Wang-Landau Improves Mean Writhe Estimates in Grid Diagrams and $\mathbb{Z}^3$ Links

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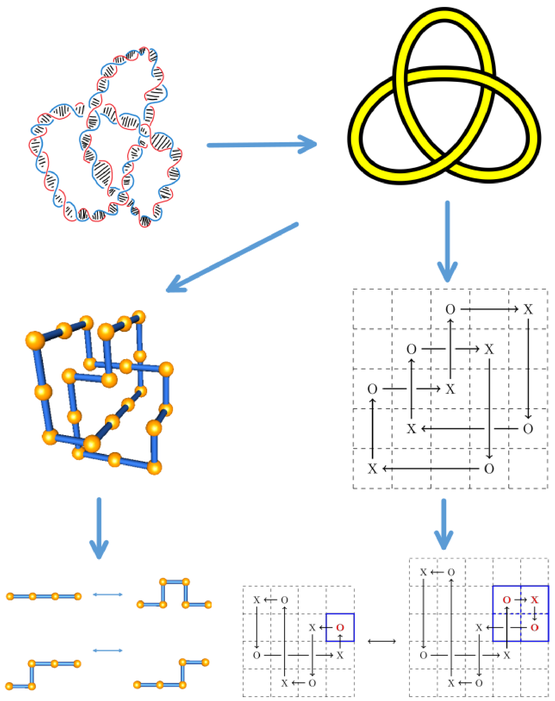
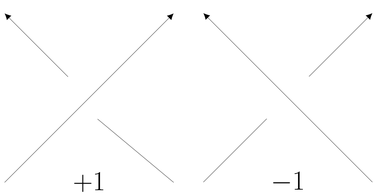
Biological Motivation and Objectives



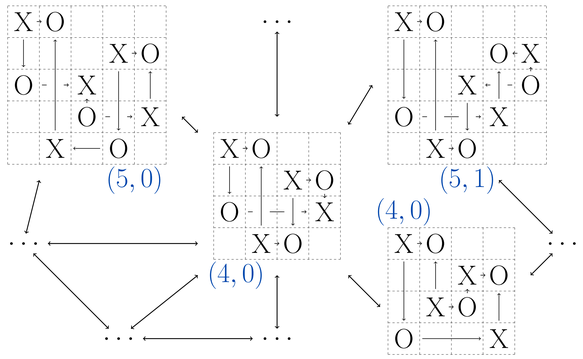
Circular DNA, as found in bacteria, can form mathematical knots, as seen above. DNA knots can be modeled by lattice links and grid diagrams. DNA knots are inherently chiral, which can be measured by writhe, calculated in planar diagrams by summing $+1$ and -1 over crossings as below, or in spatial conformations by

$$W = \frac{1}{4\pi}\int_c\int_c \frac{(dr_2 \times dr_1)\cdot r_{12}}{|r_{12}|^3} \qquad (1)$$

Here, we explore the distribution of writhe in lattice links and grid diagrams.



Markov Chains



A Markov chain of grids and their (size, writhe).

Wang-Landau Algorithm

The Wang-Landau Algorithm estimates the density of energy of a system as follows, where g_i estimates the density of energy E_i, [3]

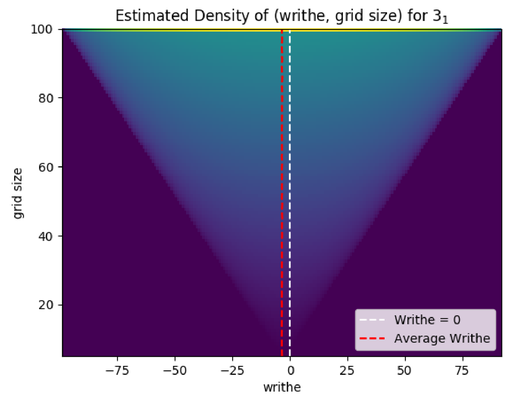
1. Specify a modification factor f, initial density estimate $\{g_i\}$, an initial state σ, and some stopping condition.
2. Perform some number of Markov steps using
$$P_{\text{acc}}(\sigma_i \to \sigma_j) = \min\left\{1, \frac{|\sigma_i|\, g_i}{|\sigma_j|\, g_j}\right\} \qquad (2)$$
for the Metropolis-Hastings step.
3. Update $g_i \leftarrow g_i \cdot f$.
4. Return to step 2 unless the stopping condition is met.

Examples of possible energies are

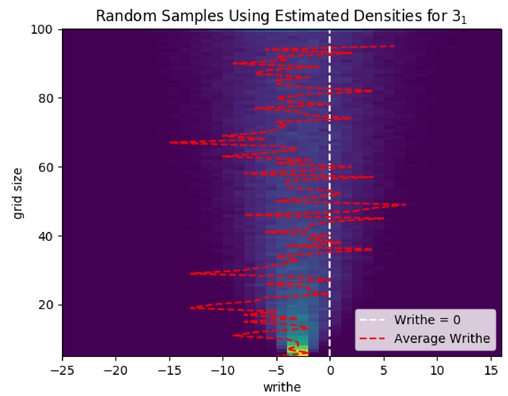
- link length,
- link component length,
- total writhe,
- component writhe,
- bending energy,
- presence of recombination sites,
- any combination of these energies.

We use grid size, lattice link length, (writhe, grid size), and (writhe, lattice link length).

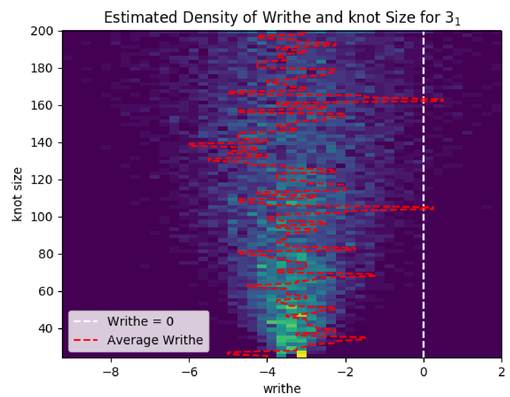
Results



Density for grid diagrams with energy = (writhe, grid size)

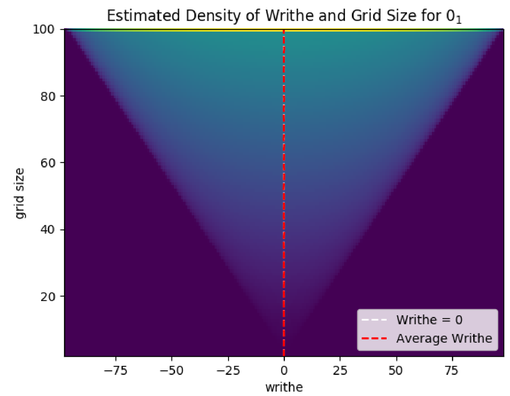


Heat map of grid diagram samples taken from a run using Wang-Landau densities trained on grid size.



Heat map of lattice link samples taken from a run using Wang-Landau densities trained on length.

Conclusions & Future Work



- Wang-Landau density estimation gives much more consistent and accurate measures of the properties of a state space than standard Markov chain Monte Carlo methods.
- We plan to generate density estimates for (writhe, lattice link length) and compare to grid estimates.
- Previous studies have found that the average of writhe for lattice links of a fixed length and link type is bounded as length varies. We wish to show the same for grid diagrams using Wang-Landau densities.

Reference

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