Randomly Sampling Grid Diagrams of Knots

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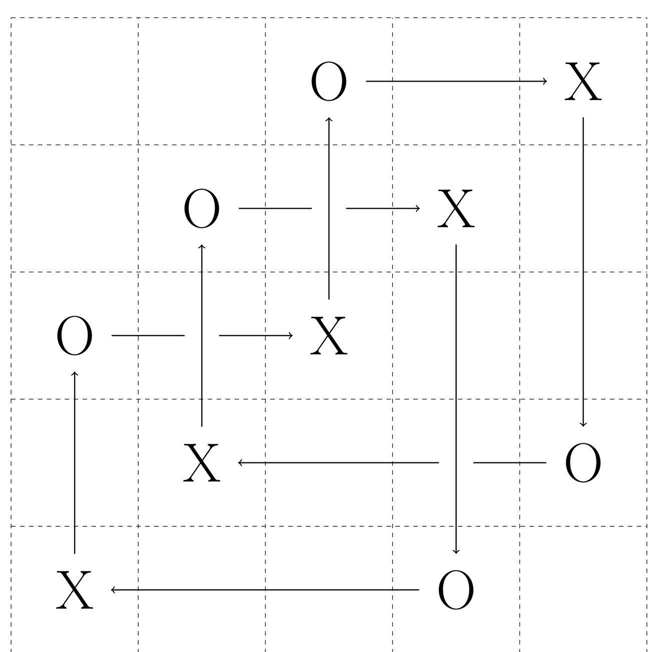
Grid Diagrams

A *grid diagram* of a link is an $n \times n$ lattice where each row and each column has exactly one "O" and one "X", where the entries in every row and column are connected so the vertical lines are overcrossings and the horizontal lines are undercrossings.

The following is an example of a trefoil in a 5×5 grid.



The following theorems due to [1] are essential:

Theorem 1

Every link can be represented in a grid diagram.

Theorem 2

If g and g' are two grid diagrams of the same link, then there exists a finite sequence of “Cromwell Moves" which takes g to g'

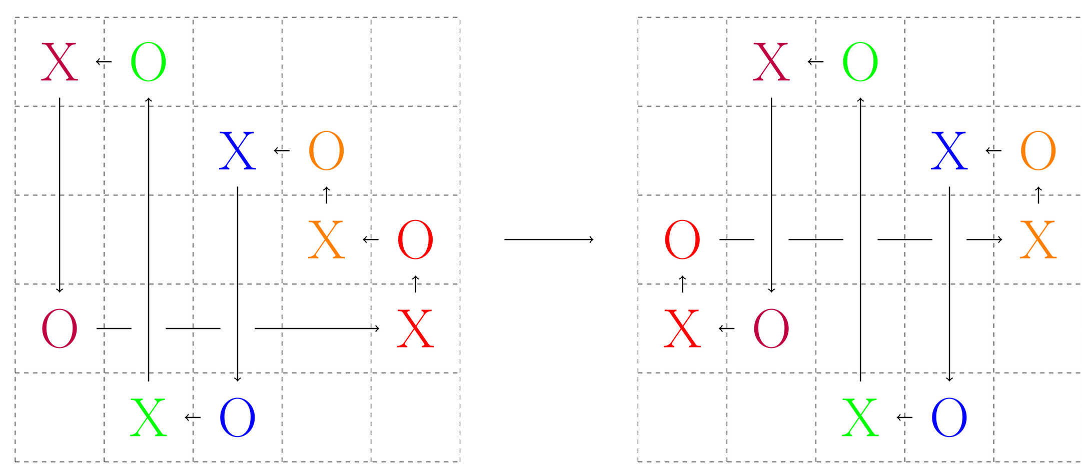
Purpose of the Algorithm

DNA knots appear to favor chiral configurations. One way of studying chirality is to examine writhe of a knot. In particular, we would like to know how the average of writhes of different configurations of the same knot behaves. To this end, the algorithm is designed generate random diagrams of a given link type, so we may sample many independent diagrams of that link for writhe calculations. This algorithm is modeled after the BFACF algorithm which operates on self-avoiding polygons in $\mathbb{Z}^3$[2].

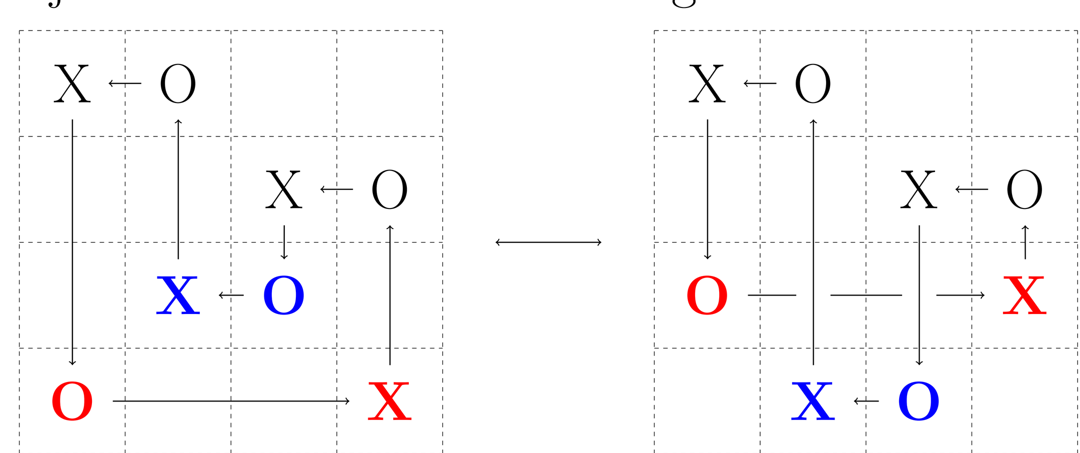
Cromwell Moves

There are four Cromwell moves:

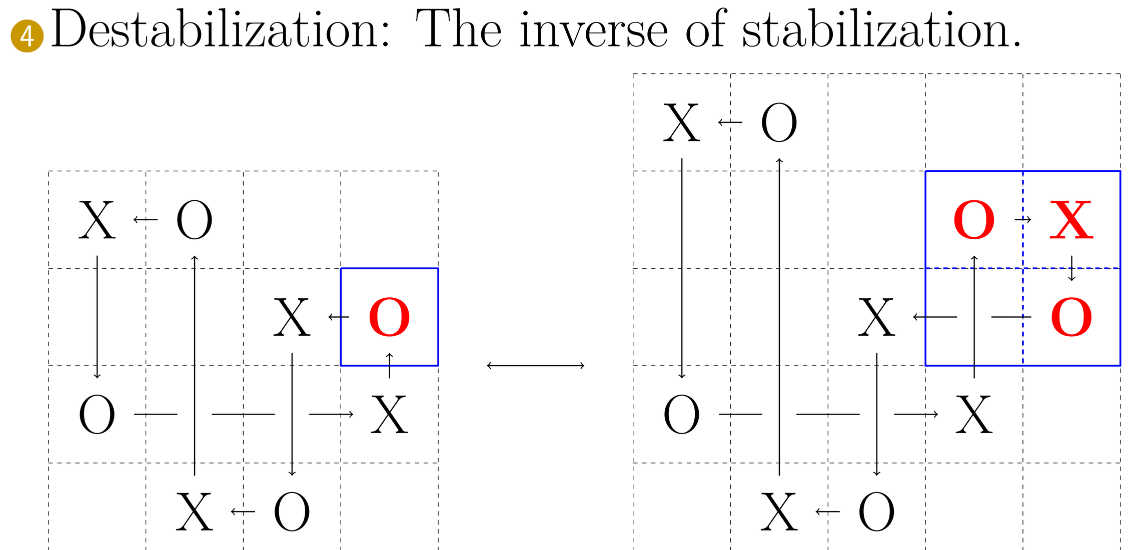
1. Translation: Moving each element of a grid cyclically up/down/left/right:



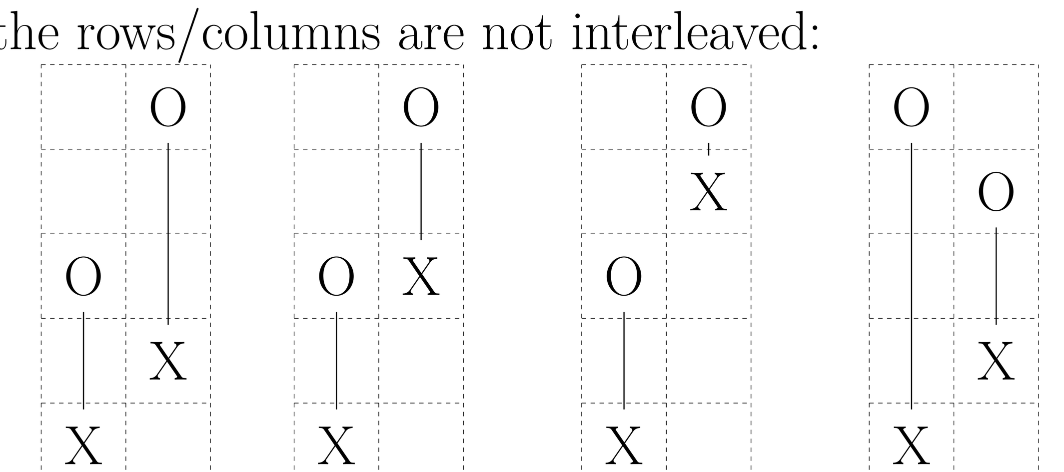
2. Commutation: Swapping two non-“interleaved" adjacent rows or columns of a grid



3. Stabilization: Replacing an entry in the grid with a 2×2 subgrid with three entries
4. Destabilization: The inverse of stabilization.



For the case of commutation, we must ensure that the rows/columns are not interleaved:



Interleaved Not Interleaved Not Interleaved Not Interleaved

Grid Algorithm

The following is a Markov chain Monte Carlo algorithm for sampling random grids of a specific link type:

1. Start with any initial grid g_0 with link type L.
2. Choose an X or O from g_t uniformly at random.
3. Choose a non-translation cromwell move σ with probability $p_{|g_t|}(|\sigma(g_t)| - |g_t|)$.
4. If σ is a valid Cromwell move, then set $g_{t+1} = \sigma(g_t)$, else $g_{t+1} = g_t$.
5. Increase t by one, and return to step 2

Distribution and Transition Probabilities

We would like to sample a link type uniformly from a chosen grid size. Hence, the probability of a getting a particular $n \times n$ grid diagram g should depend only on n (where g is an $n \times n$ grid) and some scaling parameter. We choose a distribution

$$\pi(g) = \frac{f(|g|, z)}{N(z)}$$

where $N(z)$ is a normalizing factor:

$$N(z) = \sum_{n=0}^{\infty} f(n, z) \cdot |G_n(L)|$$

Any choice of f for which N converges is a valid choice. $|G_n(L)|$ = number of $n \times n$ grid diagrams of link type L. $|G_n(L)|$ is difficult to estimate, however it is necessarily less than the number of grid diagrams representing links with the same number of components, given by

$$\sum_{k_1=2}^{n-2(c-1)} \cdots \sum_{k_j=2}^{n-2(c-j)-\sum_{i=1}^{j-1} k_i} \cdots \sum_{k_{c-1}=2}^{n-2-\sum_{i=1}^{c-1} k_i} \frac{n!(n-1)!}{\prod_{l=1}^{c-1}(n - \sum_{m=1}^{l} k_m)}$$

Specifically, for knots $|G_n(L)| < n!(n-1)!$, so we may use

$$f(n, z) = \frac{2nz^n}{n!(n-1)!}$$

To ensure convergence to this distribution, we also have

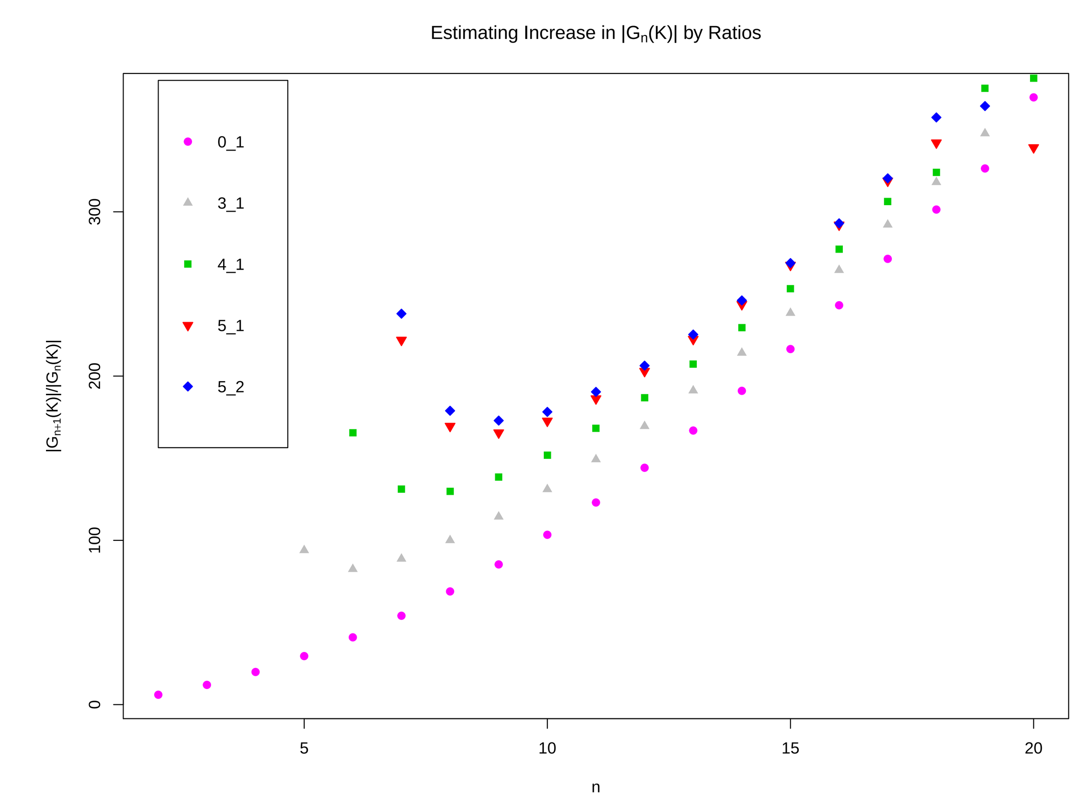
$$p_n(+1) = \frac{z}{(n+1)n} p_{n+1}(-1)$$

and

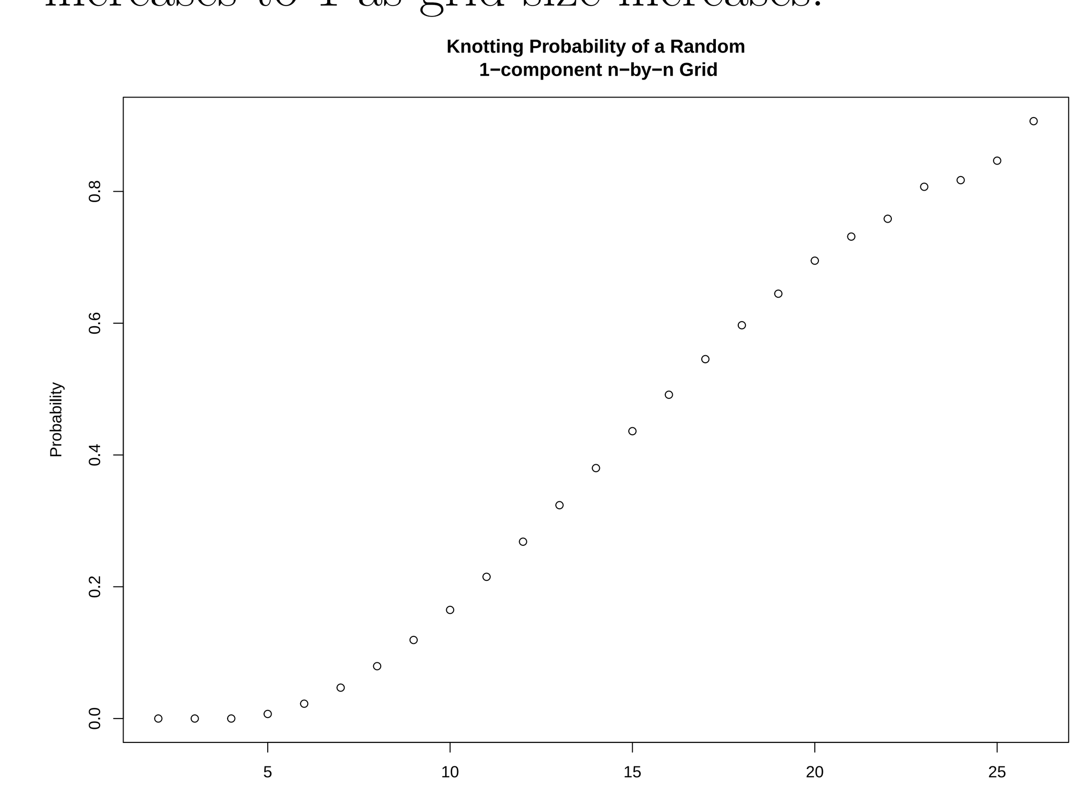
$$4p_n(+1) + 4p_n(0) + p_n(-1) \leq 1$$

Numerical Results for Grids

To understand the distribution from which the algorithm samples, we must understand $G_n(L)$. The following shows a plot of $|G_{n+1}(K)|/|G_n(K)|$ for several knot types K.



What is observed is that the ratio increases as n does, implying a faster than exponential growth. We can also see that the probability of a knotted grid increases to 1 as grid size increases:



References

[1] Peter Cromwell, *Embedding knots and links in an open book I: Basic properties*, Mathematical Proceedings of the Cambridge Philosophical Society **119** (1996), no. 02, 309.

[2] Neal Madras and Gordon Slade, *The Self-Avoiding Walk*, 1993.

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