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Methods to model (and quantify the complexity of) bio-molecular conformational dynamics

We present methods for inferring hidden Markov models from continuous data clustered around discrete values without the necessity of assuming a model architecture and as such are capable of inferring the existence of degenerate states (states with the same distribution for the observable variable but different transition probabilities). The models inferred in this way are provably optimal and minimal statistical predictors of the data. Additionally, information theoretic measures applied to the inferred model quantify the complexity of the data.

The methods have been demonstrated on the conformational dynamics of Holliday (4 way DNA) junctions (under review - http://arxiv.org/abs/1011.2969) as investigated by fluorescence resonance energy transfer spectroscopy. However, the methods are applicable to any data meeting certain criteria and as such may be applicable to many dynamical systems.