Data Analysis of RNA Model

ELD-431

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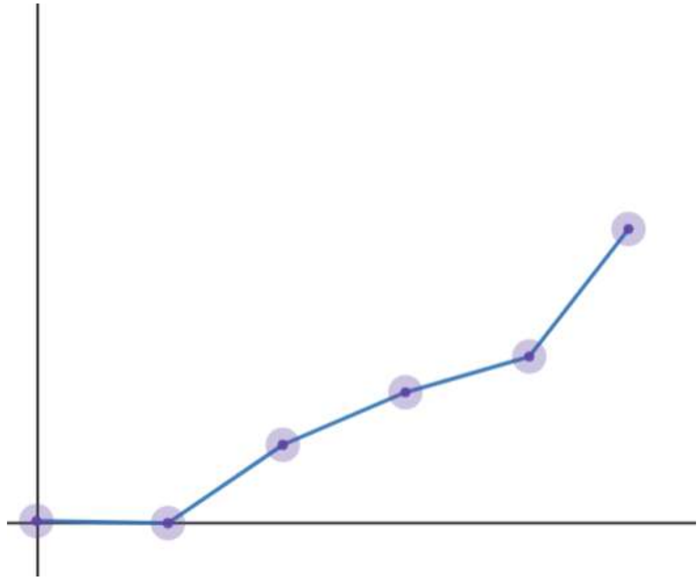
Introduction

In a 2-D plane, in a N-unit ball and stick model, the first ball is at origin and the second ball is at (1, 0). The rest of the balls can have any position, with the constraint that the distance between consecutive balls is 1.

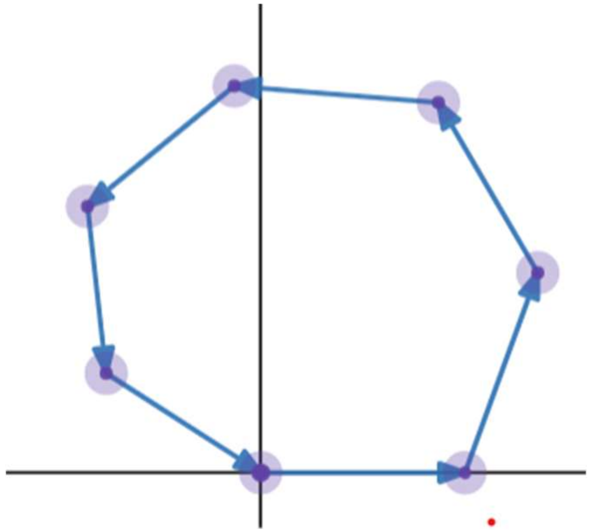
Our approach introduces a classification system based on the principle that vector representation of a n-sided polygon is unique iff n is prime. The study further categorizes configurations by vector arrangement and order, leading to a zero resultant. We methodically enumerate the total configurations, factoring in the factorial arrangement of vectors.



Problem Statement

We are trying to classify possible configurations of the model in which interaction energy of the specified balls is minimum.

1) (1, N)
2) (a, b)|a, b ∈ [1, N]; b − a > 1
3) (a1, b1), (a2, b2), (a3, b3), ...|ai, bi ∈ [1, N]; bi − ai > 1



$$V = \frac{1}{2}\left(d(b_1, a_1)^2 + d(b_2, a_2)^2 + d(b_3, a_3)^2 + ...\right)$$

Min(V)

d(1, N) = 0

Work till midterm

Equations from model in problem statement:

1. For N=3:

$$-\sin\theta_{21}$$

2. For N=4:

$$-\sin\theta_{21} - \sin\theta_{21}\cdot\cos\theta_{31} + \cos\theta_{21}\cdot\sin\theta_{31}$$

$$-\sin\theta_{31} - \sin\theta_{31}\cdot\cos\theta_{21} + \cos\theta_{31}\cdot\sin\theta_{21}$$

3. For N=5:

$$-\sin\theta_{21} - \sin\theta_{21}\cdot\cos\theta_{31} + \cos\theta_{21}\cdot\sin\theta_{31} - \sin\theta_{21}\cdot\cos\theta_{41} + \cos\theta_{21}\cdot\sin\theta_{41}$$

$$-\sin\theta_{31} - \sin\theta_{31}\cdot\cos\theta_{21} + \cos\theta_{31}\cdot\sin\theta_{21} - \sin\theta_{31}\cdot\cos\theta_{41} + \cos\theta_{31}\cdot\sin\theta_{41}$$

$$-\sin\theta_{41} - \sin\theta_{41}\cdot\cos\theta_{31} + \cos\theta_{41}\cdot\sin\theta_{31} - \sin\theta_{41}\cdot\cos\theta_{21} + \cos\theta_{41}\cdot\sin\theta_{21}$$

Solution of model obtained from problem statement:

1. For N=3:

$$[-\pi]$$

2. For N=4:

$$[\frac{2\pi}{3}, \frac{4\pi}{3}]$$

$$[\frac{4\pi}{3}, \frac{2\pi}{3}]$$

3. For N=5:

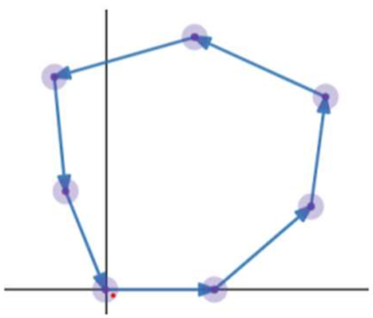
$$[-\pi, \theta, -\pi+\theta]$$

$$[\theta, -\pi, -\pi+\theta]$$

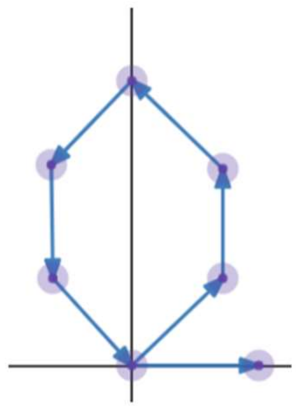
$$[\theta, -\pi+\theta, -\pi]$$

Results and Discussion

$\vec{v_1} + \vec{v_2} + \vec{v_3} + ... + \vec{v_7} = 0$



$\vec{v_1} = 0; \vec{v_2} + \vec{v_3} + \vec{v_4} + \vec{v_5} + \vec{v_6} + \vec{v_7} = 0$



$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} + \vec{v_5} + \vec{v_6} + \vec{v_7} = 0$

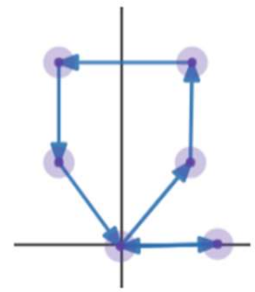
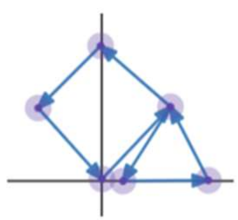
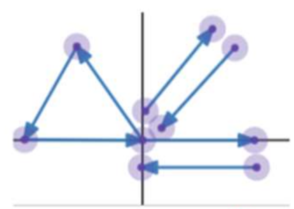


Fig. 6. For (6)

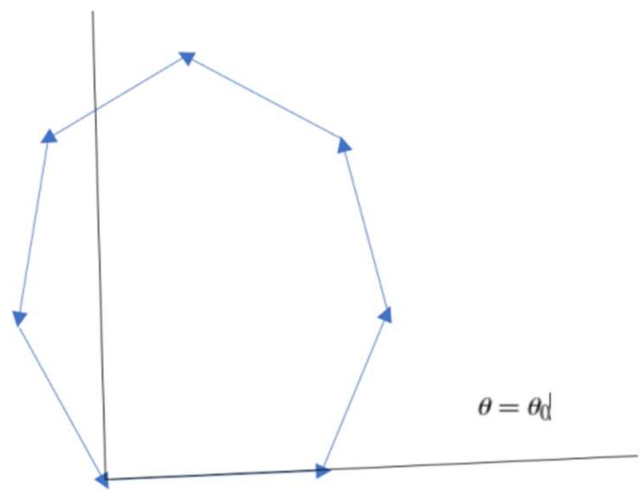
$\vec{v_1} + \vec{v_2} + \vec{v_3} = 0; \vec{v_4} + \vec{v_5} + \vec{v_6} + \vec{v_7} = 0$



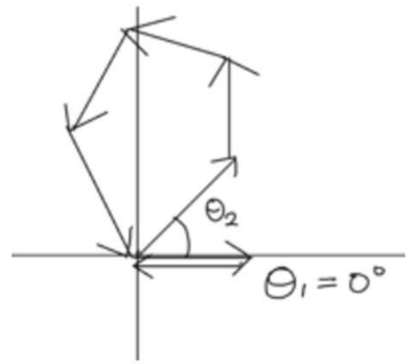
$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} = 0; \vec{v_5} + \vec{v_6} + \vec{v_7} = 0$



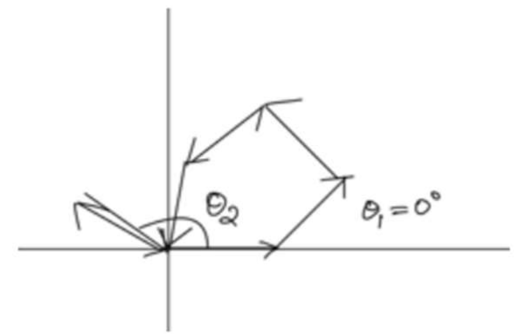
$$\vec{v_1} + \vec{v_2} + \vec{v_3} + \vec{v_4} + \vec{v_5} + \vec{v_6} + \vec{v_7} = 0; \theta_1 = 0$$



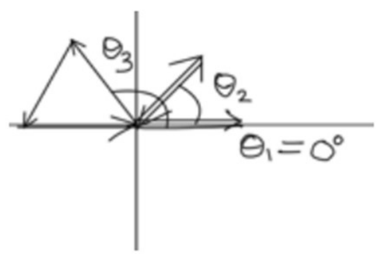
$$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} + \vec{v_5} + \vec{v_6} + \vec{v_7} = 0; \theta_1 = 0; \theta_2$$



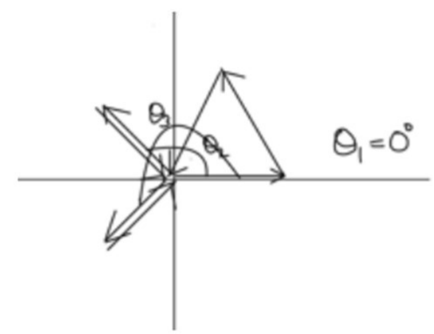
$$\vec{v_1} + \vec{v_2} + \vec{v_3} + \vec{v_4} + \vec{v_5} = 0; \vec{v_6} + \vec{v_7} = 0; \theta_1 = 0; \theta_2$$



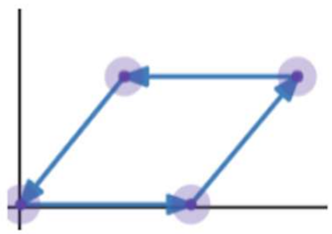
$$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} = 0; \vec{v_5} + \vec{v_6} + \vec{v_7} = 0; \theta_1 = 0; \theta_2; \theta_3$$



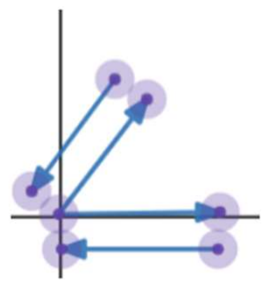
$$\vec{v_1} + \vec{v_2} + \vec{v_3} = 0; \vec{v_4} + \vec{v_5} = 0; \vec{v_6} + \vec{v_7} = 0; \theta_1 = 0; \theta_2; \theta_3$$



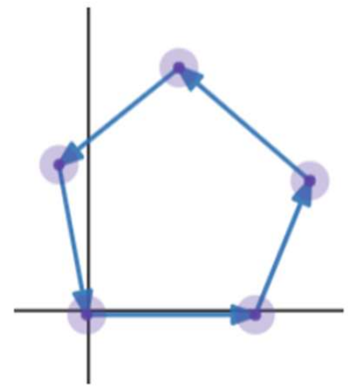
$$\vec{v_1} + \vec{v_2} + \vec{v_3} + \vec{v_4} = 0$$



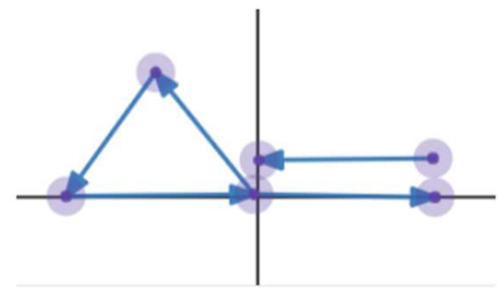
$$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} = 0$$



$$\vec{v_1} + \vec{v_2} + \vec{v_3} + \vec{v_4} + \vec{v_5} = 0$$



$$\vec{v_1} + \vec{v_2} = 0; \vec{v_3} + \vec{v_4} + \vec{v_5} = 0$$



$$e^{i\frac{2\pi 0}{4}} + e^{i\frac{2\pi\alpha}{4}} + e^{i\frac{2\pi 2}{4}} + e^{i\frac{2\pi(2+\alpha)}{4}} = 0$$

$$\left(e^{i\frac{2\pi 0}{4}} + e^{i\frac{2\pi 2}{4}}\right) + \left(e^{i\frac{2\pi\alpha}{4}} + e^{i\frac{2\pi(2+\alpha)}{4}}\right) = 0$$

$$\left(e^{i\frac{2\pi 0}{2}} + e^{i\frac{2\pi 1}{2}}\right) + e^{i\frac{2\pi\alpha}{4}}\left(e^{i\frac{2\pi 0}{2}} + e^{i\frac{2\pi 1}{2}}\right) = 0$$

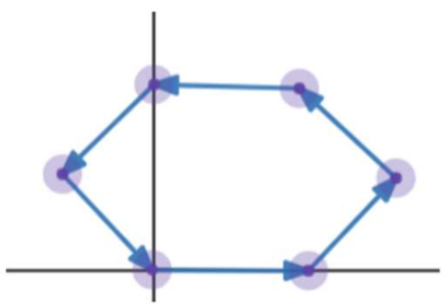
$$e^{i\frac{2\pi 0}{5}} + e^{i\frac{2\pi 1}{5}} + e^{i\frac{2\pi 2}{5}} + e^{i\frac{2\pi 3}{5}} + e^{i\frac{2\pi 4}{5}} = 0$$

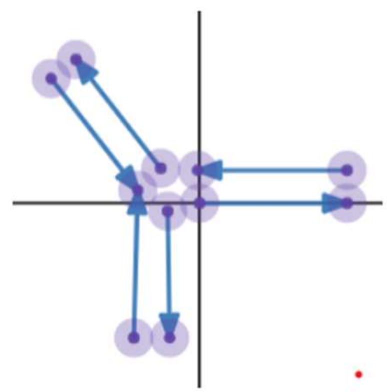
$$\left(e^{i\frac{2\pi 0}{2}} + e^{i\frac{2\pi 1}{2}}\right) + e^{i\theta}\left(e^{i\frac{2\pi 0}{3}} + e^{i\frac{2\pi 1}{3}} + e^{i\frac{2\pi 2}{3}}\right) = 0$$

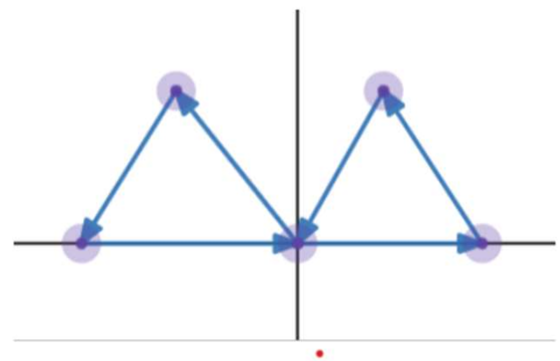
$$\vec{v_1}+\vec{v_2}+\vec{v_3}+\vec{v_4}+\vec{v_5}+\vec{v_6}=0$$

$$\vec{v_1}+\vec{v_2}=0;\vec{v_3}+\vec{v_4}=0;\vec{v_5}+\vec{v_6}=0$$

$$\vec{v_1}+\vec{v_2}+\vec{v_3}=0;\vec{v_4}+\vec{v_5}+\vec{v_6}=0$$







$$e^{i\frac{2\pi 0}{6}}+e^{i\frac{2\pi 1}{6}}+e^{i\frac{2\pi 2}{6}}+e^{i\frac{2\pi 3}{6}}+e^{i\frac{2\pi 4}{6}}+e^{i\frac{2\pi 5}{6}}=0$$

$$e^{i\frac{2\pi 0}{2}}+e^{i\frac{2\pi 1}{2}}=0$$

$$e^{i\frac{2\pi 0}{3}}+e^{i\frac{2\pi 1}{3}}+e^{i\frac{2\pi 2}{3}}=0$$

Theorem

$$\vec{v_1} + \vec{v_2} + \vec{v_3} + ... + v_n = 0$$

The above will be a unique vector equation representing the n-sided regular polygon, iff n is prime.

$$e^{i\frac{2\pi 0}{n}} + e^{i\frac{2\pi 1}{n}} + ... + e^{i\frac{2\pi(n-1)}{n}} = 0$$

$$\left(e^{i\frac{2\pi 0}{pq}} + e^{i\frac{2\pi 1}{pq}} + ... + e^{i\frac{2\pi(q-1)}{pq}}\right) * \left(e^{i\frac{2\pi 0}{p}} + e^{i\frac{2\pi 1}{p}} + ... + e^{i\frac{2\pi(p-1)}{p}}\right) = 0$$

Conclusion

From the above analysis we can conclude, the number of configurations in which the N-bead model has lowest interaction energy is based on 2 factors:

1) It is based on the distinction of which subset of the vectors has initial vector angle = 0. This is in the k factor in the answer
2) It is also based on the order in which the rest of the (N-2) vectors can be put. This is in the (N-2)! factor in the answer
3) From the above we get that the total number of configurations for our model = k(N-2)!

Future Work

There are many areas in which further computations can be made:

1) generalized form of the coordinates of a particular ball in all configurations for minimizing the interaction energy of the first and the Nth ball.
2) building a more elaborate model to allow multiple interactions between balls at the same instant [part-3 of problem statement].
3) writing code to compute k using dynamic programming