

Average length of chain molecule

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The problem:

A molecule can be described as a chain of N monomers, each monomer has the probability p to be positioned horizontally, adding length a to the molecule, otherwise the monomer is of length b . Let L be the molecule's length, define a random variable \hat{X}_n so that:

$$X_n = \begin{cases} a, & \text{the monomer is horizontal} \\ b, & \text{the monomer is vertical} \end{cases}$$

We assume that the ratio $\frac{a}{b}$ is an Irrational number.

- Express \hat{L} using \hat{X}_n . By fundamental theorems on adding independent random variables find $\langle L \rangle$, $Var(L)$.
- Find $f(L) \equiv P(L = na + (N - n)b)$. Using combinatorial considerations and calculate $\langle \hat{L} \rangle$, $Var(L)$.
- Define $\sigma_L = \sqrt{Var(L)}$ What is the behavior of $\sigma_L/\langle L \rangle$ as a function of N ?

The solution:

(a) As each monomer is of length a or b , the length of the molecule is the sum $L = \sum_{n=1}^N X_n$. The random variable $\langle \hat{X}_n \rangle = a \cdot p + b \cdot q$ where $q = (1 - p)$ can also be summed. The expectation operator E is linear in the sense that $E(X + Y) = E(X) + E(Y)$, then we can denote :

$$\langle L \rangle = \sum_{n=1}^N \langle X_n \rangle = N \langle X_n \rangle = N (ap + bq) \quad (1)$$

To find $Var(L)$ let us find the variance of X_n and use the linearity property $Var(X + Y) = Var(X) + Var(Y) + 2Cov(X, Y)$. The random variables X_n are not dependant, meaning they have a Covariance of 0. the variance of L is the sum

$$Var(L) = \sum_{n=1}^N Var(X_n) = N ((pa^2 + qb^2) - (pa + qb)^2) \quad (2)$$

(b) The number of ways to choose n out of N objects with no importance to the order in which they were chosen is $C_N^n = \frac{N!}{n!(N-n)!}$. So the probability for a molecule to be of length L takes the form of binomial distribution

$$f(L) = P(L = na + (N - n)b) = \sum_{n=1}^N C_N^n p^n q^{N-n} (na + (N - n)b) \quad (3)$$

The expectation value and variance can be found by use of the moment generating function of the binomial distribution $M(v) = (pe^{av} + qe^{bv})$ and the linearity properties.

$$\langle L \rangle = \sum_{n=1}^N \langle X_n \rangle = N \frac{\partial M(v)}{\partial v} (pe^{av} + qe^{bv}) \Big|_{v=0} = N(pa + qb) \quad (4)$$

In a similar way using the second moment (second derivative) we can find the variance:

$$Var(L) = \sum_{n=1}^N Var(X_n) = \sum_{n=1}^N \left[\frac{\partial^2 M(v)}{\partial v^2} - \left(\frac{\partial M(v)}{\partial v} \right)^2 \right] = N((pa^2 + qb^2) - (pa + qb)^2) \quad (5)$$

(c) by inspecting the behavior of the function with respect to N one can see that:

$$\frac{\sigma}{\langle L \rangle} = \frac{\sqrt{N(pa^2 + qb^2 - (pa + qb)^2)}}{N(pa + qb)} \sim \frac{1}{\sqrt{N}} \quad (6)$$