Short vs Long Modelling

Spyros Koumarianos

February 9, 2020

Formulas and Expressions

Draft Page 20-21

For an n-mer free in Solution scenario

$$Z_F = Z_{vol} N_{tot} \; with \; E_n = n\epsilon$$

now lets consider the scenario where it is bound to a 2D surface Lattice of chain length L, where the sum is the union of partial surface contact permutations, for n$\in [1, L]$ where n, is the number of discrete contacts of the bound-chain,this considering the possibility of Looping

$$Z_B = Z_surf \sum_{n=1}^{L} N_n exp\left\{ \frac{-n\epsilon}{kT} \right\}$$

where equlibrium constant is just the ratio

$$\frac{Z_{Bound}}{Z_{Free}} = K$$

so we take $\frac{Z_{Bound}}{Z_{Free}} = \frac{Z_{surf}}{Z_{vol} N_{tot}} \sum_{n=1}^{L} N_n exp\left\{ \frac{-n\epsilon}{kT} \right\} = \frac{Z_{surf}}{Z_{vol}} \sum_{n=1}^{L} \frac{N_n}{N_{tot}} exp\left\{ \frac{-n\epsilon}{kT} \right\}$

now let $f_n := \frac{N_n}{N_{tot}}$

$$K := \frac{Z_{surf}}{Z_{vol}} \sum_{n=1}^{L} f_n exp\left\{ \frac{-n\epsilon}{kT} \right\}$$

normalizing by dividing by fn both sides

$$K' := K \frac{1}{f_n} = \frac{Z_{surf}}{Z_{vol}} \sum_{n=1}^{L} \frac{f_n}{f_n} exp\left\{ \frac{-n\epsilon}{kT} \right\}$$

The author of Draft used Boltzman Statistics, where the probability a chain contacts surface, is the cardinality of set of m-mers contacting to cardinality of all possible n-mers making discrete partial contacts, otherwise known as looping
(Aside: this applies for either long or short)

$$p_n(m) := \frac{\left| \left\{ \text{m-mers of chain contacting surface} \right\}_{\text{fixed m}\in n} \right|}{\left| \bigcup_{n=1}^{L} \left\{ \text{n-mers of chain contacting surface} \right\}_n \right|}$$

Whereas Professor Madras focused on the Summand of n=L, as opposed to incorporating all possible mers in the "1st level model"

page 23

Graph 1

The % total conformations possible to the # of contacts we are outputting for
LONG vs SHORT ie; as the variation of conformations increases the less contacts we will get
for both long and short. Obviously, the long drops off extremely quick.

Graph 2

The zoomed in graphic says that between 2% and 22% of potential conformations either or can win
By diversifying our conformations iteratively, in essence progressing our random walk
we produce all sorts of line-segment (chain) conformations and see who wins in # of
surface contacts, the long or the short?
So what the iterations are simulating are essentially the levels of entropy.

Understanding Methods Used by A. Mittermaier

Comments on Differences: Mittermaier vs Madras

In order to model the fn's by MC we would require values for everything but fn
So from our partition function (which is the (literal) distributions of particles
in the space, or ensemble

So K' is the best candidate for modelling, but I must calculate the K' from ΔA

There are also questions about how to compile the model because we aren't sure
if we should proceed directly with the complex case before trying it without
looping, because Anthony, from the very first level considering loops in the calculation
from the summand, and Professor Madras said that wouldn't be required
needed as they cancel out, in the comparison, which also happens to be
the normalized Equilibrium constant for chain binding

References

They are referring to an 80 page document and are giving very little
in regards to methods and algorithms in specific,
it would be very hard to reproduce their results

Few words on MC

take a bound and a distribution and randomly take values from it and
see what the area below the curve is. For example, the area of a circle
can be found using even distr. eg raindrops falling uniformly in the bounds of a
chalked in circle of pavement