Boltzmann Probability

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1 Introduction

The Boltzmann Probability is used to calculate the likelihood of a protein being within a certain state.

This can be applied to ensemble design, where each backbone template is the state, and the ensemble is the set of all possible states (a discrete approach to modelling protein dynamics). Represent each backbone template as E_i, where i is the state number. Hence we have

$$E_T = \{E_1, E_2, ..., E_N\} \tag{1}$$

Where N is the total number of ensembles, and $E_i \in \mathbb{R}$.

Using Boltzmann's probability, we can write the likelihood of finding the protein with a certain backbone E_i, as $P_{E_T}(E_i)$:

$$P_{E_T}(E_i) = \frac{e^{-E_i/k_B T}}{\sum_{i=1}^{N} e^{-E_i/k_B T}} \tag{2}$$

Where k_B is the Boltzmann constant, T is the temperature.

Now, let's add in a single template E_{N+1} to our set of backbones, to form E_T':

$$E_T' = \{E_1, E_2, ..., E_N, E_{N+1}\} \tag{3}$$

Hence, the new probability becomes $P_{E_T'}(E_i)$:

$$P_{E_T'}(E_i) = \frac{e^{-E_i/k_B T}}{\sum_{i=1}^{N+1} e^{-E_i/k_B T}} \tag{4}$$

Notice that the denominator in (4) will always be greater than the one in (3).

Hence,

$$P_{E_T'}(E_i) < P_{E_T}(E_i) \tag{5}$$

Which makes sense upon further examination - since nothing has changed apart from adding a new template, the probability of extracting any E_i will be smaller in the new case (4) rather than the original (3).