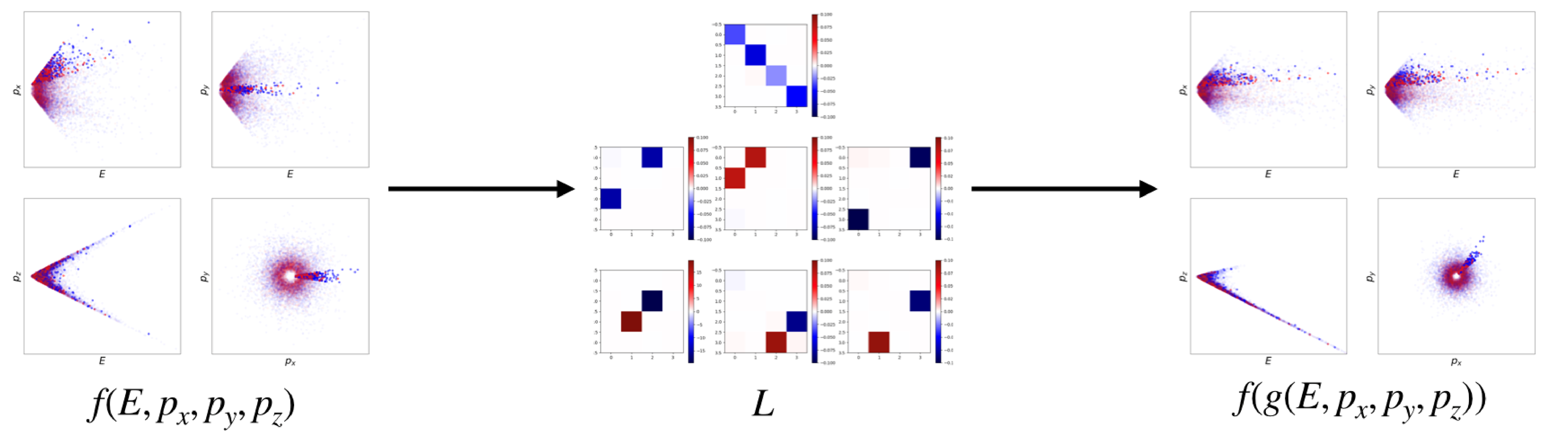
Equivariant MLP. There is a simple interface for building equivariant multi-layer perceptrons (MLP) for arbitrary matrix groups [2]. The discovered Lie algebra basis can be directly used to construct an equivariant model to the corresponding connected Lie group.

Model	EMLP	Data Aug.
LieGAN	6.43e-5	3.79e-5
LieGAN-ES	2.41e-4	6.17e-5
Augerino+	9.41e-4	1.47e0
SymmetryGAN	-	6.79e-4
Ground truth	**9.45e-6**	**1.39e-5**
HNN	3.63e-4	
MLP	8.49e-2	

Task #2: Top Quark Tagging

Task: Binary classification between top quark jets and lighter quarks. The input is the four-momenta of the constituents of the particle jets.

Discovery: LieGAN discovers the symmetry of restricted Lorentz group, $\mathrm{SO}(1,3)^+$. It learns the boosts along different spatial dimensions (row 2 of L) and the rotations within spatial dimensions (row 3 of L). The figure shows how the data distribution is transformed by one group element sampled from LieGAN.



LieGNN Prediction: Equivariance can be introduced into graph neural networks (GNN) through invariant edge features [3, 4]. We extend these methods to construct LieGNN, which can be equivariant to arbitrary symmetry discovered by LieGAN, based on the following proposition:

Proposition: *Given a Lie algebra basis* $\{L_i \in \mathbb{R}^{k\times k}\}_{i=1}^c$, $\eta(u,v) = u^T J v$ $(u, v \in \mathbb{R}^k, J \in \mathbb{R}^{k\times k})$ *is invariant to infinitesimal transformations in the Lie group G generated by* $\{L_i\}_{i=1}^c$ *if and only if* $L_i^T J + J L_i = 0$ *for* $i = 1, 2, ..., c$.

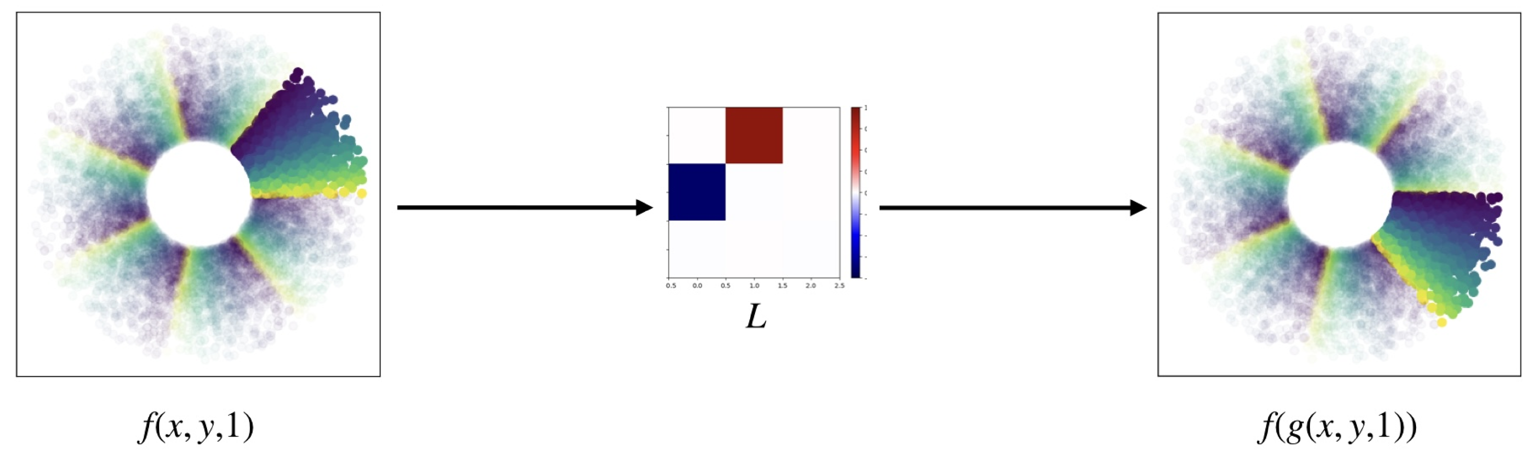
Model	Accuracy	AUROC
LorentzNet	**0.940**	**0.9857**
LieGNN	0.938	0.9848
LorentzNet (w/o)	0.934	0.9832
EGNN	0.922	0.9760

The table shows the test accuracy and AUROC on top tagging. Without requiring any prior knowledge, LieGNN almost reaches the performance with LorentzNet which explicitly encodes Lorentz symmetry.

Task #3: Synthetic Regression

Task: Regression on a synthetic function: $f(x,y,z) = z/(1 + \arctan\frac{y}{x} \mod \frac{2\pi}{7})$.

Discovery: LieGAN can discover a discrete C_7 rotation symmetry by using a discrete coefficient distribution $\gamma_\beta(w)$. The figure shows how the original samples on $z = 1$ plane are transformed by $g = \exp(L)$.



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