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Sampling with generative models

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In probability theory, the notion of "weak convergence" is often used to describe two equivalent probability distributions. This metric requires equivalence of the average value of well-behaved functions under the two probability distributions being compared. In coarse-grained modeling, Noid and Voth developed a thermodynamic equivalence principle that has a similar requirement. Nevertheless, there are many functions of the fine-grained system that we simply cannot evaluate on the coarse-grained degrees of freedom. In this talk, I will describe an approach that combines accelerated sampling of a coarse-grained model with invertible neural networks to invert a coarse-graining map in a statistically precise fashion. I will show that for nontrivial biomolecular systems, we can quantitatively recover the fine-grained observables from coarse-grained sampling. Finally, I will discuss the general framework of using auxiliary models for mode discover when sampling with generative models.

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Classification de Session: Challenge and Perspective