DEEP NEURAL NETWORKS AND MOLECULAR DYNAMICS

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Multilayer neural networks (NN), commonly called deep NN, have demonstrated an unprecedented capability of learning complex and highly nonlinear functional dependence. This feature prompted several groups to use machine-learning techniques to generate potentials that faithfully reproduce the trajectories of *ab-initio* molecular dynamics (AIMD) simulations, either classical or quantum mechanical (path-integral).
These approaches eliminate the need of carrying electronic structure information on the fly, and allow us to perform simulations of AIMD quality at the cost of empirical force fields. In this context, I will discuss an approach that uses a novel symmetry preserving ordering of the atomic coordinates in a local environment. In this scheme the many-body potential energy is a sum of the energies associated to the individual atoms in the system.
Each one of these "atomic" energies depends analytically, via the deep NN representation, on the coordinates of the atoms belonging to the local environment of each given atom. The approach can be further generalized by systematically coarsegraining the atomic coordinate dependence to greatly speed up free energy computations.
Open problems and future perspectives will be discussed in the concluding remarks.