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Information Theory and Statistical Mechanics Revisited

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The statistical mechanics of Gibbs is a juxtaposition of subjective, probabilistic ideas on the one hand and objective, mechanical ideas on the other. In this paper, we follow the path set out by Jaynes, including elements added subsequently to that original work, to explore the consequences of the purely statistical point of view. We show how standard methods in the equilibrium theory could have been derived simply from a description of the available problem information. In addition, our presentation leads to novel insights into questions associated with symmetry and non-equilibrium statistical mechanics. Two surprising consequences to be explored in further work are that (in) distinguishability factors are automatically predicted from the problem formulation and that a quantity related to the thermodynamic entropy production is found by considering information loss in non-equilibrium processes. Using the problem of ion channel thermodynamics as an example, we illustrate the idea of building up complexity by successively adding information to create progressively more complex descriptions of a physical system. Our result is that such statistical mechanical descriptions can be used to create transparent, computable, experimentally-relevant models that may be informed by more detailed atomistic simulations. We also derive a theory for the kinetic behavior of this system, identifying the nonequilibrium `process' free energy functional. The Gibbs relation for this functional is a fluctuation-dissipation theorem applicable arbitrarily far from equilibrium, that captures the effect of non-local and time-dependent behavior from transient driving forces. Based on this work, it is clear that statistical mechanics is a general tool for constructing the relationships between constraints on system information.

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