Snowmass2021 – Letter of Interest

Symmetry Group Equivariant Architectures for Particle Physics

Computational Frontier – Thematic Areas:

☐ (CompF1) Experimental Algorithm Parallelization
☐ (CompF2) Theoretical Calculations and Simulation
■ (CompF3) Machine Learning
☐ (CompF4) Storage and processing resource access
■ (CompF5) End user analysis
☐ (CompF6) Quantum computing
☐ (CompF7) Reinterpretation and long-term preservation of data and code

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Abstract:

This *Letter of Interest* aims to communicate the potential and the need for a concerted effort to consider the role that physical laws and, more specifically, *symmetries*, may have in the design and development of machine learning architectures for physics. As the field of particle physics moves inexorably towards the widespread use of sophisticated, powerful, and yet often intractably complex algorithms, it is likely to prove advantageous, both practically and scientifically, to imbue these systems with the understanding of the symmetries that we believe underlie them. Several examples of neural networks, graph networks, and other architectures that respect global and/or gauge symmetries have been developed very recently, and the lessons learned from these efforts may help both to guide future architecture designs, as well as to suggest infrastructure and resources that may be necessary for efficient usage of such approaches (e.g. dedicated CUDA kernels or IP blocks for embedded systems). We hope that these ideas can be incorporated into either a dedicated *White Paper* on equivariant architectures for physics, or a joint report for Snowmass summarizing plans and novel ideas for new directions in machine learning for future physics facilities.

***Letter of Interest*:**

Nearly all areas of physics are witnessing a renaissance in the development, application, and results of machine learning applied to both old and new problems. Sophisticated, complex, and extremely diverse sets of algorithms based on a wide array of architectures and design principles are breathing new life into issues ranging from silicon sensor readout [1] to parsing the landscape of string theories [5], from distinguishing quarks from gluons [11] to controlling telescopes searching the cosmos. One of the driving principles that has often guided the emergence of new theoretical directions and placed constraints on the experimental methods used to test them is that of *symmetries*. Global and gauge symmetries, continuous and discrete symmetries, internal and external symmetries: the existence of any one of these can place constraints on the dynamics of a system, require conservation of quantities and quantum numbers, or reduce the dimensionality of the phase space in which the system may live. However, it is rare to see their explicit inclusion into the complex algorithms that are so often used to analyze particle collisions, or constrain the identification of particle decays, for example. In this *Letter of Interest* we aim to highlight the potential for such approaches at both current and future physics facilities and argue for the need for the community to consider the possible benefits to the tools of machine learning as they are applied to physics problems.

There are many relevant problems in physics that exhibit rich and complex symmetries, and in many cases several such symmetries. These problems may require or at least benefit from models that exhibit latent space representations that are intimately connected with the theory of the specific underlying symmetry group. Indeed, these symmetries are often manifest in the data itself, as each data point is generated by a symmetric process or model. Following this approach, elegant architectures can be informed by fundamental principles, and the "building blocks" of such architectures may be greatly restricted by the imposed symmetries. This is a highly sought-after property in neural network design since it may – perhaps counterintuitively – improve generality, interpretability, and uncertainty quantification, while also allowing for certainly simplifications of the model itself.

These general ideas have already led to the development of multiple equivariant architectures for sets (permutation invariance) [14], graphs (graph isomorphisms), 3D data (spatial rotations) [12], homogeneous spaces of Lie groups such as the two-dimensional sphere [6], and even gauge invariant systems [4, 10].

Symmetries play a central role in any area of physics [9], and as such physics provides may provide one of the widest variety of symmetry groups relevant in computational problems. In particular, high energy and particle physics involve symmetry groups ranging from $\mathrm{U}(1)$, $\mathrm{SU}(2)$ and $\mathrm{SU}(3)$ to the Lorentz group $\mathrm{SO}(1,3)$, and even more exotic ones like E_8 and conformal Lie algebras. Architectures that respect these symmetries may be able to provide more sensible and tractable models, whose parameters have the potential be directly interpreted in the context of known physical models, as is often the case with convolutional neural networks (CNNs) used in image recognition.

Harmonic analysis provides two parallel but closely related implementations of group equivariance in neural networks. The first is a natural generalization of CNNs to arbitrary Lie groups and their homogeneous spaces [8], where activations are functions on the group, the nonlinearity is applied point-wise, and the convolution is an integral over the Lie group. The second approach works entirely in the Fourier space [2, 13], that is, on the set of irreducible linear representations of the group, and the nonlinearity is based on tensor products and Clebsch-Gordan decompositions.

These ideas are general and may be applied in any field of computational physics. In this *Letter of Interest* we focus on a particular subset of applications in particle physics where the data typically contain the energy-momentum 4-vectors of particles produced in collision events at high energy particle accelerators, or by simulation software used to model the collision events. As 4-vectors, these data naturally support an action of the Lorentz group, therefore architectures that are Lorentz-invariant or Lorentz-equivariant are a major step towards understanding the ways in which machine learning can solve physical problems with such inputs. The first successful application was for the Lorentz-invariant task of top-tagging [3], where a competitive performance was reached despite a dramatic decrease in the number of parameters. We are confident that in the near future these applications will be extended to complex regression tasks and tasks with vector targets.

As can be seen in the literature referenced above, the development of equivariant architectures requires an understanding of group theory, representation theory, and numerical methods associated with them. Until recently, these areas have have existed on the periphery the machine learning community within physics, but we hope that by building a catalog of basic machine learning tools (and "building blocks") for specific common symmetries, we can usher in a new level of sophistication for applications in this, and related, domains. Here are some of the basic areas that require more work:

- Efficient Clebsch-Gordan decompositions of tensor products for representations of compact Lie Groups (e.g. $\mathrm{SU}(N)$), to be used as equivariant nonlinearities;
- Combining Lie Group equivariance with complete equivariance w.r.t. discrete symmetries such as permutations or graph isomorphisms ([2] and [3] only achieved permutation *invariance*, and not in the most general way);
- Efficient convolutions on compact Lie Groups and their induced representations, as an extension of CNN's to other symmetries, including gauge groups;
- Extensions to symmetries that are direct or semi-direct products of simple groups (such as the group of Euclidean motions [7], or the full Standard Model symmetry group);
- Extensions to non-compact groups with completely reducible finite-dimensional representations (such as the Lorentz group [3]). This task is very similar to that for compact groups;
- Extensions to infinite-dimensional representations of non-compact group (such as conformal symmetries in e.g. image recognition). This requires new advanced methods, such as an efficient truncation of representations, and dealing with continua of irreducible representations.

By imbuing machine learning architectures with the fundamental symmetries that underlie the systems to which we are applying them, we aim to improve their performance, reduce unnecessary computational complexity, and enhance the interpretability of their outputs. By exploring the space of possible applications and avenues of investigation – symmetry groups, compute kernels, technical implementation, applications – we hope to identify new directions and highlight priorities in theoretical physics, computational physics, and instrumentation for incorporating these fundamental principles into our machine learning toolkits. We believe that this work may be best represented in the Snowmass process through either a dedicated *White Paper* on equivariant architectures for physics, or a joint report for Snowmass summarizing plans and novel ideas for new directions in machine learning for future physics facilities.

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