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: \( \check{1} = -1 \), \( \check{3} = +1 \).

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]:

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 mimics the BFACF algorithm (detailed in [2]), which is another Monte Carlo algorithm used to sample knots represented in \( \mathbb{Z}^2 \). 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.

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 over-crossings and the horizontal lines are under-crossings. The following is an example of a trefoil in a 5 x 5 grid.

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 x 2 subgrid with three entries:


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

Distribution and Probabilities

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 \( g_t \) with knot type \( K \) and uniform probability.
3. Choose a non-translation cromwell move \( \sigma \) with probability \( p(\sigma) \).
4. If \( \sigma \) 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 \( 0 \leq i, j \leq |g_t| \), and sample \( g_t \) translated \( i \) units horizontally and \( j \) units vertically.
7. Return to step 2.

Theorem 2 considers the grid size of a knot with the probability \( \pi(g) \) of \( g \). So we may choose the following distribution:

\[
\pi(g) = \frac{1}{2^{|G(z)|}} \left( \frac{|G(z)|}{n!(n-1)!} \right)^{|G(z)|}
\]

with

\[
N(z) = \sum_{n=0}^{\infty} \frac{2^{zn}|G_n(K)|}{n!(n-1)!}
\]

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

\[
p(+1) = \frac{2}{(|G(z)|+1)}p(-1), \quad p(+1) \leq \frac{1}{4}, \quad p(-1) \geq \frac{1}{4} + \frac{2p(0)}{3}.
\]

Optimal choices for these probabilities are not yet known.

References


Acknowledgements

- Funding from NSF DMS 1057284 grant
- UC Davis department of mathematics