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Building phenomenological models of complex biological processes[1] BRYAN DANIELS, Cornell University, ILYA NEMENMAN, Emory University — A central goal of any modeling effort is to make predictions regarding experimental conditions that have not yet been observed. Overly simple models will not be able to fit the original data well, but overly complex models are likely to overfit the data and thus produce bad predictions. Modern quantitative biology modeling efforts often err on the complexity side of this balance, using myriads of microscopic biochemical reaction processes with a priori unknown kinetic parameters to model relatively simple biological phenomena. In this work, we show how Bayesian model selection (which is mathematically similar to low temperature expansion in statistical physics) can be used to build coarse-grained, phenomenological models of complex dynamical biological processes, which have better predictive powers than microscopically correct, but poorely constrained mechanistic molecular models. We illustrate this on the example of a multiply-modifiable protein molecule, which is a simplified description of multiple biological systems, such as an immune receptors and an RNA polymerase complex. Our approach is similar in spirit to the phenomenological Landau expansion for the free energy in the theory of critical phenomena.

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