

# 1 The Model

# A Simple Markov Model Of A Chain with A Single Loop

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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  $j = 2, 3, \dots, N$ . 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

$$\begin{aligned} [1, j] &\rightarrow [1, j + 1] = \lambda \\ [1, j] &\rightarrow [1, j - 1] = \mu \\ [1, 0] &\rightarrow [1, j] = \alpha \\ [1, j] &\rightarrow [1, 0] = \beta \\ [1, 0] &\rightarrow [1, 0] = 1 - \alpha \end{aligned}$$

where  $j = 2, 3, \dots, N$ . The  $\alpha$  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  $\alpha$  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:

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

in short notation we write

$$[P(t)] = [M] [P(t)].$$

the solution to the equation above is given by

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

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

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

choosing  $x = 1/3$ ,  $d = b/2$ , and simulating the system until steady-state (note that  $\alpha$  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 ( $\beta$ ), decreasing ( $\mu$ ) or increasing ( $\lambda$ ) the loop size are decreased in relation to other beads.

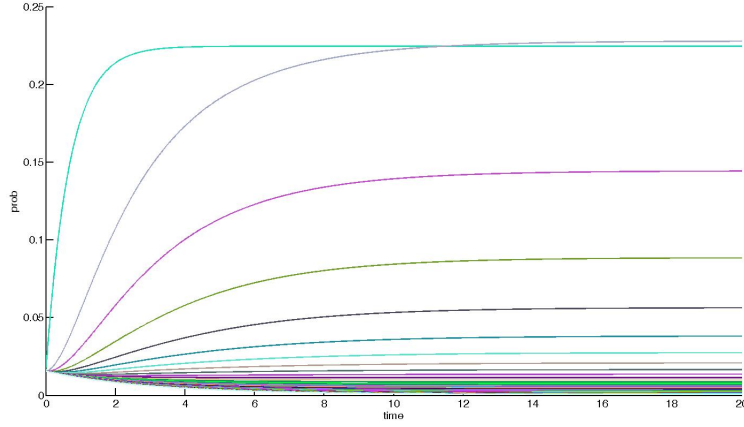


Figure 1: The time evolution of the Markov chain, with  $x = 1/3$ . The values of  $\alpha$  remained as defined above. The thick cyan curve represents the probability of no loop. The curves are decreasing (at steady states) with bead number

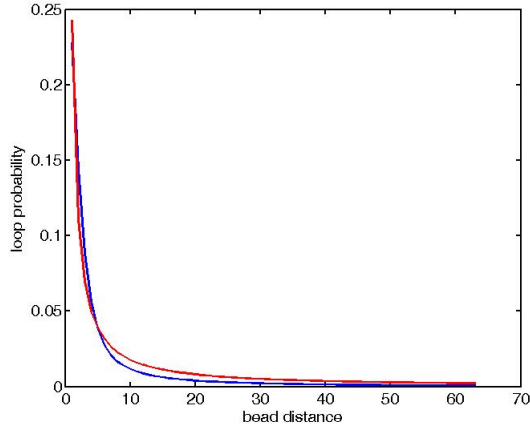


Figure 2: The steady state values of the loop probability (blue curve), with  $x = 1/3$ , and  $\alpha$  as defined above. To test the theoretical results, that the looping probability is proportional to the bead distance, we fit a model of the kind  $y = ax^{-b}$  (red curve). The fitted values are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