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Efficient Parameterization of Many-body Interaction

I will review the atomic cluster expansion (ACE), which provides a systematic, efficient, and interpretable parameterisation of many-body interaction in particle systems. It can be thought of as a method to enlarge the design space of equivariant neural network architectures. ACE is well-suited for parameterising surrogate models of particle systems where it is important to incorporate symmetries and geometric priors into models without sacrificing systematic improvability. The most successful application so far is “learning” interatomic potentials (or, force fields) but the applicability is much broader; it has been adapted to other contexts such as electronic structure (parameterising Hamiltonians), quantum chemistry (wave functions), and elementary particle physics (e.g., jet tagging). The main purpose of my talk will be to explain the framework that enables this breadth of applications, and point out theoretical questions and challenges.