

Supervised Learning for Untangling Braids

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Abstract: Untangling a braid is a typical multi-step process, and reinforcement learning can be used to train an agent to untangle braids. Here we present another approach. Starting from the untangled braid, we produce a dataset of braids using breadth-first search and then apply behavioral cloning to train an agent on the output of this search. As a result, the (inverses of) steps predicted by the agent turn out to be an unexpectedly good method of untangling braids, including those braids which did not feature in the dataset.

1 INTRODUCTION

Braids are mathematical objects which are studied using knot theory and group theory. For us in our study, braids are a type of mathematical objects to which machine learning can be usefully applied. See more on the problem of untangling braids in Section 3. In our earlier research we attempted to apply reinforcement learning to the problem of untangling braids, with limited success. In this study we develop and successfully apply a new approach which is inspired by behavioral cloning and includes supervised learning as one of its parts, see Section 2 for more details.

The contribution of the study is two-fold, combining a new insight in the problems related to braids, on the one hand, and a new machine learning technique which can be used in place of reinforcement learning, on the other hand.

2 GENERAL IDEA

Consider a network having a certain regular structure (for example, a grid), like the one in Figure 1.

We want to train an agent to find a path, starting from an arbitrary node in this network, to the node O . There are many approaches which can be used, including several flavours of reinforcement learning (Sutton and Barto, 2018). However, in this study we

use supervised learning, namely, a version of behavioral cloning (Ho and Ermon, 2016).

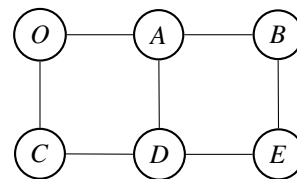


Figure 1: A sample network to apply breadth first search to.

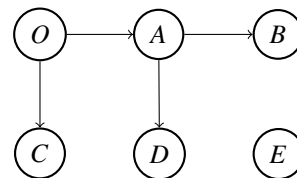




Figure 2: Breadth first search has been applied.

Starting from node O , we perform a breadth first search of a given depth. As a result of this search, we obtain a tree within the network, which stores, for each node in the tree, one of possible shortest ways of reaching this node from O . Figure 2 shows such a tree, with depth 2, in the network shown in Figure 1. Then we train a neural network to predict, for a given node picked from the tree, what was the last move between two nodes in the tree that has reached this node. For example, for node D in Figure 2 the correct answer would be ‘reach it by moving from A to D ’. To be more precise, note that the network might contain a large number of nodes, but only a very small number of different kinds of moves; for example, in a grid the

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moves are ‘move up’, ‘move right’, ‘move down’, and ‘move left’. Thus, for node D in Figure 2 the correct answer would be ‘reach it by moving down’.

Below, we will refer to the trained neural network predicting the last step in the tree as Lara (for ‘last’). After we have trained Lara, we use another piece of code to find a path from a given node to O ; we call this code Una (for ‘untangle’). Starting from a given node, Una asks Lara how this node is classified, and then performs the opposite move; then the same step is repeated until O is reached. For example, if Una starts at node D , Lara classifies this node as ‘move down’, thus, Una applied the opposite move, ‘move up’, reaching node A , then asks Lara again, etc., until O is reached.

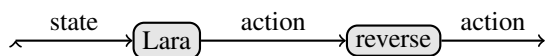


Figure 3: Diagram showing how Una works. A trained classifier Lara is applied to a state to produce an action; then the action is reversed.

Note that the tree does not include all nodes in the network, for example, node E in Figure 2 is not in the tree. Lara is not trained on the nodes which are not in the tree. However, due to the regular structure of the network, we can hope that Lara will be able to generalize to these nodes and produce a reasonable recommendation for Una. For example, for node E one can hope that Lara will conjecture that this node can be reached from above or from the left, thus directing Una, correctly, up or to the left.

In this paper we apply this idea to untangling braids. However, before we delve into braid theory, let us explain how this idea could potentially work on another, more familiar example. Suppose we want to train an agent to solve the Rubik’s cube. Visualise a network in which nodes are all possible positions of the Rubik’s cube (there are about 10^{20} of them), and in which two nodes are connected with an edge if the nodes can be produced from one another by one move (that is, one face turn). The network has a regular structure, with each node connected to its neighbors by a small number of possible moves. Denote the solved position of the Rubik’s cube by O . As described above, we can perform a breadth first search in the network starting from O . As a rough estimation, conducting this breadth first search up to depth d reaches 10^d nodes. It is known that one needs 20 moves (or 26 moves, depending on the exact definition of moves (Kunkle and Cooperman, 2007)) to reach every node from O , and it is not feasible to build a tree containing 10^{20} nodes. Realistically, a tree that one can build would be much smaller, for example, a tree can contain about 10^7 nodes. Thus, it is impor-

tant that Lara can generalize well from this relatively small tree to the unfathomably large network.

3 BRAIDS

Braids are mathematical objects from low-dimensional topology or, to be more precise, knot theory (that is, the study of the relative position of curves in the space). A *braid* on n strands consists of n ropes whose left-hand ends are fixed one under another and whose right-hand ends are fixed one under another; you can imagine that the braid is laid out on a table, and the ends of the ropes are attached to the table with nails. Figures 4, 5 show examples of braids on 3 strands with 10 crossings. Braids are important because, on the one hand, they are useful building blocks of knots and other constructions of low-dimensional topology and, on the other hand, have a simple structure and can be conveniently studied using mathematics and, as in this study, experimented with using computers.

The braids in Figures 4, 5 can be untangled, that is, all crossings can be removed by moving certain parts of strands up or down, as needed (without touching the ends of the ropes); after the braid is untangled, the braid diagram will look as in Figure 6, which shows what we will call the *canonical trivial braid*. Not every braid can be untangled. Those braids that can be untangled are called *trivial* braids. The task that we explore in this research is untangling braids using ideas from Section 2.

When one studies braids (or knots) and how to untangle them, the untangling process is split into elementary local changes, affecting 2 or 3 consecutive crossings, called Reidemeister moves (Kassel and Turaev, 2008). Somewhat confusingly, the moves for untangling braids are called the second Reidemeister move and the third Reidemeister move; there exists a move called the first Reidemeister move, but it is used only with knots and not with braids (Lickorish, 2012). Please see all forms of the second Reidemeister move in Figures 7, 8. The meaning of each of these figures is that a braid fragment shown on the left can be replaced by a braid fragment shown on the right, or vice versa.

All forms of the third Reidemeister move are shown in Figures 9, 10, 11, 12, 13, 14.

As you can see, the second Reidemeister move, when applied to one of directions, removes two crossings from a braid; thus, if our aim is to untangle the braid, it seems like a good move to use. However, not every Reidemeister move removes crossings from a braid; one can say that some Reidemeis-

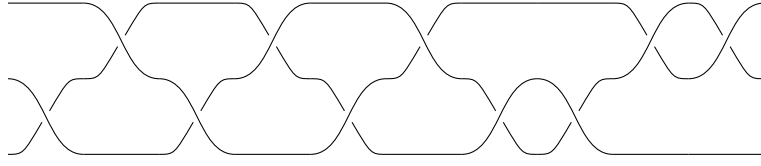


Figure 4: An example of a trivial braid which our agent successfully untangles.

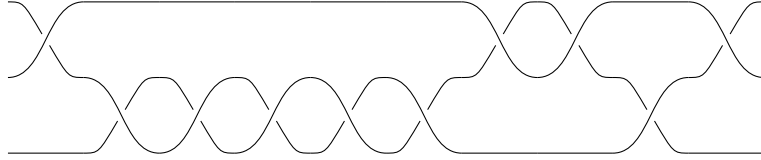


Figure 5: An example of a trivial braid which our agent cannot untangle.

ter moves (including all versions of the third Reidemeister move) only prepare groundwork for removing crossings. Thus, the challenge for artificial intelligence is to learn which Reidemeister moves it should use to untangle a braid, even though initially it might not be clear how these moves contribute to untangling the braid.

Here is how we encode braids in the computer. Considering a braid from left to right, we record a clockwise (or anti-clockwise) crossing of strands in positions i and $i + 1$ (counting from the bottom) as the number i (or $-i$). Thus, for example, the braid in Figure 5 is encoded as the list of numbers $-2, 1, -1, -1, 1, 1, 2, -2, -1, 2$. We were prepared to transform this encoding into one-hot encoding, if needed, but so far, we are reasonably successful with this simple encoding. This list of numbers is fed into a neural network when Lara is trained. As to Reidemeister moves, each of them is re-interpreted as an instruction stating that a certain two-digit or three-digit fragment within the braid can be replaced by another fragment of the same length. For example, the Reidemeister move in Figure 7 states that 00 can be replaced by $1-1$ (or $2-2$, etc., depending on which strands the move is applied to) or vice versa.

For our experiments, we fix the length of the braid, as we did in our previous research (Khan et al., 2021). If there is no intersection of strands in a certain part of a braid, this part of the braid is denoted by 0 . Thus, for example, in the context of braids with up to 10 crossings, the canonical trivial braid (shown in Figure 6) is encoded by the list of 10 0 s. Because of this encoding, we need to add one more kind of moves in addition to Reidemeister moves, namely, shifting zero entries in the braid to the left or to the right, as needed; that is, the fragment $i0$ in the braid can be replaced by $0i$ or vice versa.

Not every type of Reidemeister move can be applied at every position in a given braid; for example, the Reidemeister move in Figure 7 cannot be applied

to the first and the second crossing (counting from the left) of the braid in Figure 5, but can be applied to the second and the third crossing of this braid. When Lara predicts the last move, it predicts a pair, consisting of the type of the move and the position in the braid where it was applied. Sometimes Lara is wrong in the sense that this move could not have been applied at this position in the braid. In this sense, below, when we discuss how Una should interpret Lara’s predictions, we discuss how to interpret valid and invalid moves.

4 MODEL STRUCTURE

As we said in Section 2, our code consists of two main parts, Lara and Una. The first one, Lara, is a Multi-Layered Perceptron (MLP) network that predicts the last move that was made to obtain a given braid. The second one, Una, is an algorithm that attempts to untangle a given braid by executing a series of moves.

4.1 LARA

This model is used to predict the last move made to a certain braid. The data generated for Lara comes from a breadth first search tree, as in Figure 2, where there is only one path from O to any other node. In this sense, Lara is a single-label multi-class model. The configuration of this MLP is given by:

- Input layer that receives the array of an encoded braid.
- Three hidden layers of size 128, 64 and 32, respectively. Each one with ReLU as activation function.
- Output layer of the the encoded action array, of length $(strands * 2 + 4) * length$. with a *softmax* activation function.



Figure 6: The canonical trivial braid contains no crossings.

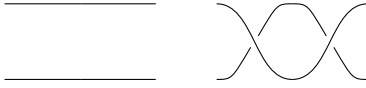


Figure 7: Second Reidemeister move (form 1).



Figure 8: Second Reidemeister move (form 2).

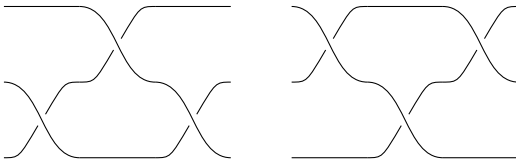


Figure 9: Third Reidemeister move (form 1).

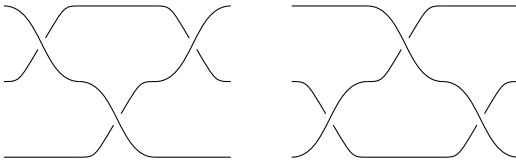


Figure 10: Third Reidemeister move (form 2).

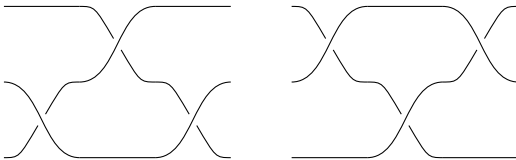


Figure 11: Third Reidemeister move (form 3).

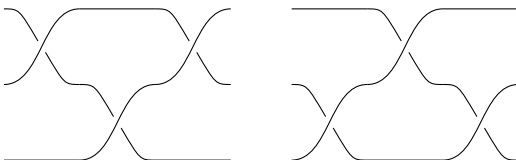


Figure 12: Third Reidemeister move (form 4).

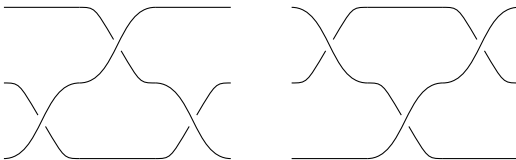


Figure 13: Third Reidemeister move (form 5).

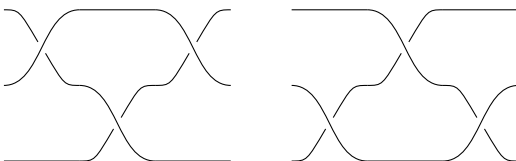


Figure 14: Third Reidemeister move (form 6).

We could have trained Lara on all nodes of the tree; however, we not only train Lara, but also test its accuracy on a test set. The training and test sets come from the tree dataset, being randomly chosen 80% and 20% of the nodes, respectively. As you can see in Table 1, the performance of Lara is very promising, maintaining overall accuracy above 99%.

After Lara has been trained, the predictions of Lara need to be sequenced and inverted to use them to untangle braid, as described below.

4.2 UNA

The purpose of this code is untangling a given braid by executing a series of moves, namely, the inverses of the moves produced by Lara. In order to test our Lara/Una architecture, We wrote several versions of Una, depending on how much they trust Lara's output and how they interpret it:

- Random (UNA_R): Una performs a randomly chosen valid move without consulting Lara.
- Valid or random (UNA_V): Una executes the recommended move from Lara if the recommended move is valid; otherwise, Una performs a randomly chosen valid move (like UNA_R).
- Best valid move (UNA_B): Una executes, out of all valid moves available, the one that is ranked most highly by Lara.
- Tree only (UNA_T): Una executes the recommended action from Lara (like UNA_B) if the currently considered braid belongs to the tree on which Lara was trained. If the braid does not belong to the tree, Una executes a random valid move (like UNA_R).

Every version works until it reaches one of two situations. The first one is when the braid is completely untangled; then it is a success. The second one is when the current braid has already been visited; then it is a failure ¹.

¹We could have expanded our experiments to allowing Una to visit the same node repeatedly and choose a different random action each time it happens. However, these non-deterministic approaches are of little interest to us, because our main aim is to test how much Lara's advice helps Una in untangling the braid.

5 EXPERIMENTS

To test the different versions of Una, we used a dataset of randomly generated braids that do not necessarily belong to the tree of braids created to train Lara. (To be more precise, the randomly generated braids in the test set are unlikely to be in the tree because we only include braids without 0s, in other words, braids with the maximal number of crossings, in the test set.) In Table 1, we show the size of the braids used in the experiments (the length and the number of strands), the size of the tree used to train Lara (the depth and the number of nodes), the total number of trivial braids in the network containing the tree, Lara’s accuracy (on the test set separated within the tree), and the success rate of different implementations of Una.

The training set of Lara is represented in the Tree size column. For length 8, this training set goes from 11% to 61% of the all braids. The test set of Una is represented in the Test size column, and for length 8 it is 21% of all braids. For length 10, Lara’s training set goes from 2% to 30%, with a test set of Una of around 5% of all braids. Finally, with length 12 the training set of Lara goes from 0.2% to 3.2% with the test set of Una of 0.6% of all braids.

This data enables us to answer two research questions which we asked ourselves. Do Lara and Una, between the two of them, learn something useful about untangling braids? The answer is yes, because the performance of the version of Una making random moves, UNA_R , is much lower than the performance of all other versions of Una, which benefit from learning. Can Lara, after having been trained on a tree, generalize this knowledge usefully to the braids it has not been trained on? The answer is yes, because the performance of the versions of Una that use Lara’s advice outside the tree, UNA_V and UNA_B , are noticeably better than the performance of the version of Una that does not use Lara’s advice outside the tree, UNA_T .

The performance of these models is calculated with an accuracy ratio of the successfully untangled braids over the total braids tested. For example, with length 8 and depth 7, UNA_V is able to untangle 74% of the testing set braids.

Although our experiment results make us sufficiently confident to formulate the general conclusions stated in the previous paragraph, we can report that specific numbers are noisy and depend on the randomness in the training of Lara. For braids of length 8, we ran each experiment (including training Lara) several times, and results are different; please see Table 2 showing how the performance of Una changes depending on Lara. The first 4 rows in Table 2 are the numbers from Table 1, and the next 4 rows are the

same experiments, but repeated with newly trained Lara’s neural networks. The bottom 4 rows in Table 2 are the same experiments again, with longer trained Lara’s neural networks.

From the mathematical point of view, we know that only at the distance of 6 moves from O the third Reidemeister move can be first applied. For instance, for length 10, the 24,191 braids in the tree of depth 5 do not include any braids that require the third Reidemeister move to be untangled, so Lara trained on this dataset has never encountered any version of the third Reidemeister move applied. Accordingly, we can see, for example, that for length 10 there is a clear improvement between depth 5 and 6, with the success rate of both UNA_V and UNA_B improving almost two times.

6 RELATED WORK

A Reinforcement Learning approach was attempted for the same problem in previous research that we developed. Using Policy Gradient with a MLP we gave a negative reward for every step the agent made in order to encourage time efficiency. A comparative result is the RL approach obtained an accuracy of 22% for untangling braids of 3 strands and 12 crossings. In this sense, this Supervised Learning approach improves that accuracy to 27% with UNA_B , for example.

Multiple- and single-agent reinforcement learning was applied to untangling braids in our earlier work (Khan et al., 2021; Khan et al., 2022). The method proposed in this paper demonstrates better performance of untangling on comparable sizes of braids.

A closely related problem (with a slightly extended list of Reidemeister moves) is untangling knots presented as closed braids. A range of single-agent reinforcement learning methods was used in (Gukov et al., 2021) to solve that problem. The best accuracy (about 85% of braids untangled) was reported for the trust region policy optimization (TRPO) method. Although that is a not the same untangling problem as the one we consider in this paper, it is encouraging to see that this accuracy is comparable with the best results we have achieved in our experiments, with arguably a simpler off-line learning approach.

7 CONCLUSION

We demonstrate that although Lara is only trained on a small tree inside the network (that is, the network of braids connected by actions), using Lara’s advice

Length	Depth	Tree size	Total braids	Test size	LARA	UNA_R	UNA_V	UNA_B	UNA_T
8	3	1,271	11,317	2,400	99.30%	16%	52%	18%	30%
8	5	3,919	11,317	2,400	99.48%	16%	46%	59%	43%
8	6	5,639	11,317	2,400	97.36%	16%	64%	80%	62%
8	7	6,963	11,317	2,400	99.44%	16%	74%	64%	57%
10	3	3,455	191,645	10,000	99.12%	6%	32%	16%	18%
10	5	24,191	191,645	10,000	99.92%	6%	26%	33%	14%
10	6	38,759	191,645	10,000	99.85%	6%	51%	65%	36%
10	7	57,947	191,645	10,000	99.63%	6%	60%	54%	35%
12	3	7,367	3,427,517	20,000	99.52%	2%	18%	11%	8%
12	5	112,559	3,427,517	20,000	99.07%	2%	20%	27%	10%

Table 1: Results of Una versions using different depths to train Lara. All experiments are with braids with 3 strands.

Depth	UNA_R	UNA_V	UNA_B	UNA_T
3	16%	52%	18%	30%
5	16%	46%	59%	43%
6	16%	64%	80%	62%
7	16%	74%	64%	57%
3	16%	53%	27%	40%
5	16%	61%	77%	56%
6	16%	58%	72%	51%
7	15%	41%	37%	32%
3	16%	53%	27%	40%
5	16%	65%	77%	56%
6	15%	70%	85%	63%
7	15%	81%	81%	69%

Table 2: Experiments run two times with different NNs

when performing actions considerably increases the probability of reaching the canonical trivial braid (that is, untying the braid).

As described in the end of Section 2, this approach can be applied to other problems, too, in place of reinforcement learning.

In the future, we will extend our approach to untying knots presented as closed braids, as in (Gukov et al., 2021); one specific challenging example to tackle is the one presented in (Morton, 1983). In addition to this, we want to untangle knots presented in a different form, called the plat representation of knots (Birman, 1976).

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