Automatic Symmetry Detection: A Pivot for AI-Guided Scientific Discovery

Jianke Yang UCSD
Nima Dehmamy IBM Research
Robin Walters Northeastern University
Rose Yu UCSD

We focus on the problem of automatic symmetry discovery from data. We define symmetry as the equivariance of a function under group transformations. Formally, G is a symmetry group of function $f : \mathcal{X} \to \mathcal{Y}$ if $g \cdot f(x) = f(g \cdot x), \forall g \in G, x \in \mathcal{X}$. The group action $\cdot$ characterizes how the group elements transform each point. Invariance is a special case of equivariance when the group action on $\mathcal{Y}$ is identity. Given a paired dataset $\{(x_i, f(x_i))\}$, we aim to discover its symmetry group G and the group action.

Symmetry is closely related to other physical properties. For instance, Noether's theorem states that continuous symmetries lead to conserved quantities; Sophus Lie's theory indicates that symmetries of a PDE constrain its equation form. Given the prevalence of symmetry in the natural world, we promote symmetry to a pivotal role in our workflow for scientific discovery. In our recent works, we have (i) developed a common framework for symmetry discovery for various types of data and group action (1; 2), (ii) derived useful inductive biases from the discovered symmetries via their connections to other physical properties (1; 3), and (iii) applied the symmetry-based inductive biases to downstream tasks, such as learning symbolic governing equations and long-term forecasting of dynamical systems (3).

Symmetry Discovery. Given the observed data $\{(x_i, y_i)\}$, we use an adversarial training approach to discover symmetry (1). A symmetry generator produces the transformations acting on data, and a discriminator is trained to distinguish the difference between the data distribution $p(x, y)$ and the transformed distribution $p(gx, gy)$. Our previous works have proposed different symmetry generator architectures to represent distinct types of symmetries, such as Lie group equivariance in terms of linear (1) and nonlinear group actions (2).

Symmetry-Informed Equation Discovery. Equation discovery aims to learn closed-form equations from numerical data. We focus on its application to first-order ODE systems: $\dot{\mathbf{x}} = \mathbf{h}(\mathbf{x})$. Our dataset consists of the observed trajectories: $\{\mathbf{x}_{0:T}^{(i)}\}_{i=1}^{N}$. We discover the ODE flow $\mathbf{h}$ in a closed form with sparse regression and genetic programming. We show that incorporating symmetry into these equation discovery algorithms can significantly increase the success probability of finding the correct equations, especially when the data is highly noisy (3).

Incorporating Symmetry-Based Inductive Biases. Depending on the type of symmetry, we propose a general guideline on how to incorporate symmetry into equation discovery (3). For linear symmetries, we solve the symmetry constraints as a linear system and obtain a lower-dimensional equation parameter space, thereby expediting the discovery process and promoting parsimony. For nonlinear symmetries, we construct regularization terms based on infinitesimal transformations, which is shown to improve the robustness of equation discovery methods to high measurement noise.

Discovery Results. We have re-discovered classical symmetries such as rotational symmetry in classical mechanics and Lorentz transformation invariance in high-energy physics (1). We have also discovered symmetries of nonlinear group actions in a wide range of differential equation systems, such as $\lambda - \omega$ reaction-diffusion system, nonlinear pendulum, Lotka-Volterra equations, and Sel'Kov glycolytic oscillator (2; 3). The discovered symmetry makes it much more likely to recover the correct equations with highly noisy data (3).

While our works (1; 2; 3) focus on different aspects of discovery, we will present them as components of the integrated discovery pipeline proposed in (3). We will show that the automatic detection of symmetry can lead to more robust and principled scientific discovery with machine learning approaches.

References

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