A Dynamic Monte Carlo Algorithm for Sampling Grid Diagrams of Knots

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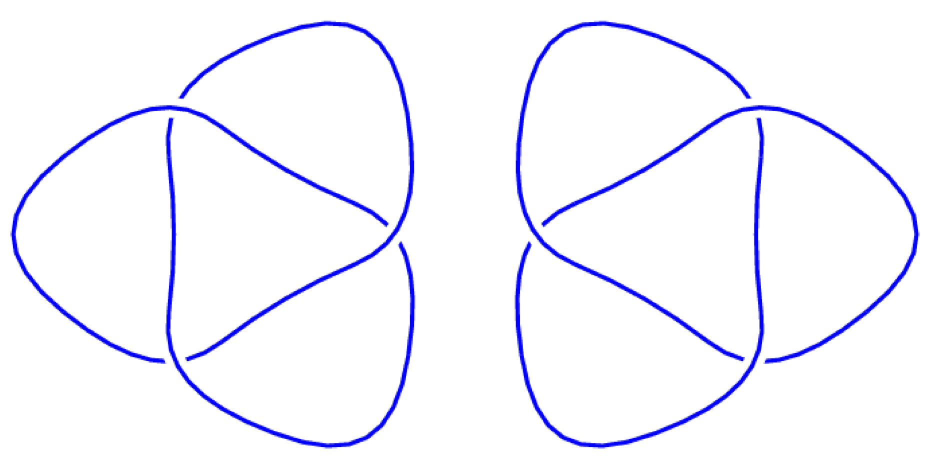
Motivation

A knot is *chiral* if it is not isotopic to its mirror image. For example, the following trefoils are not isotopic.



One feature that changes in a mirror image of a knot is a value called *projected writhe*. Projected writhe is the sum over the crossings of a planar projection of a knot using the following convention: $= -1$, $= +1$.

This yields a projected writhe of $+3$ for the trefoil on the left and -3 for the trefoil on the right. Projected writhe is not a topological invariant, however

Proposition 1

If $w(D)$ is the writhe of a knot diagram D, and D^* is its mirror image, it is always true that $w(D) = -w(D^*)$

What this gives is that if most of the diagrams of a knot have positive projected writhe, then most of the diagrams of its mirror have negative projected writhe. To formalize this notion into a classification of chiral knots, we turn to grids and a modification of conjectures from [3]:

Conjecture 1

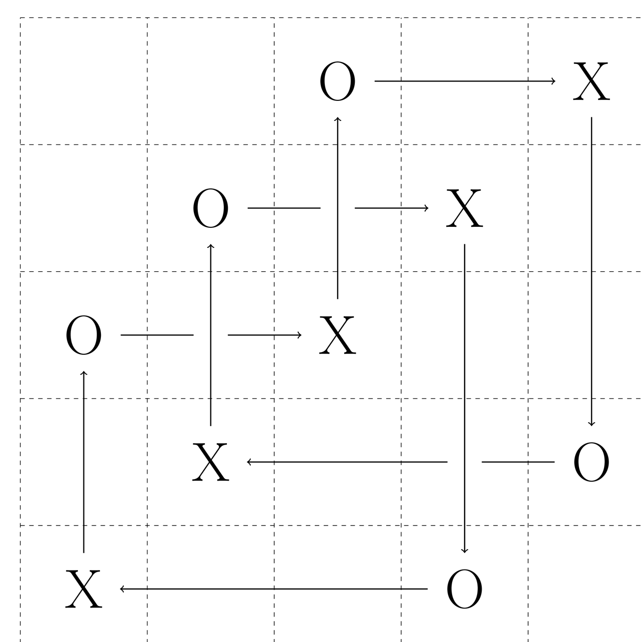
The average of the writhes of all $n \times n$ grids of a specific knot type is contained in a finite interval (a, b)

Conjecture 2

If a knot is chiral, then the interval (a, b) in the first conjecture does not contain 0.

Grid Diagrams

A *grid representation* of a knot 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 knot can be represented in a grid diagram.

Theorem 2

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

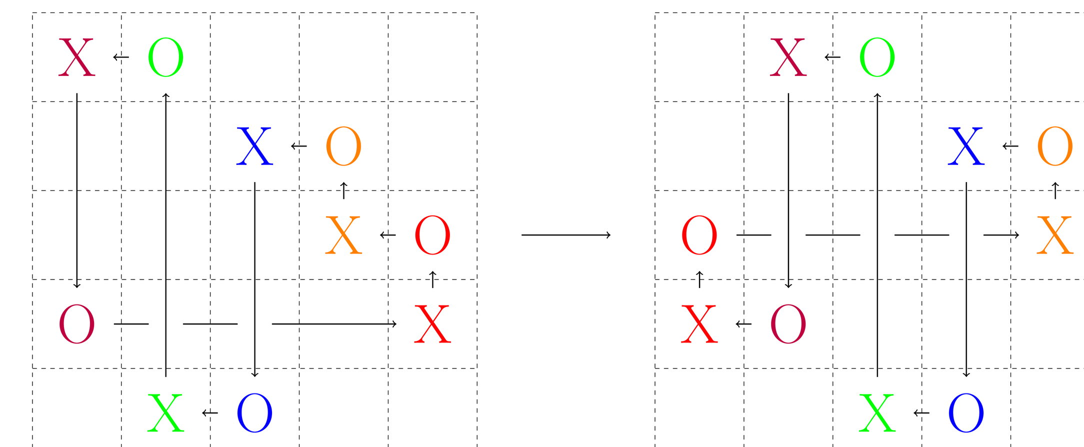
Purpose of the Algorithm

For an initial test of the conjectures, we seek significant numerical results. The algorithm is meant to sample random grids of a specific knot type. This algorithm imitates the BFACF algorithm (detailed in [2]), which is another Monte Carlo algorithm used to sample knots represented in $\mathbb{Z}^3$. The benefit of using grids and a grid algorithm is that projected writhe behaves in predictable ways under Cromwell moves, whereas measures of writhe are less predictable under BFACF moves.

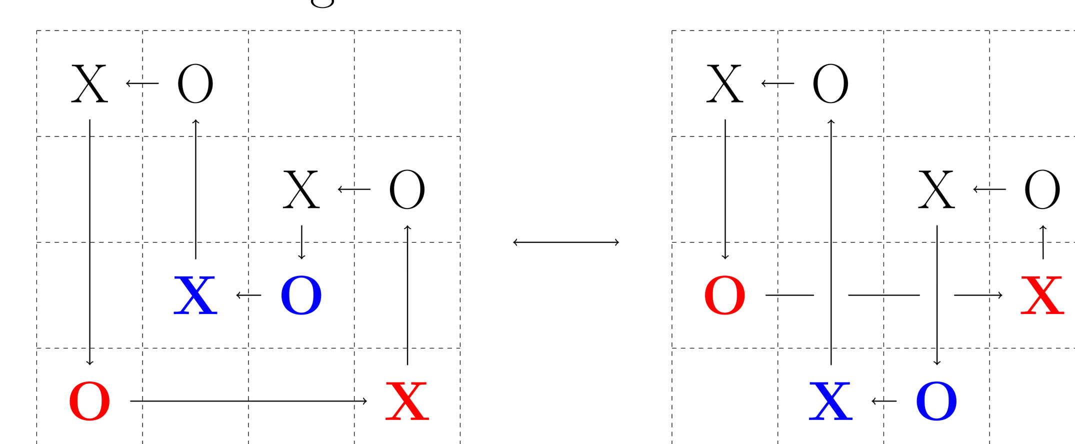
Cromwell Moves

There are four "Cromwell" moves:

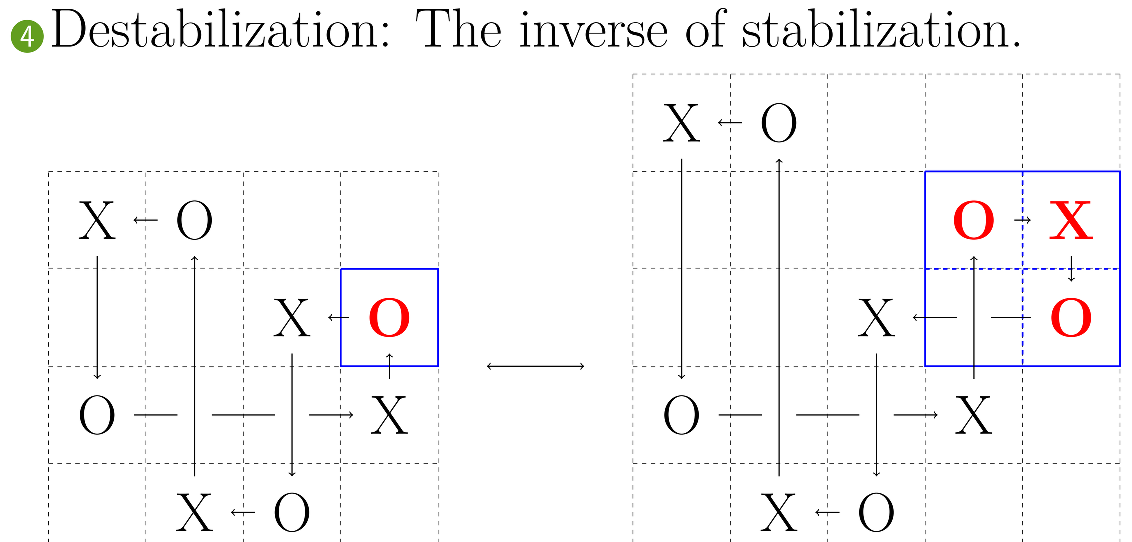
1. Translation: Moving each element of a grid cyclically up/down/left/right:



2. Commutation: Swapping two 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.



Note that stabilization increases the grid size and destabilization decreases it.

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.

[3] J Portillo, Yuanan Diao, R Scharein, Javier Arsuaga, and Mariel Vazquez, *On the mean and variance of the writhe of random polygons*, Journal of Physics A: Mathematical and Theoretical **44** (2011), no. 27, 275004.

Grid Algorithm

The following is a proposed monte carlo algorithm for sampling random grids of a specific knot type to numerically test the conjectures:

1. Start with any initial grid g_0 with knot type K, let $t = 0$, and set sampling frequency n.
2. Choose a vertex of g_t uniformly at random.
3. Choose a non-translation cromwell move σ with probability $p(|\sigma(g_t)| - |g_t|)$.
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.
6. If t is a multiple of n, then choose two random integers $0 \leq i, j < |g_t|$, and sample g_t translated i units horizontally and j units vertically.
7. Return to step 2

Distribution and Probabilities

It is important to note that, because of theorem 2, every grid of the given knot type can be achieved, i.e. for all grids g of a knot type, their probability $\pi(g) \neq 0$. So we may choose the following distribution:

$$\pi(g) = \frac{1}{N(z)} \frac{2|g| z^{|g|}}{n!(n-1)!},$$

with

$$N(z) = \sum_{n=0}^{\infty} \frac{2nz^n |G_n(K)|}{n!(n-1)!}.$$

To satisfy detailed balance, guaranteeing convergence to this distribution, we choose the probabilities from 3 to satisfy

$$p(+1) = \frac{z}{(n+1)n} p(-1),$$

$$p(+1) \leq \frac{1 - 2p(0)}{4 + \frac{n(n+1)}{z}}.$$

Optimal choices for these probabilities are not yet known.

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