A Neural Network architecture for data-driven symmetry discovery and inverse design, with application to twistoptics.

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Symmetries play an essential role in the understanding of physical theories. A paradigmatic example is the conservation laws arising from continuous symmetries in classical mechanics. Discrete symmetries, such as parity or time reversal, do not depend on any continuous parameter and are key in studying degeneracies in the energy spectrum of quantum mechanical systems, for instance. Unveiling hidden discrete symmetries is of enormous interest in many fields of physics. Until recently, this task relied solely on human intuition. However, recent advances in machine learning (ML), especially in neural networks (NNs), have opened up new and efficient data analysis methods. For example, ML models have been exploited to uncover physical insights in unknown or partially known physical systems, including symmetries, governing equations, conservation laws, or physically relevant quantities.

If a given system presents discrete symmetries, there is a group of transformations acting on the physical parameters that leave the physical response invariant. Calculating the parameters from a given response is thus a multivalued problem. Here, we introduce a novel NN architecture that, provided only with experimental or numerical data, is capable of finding all these symmetry-related multivalued solutions and the corresponding representation of the group of symmetry transformations. We also provide a group-theoretic-based validation procedure that corroborates the finding of the unknown symmetry group.

Furthermore, our NN-based technique is generalizable for solving any multivalued inverse design problem (for example, when the degenerated solutions are not related to a symmetry inherent to the physical system). As an example, we provide an actual application in the emergent field of "twistoptics". Here, the systems under study comprise stacked van der Waals material layers, which present hyperbolic 2D propagation of phonon polaritons. An interesting phenomenon is that these materials present a topological transition between elliptic and hyperbolic propagation when twisting the layers at certain relative angles. At some specific "magic angles" where that transition occurs, light can be canalized, propagating at a given unique direction. This light canalization can arise in different material configurations, as relative angles, layer thicknesses, etc, can control it. Given a set of simulated data, our method can calculate several different setups of twisted layers that produce the same desired polariton propagation at a given frequency.

Our approach is a powerful tool because (i) discovering symmetries on data sets is highly nontrivial (especially if the data is high-dimensional), and (ii) it accurately solves multivalued inverse design problems where traditional NNs present significant prediction errors. Our algorithm is general and has been validated by several application examples.

References

[1] Calvo-Barlés, P., Rodrigo, S. G., Sánchez-Burillo, E., & Martín-Moreno, L. (2024). Finding discrete symmetry groups via machine learning. *Phys. Rev. E, 110, 045304*.

Figures

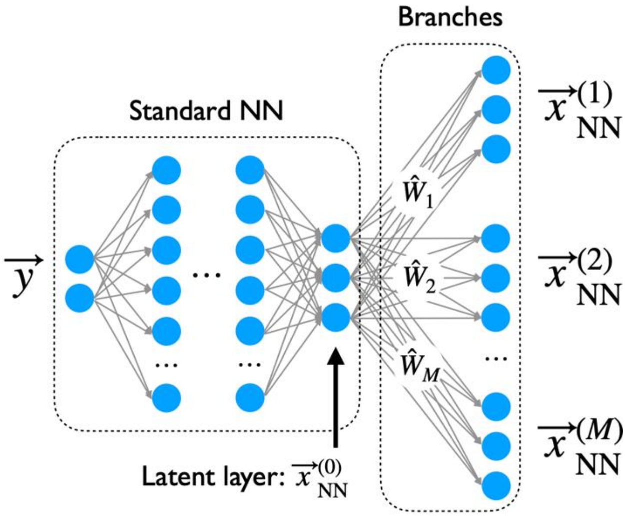

Figure 1. ML-based approach for symmetry detection: Symmetry Seeker Neural Network (SSNN).