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Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

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Computing equilibrium states in condensed-matter many-body systems, such as solvated proteins, is a long-standing challenge. Lacking methods for generating statistically independent equilibrium samples in "one shot," vast computational effort is invested for simulating these systems in small steps, e.g., using molecular dynamics. Combining deep learning and statistical mechanics, we developed Boltzmann generators, which are shown to generate unbiased one-shot equilibrium samples of representative condensed-matter systems and proteins. Boltzmann generators use neural networks to learn a coordinate transformation of the complex configurational equilibrium distribution to a distribution that can be easily sampled. Accurate computation of free-energy differences and discovery of new configurations are demonstrated, providing a statistical mechanics tool that can avoid rare events during sampling without prior knowledge of reaction coordinates.