We propose a new flexible method of calculating conformational entropy of lattice polymer and random walk models and apply it to reconstruct phase diagram of a novel model of non-Markovian discrete random walk on a three-dimensional lattice, which we call volume and surface reinforced random walk.

Consider a random walk on some graph \( G \) defined by its sets of vertices and edges \( G = (V, E) \). Let \( V_N \) be a set of vertices visited up to step \( N \) of the walk, and \( V_N \) – the position of the walker at step \( N \). For each site \( v_i \) which is neighbor of \( v_N \), define a weight

\[
W(v_i) = I(e_{v_i} \in E) \times \begin{cases} \exp a, & \text{if } v_i \in V_N; \\ 1, & \text{if } v_i \notin V_N \text{ and } v_{N-1} \text{ is the only neighbor of } v_i \text{ from } V_N; \\ \exp b, & \text{if } v_i \notin V_N \text{ and there are other neighbors of } v_i \text{ in } V_N. \end{cases}
\]

where \( e_{v_i} \) denotes the edge connecting \( v_i \) and \( v_{N-1} \), and \( I \) is the indicator function. Now the probability of a walker going from \( v_{N-1} \) to \( v_i \) on step \( N+1 \) is proportional to \( W(v_i) \):

\[
P(v_{N+1} = v_i | v_N) = \frac{W(v_i)}{\sum_j W(v_j)}
\]

This model has two parameters: \( a \) (volume reinforcement) and \( b \) (surface reinforcement). Case of \( b = 0 \) was earlier discussed in [1, 2]. Our goal is to estimate conformational entropy of the model trajectories for \( G = Z^d \).

### Method of conformational entropy estimation

The method approximates the full-dimensional probability density function over all possible conformations by deep autoregressive generative model resembling the conditional PixelCNN [3]. The joint distribution \( p(x|\theta) \) of a trajectory conditioned on a vector \( \theta \) of macroscopic parameters is expanded as

\[
p(x|\theta) = \prod_{t=1}^T p(x_t|\theta),
\]

where conditional distributions are modelled by a 3d fully convolutional neural network with locally masked weights.

We present an adaptive masking mechanism which takes into account sequential nature of the trajectory generation process and allows to define sparse three-dimensional generalization of conditional PixelCNN capable of computing all conditional distributions in a single forward pass. The network then is trained on the ensemble of trajectories generated for different macroscopic parameters using maximum likelihood estimation. Given a trained network we compute conformational entropy by averaging negative log-likelihood over ensemble of trajectories generated at fixed values of macroscopic parameters

\[
S(\theta) = -E_x \log p(x|\theta).
\]

### References