# Analysis of Molecular Simulation by Adversarial Autoencoder

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Machine learning and artificial neural networks are intensively studied in connection with molecular simulations. This research is often motivated by acceleration. Molecular simulations, namely, the molecular dynamics simulation or Monte Carlo method, have a great potential in designing new drugs, proteins, enzymes, or materials. In principle, it is possible to simulate drug-target complexes, proteins or new materials to predict their stability and other properties from the evolution of molecular structure. However, the practical application of molecular simulations is complicated by their large computational costs. A typical biomolecular system consists of thousands of atoms interacting with each other via short-range and long-range non covalent interactions. This vast number of mutual interactions must be evaluated in every step of the simulation. Furthermore, a simulation step must be relatively short (femtoseconds in molecular dynamics) to assure numerical stability. As the results, typical molecular dynamics simulations can sample only a small fraction of the states available to the simulated system, with the likely loss of some slow or rarely occurring processes. There are numerous opportunities for machine learning and artificial neural networks to address this problem. For the reasons mentioned above, we apply autoencoders, generative neural networks and their combination as a platform for analysis of simulation data. The potential of this fusion was demonstrated on microsecond trajectory of Alanine Dipeptide and Trp-cage.

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