A Simple Markov Model Of A Chain with A Single Loop

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1 The Model

In this document we summarize a simple Markov chain describing a chain having N monomers (beads) and one occasion of a loop. Only the first monomer can create a loop with all other $j = 2, 3, .., N$. We consider bead N to be fixed. There are several states for the model. Assuming a loop $[1, j]$, indicating bead 1 is connected to bead j, we can form the loops $[1, j+1], [1, j-1]$, or detach, indicated by $[1, 0]$.

Using this terminology, we write
$[1, j] \rightarrow [1, j+1] = \lambda$
$[1, j] \rightarrow [1, j-1] = \mu$
$[1, 0] \rightarrow [1, j] = \alpha$
$[1, j] \rightarrow [1, 0] = \beta$
$[1, 0] \rightarrow [1, 0] = 1 - \alpha$
where $j = 2, 3, ..., N$ The α value represent the probability of attaching bead 1 to bead j given that there is no loop at time t. At first approximation we vary α according to the probability that the beads are closer than some distance, given by the function:

$$\alpha_{nm} = \Phi(|R_n - R_m| < \epsilon, n-m) = \left[\frac{3}{2\pi b^2 |n-m|}\right]^{3/2} \int_0^{\epsilon} \exp\left[-\frac{3k^2}{2|n-m|b^2}\right] dk$$

where $b > 0$ is the connection length, R_n is the position of bead n, and $\epsilon > 0$ is the maximal distance in which two beads are considered to have met. We indicate the probability to create a loop $[1, j]$ by p_j. Thus, the master equation is given by:

$$
\begin{bmatrix} \dot{p}_0 \\ \dot{p}_2 \\ . \\ . \\ . \\ \dot{p_N} \end{bmatrix} = \begin{bmatrix} -N\alpha & \beta & \beta & ... & ... & \beta & \beta \\ \alpha & -(\beta+\lambda) & \mu & ... & ... & ... & 0 \\ \alpha & \lambda & -(\beta+\lambda+\mu) & \mu & ... & ... & 0 \\ \alpha & 0 & \lambda & -(\beta+\lambda+\mu) & \mu & ... & 0 \\ . \\ . \\ . \\ \alpha & 0 & 0 & ... & \lambda & -(\beta+\mu+\lambda) & \mu \\ \alpha & 0 & 0 & ... & 0 & \lambda & -(\beta+\mu) \end{bmatrix} \begin{bmatrix} p_0 \\ p_2 \\ . \\ . \\ p_N \end{bmatrix}
$$

in short notation we write

$$[\dot{P(t)}] = [M]\,[P(t)]\,.$$

the solution to the equation above is given by

$$[P(t)] = [P(0)]\exp[Mt] = [U]\,exp([D]\,t)\,\left[U^{-1}\right][P_0]$$

where $[P(0)]$ is the initial distribution of states, U is a matrix of the eigenvectors in its columns, and D is a diagonal matrix with the corresponding eigenvalues in the diagonal entries.

2 Simulations

Setting $\beta = \mu = \lambda = x$ we get

$$
[M] = \begin{bmatrix} -N\alpha & x & x & ... & ... & x & x \\ \alpha & -2x & x & ... & ... & ... & 0 \\ \alpha & x & -3x & x & ... & ... & 0 \\ \alpha & 0 & x & -3x & x & ... & 0 \\ . \\ . \\ . \\ \alpha & 0 & 0 & ... & x & -3x & x \\ \alpha & 0 & 0 & ... & 0 & x & -2x \end{bmatrix}
$$

choosing $x = 1/3$, $d = b/2$, and simulating the system until steady-state (note that α remains as defined above), we find, for a chain of $N = 64$ beads that the probability to find a loop $[1, j]$ at steady-state is proportional to $|j-1|$ see Figure 2 and Figure 2.

The steady state probability of loops $[1, j]$ is shown in Figure 2

2.1 Introducing 'hot spots' in the chain

We next introduce some beads for which bead 1 have more affinity to, in the sense that once a loop $[1, j]$ is formed,with j being the affine bead to 1, the probability of either detachment (β), decreasing (μ) or increasing (λ) the loop size are decreased in relation to other beads.

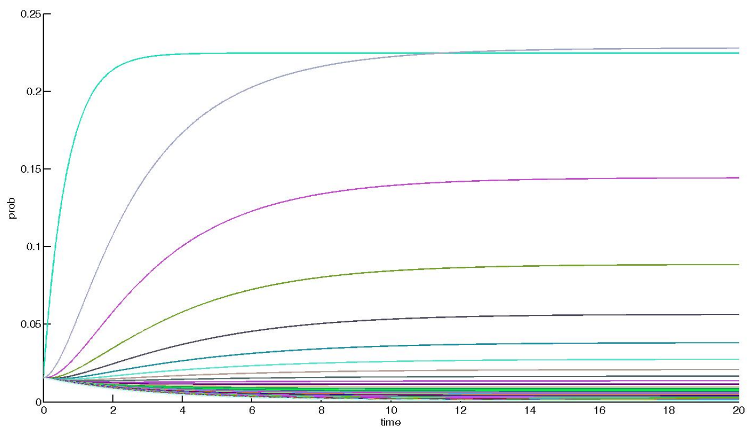

Figure 1: The time evolution of the Markov chain, with $x = 1/3$. The values of α remained as defined above. The thick cyan curve represents the probability of no loop. The curves are decreasing (at steady states) with bead number

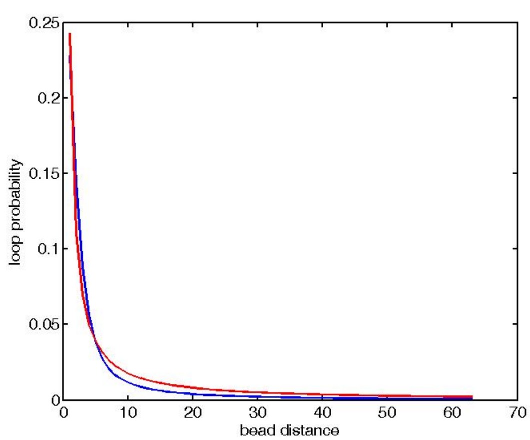

Figure 2: The steady state values of the loop probability (blue curve), with $x = 1/3$, and α as defined above. To test the theoretical results, that the looping probability is proportional to the bead distance, we fit a model of the kind $y = ax^{-b}$ (red curve). The fitted values are $a = 0.2429$, $b = 1.137$. The R-square value of the fit is 0.9687