# Solving the 15-Puzzle & Rubik's Cube

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September 12, 2022

# Declaration

This report has been prepared on the basis of my own work. Where other published and unpublished source materials have been used, these have been acknowledged.

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# Abstract

**Motivation** – Reinforcement Learning (**RL**), exposed with brilliant clarity in Sutton and Barto, 2018, has until recently known less success than we might have hoped for. Its framework is very appealing and intuitive. In particular, the mathematical beauty of Value iteration and Q iteration (Watkins, 1989) for discrete state and action spaces, blindly iterating from *any* initial value, is quite profound. Sadly, it had until recently proven hard to achieve practical success with these methods. Inspired however by the seminal success of Deep Mind's team in using Deep Reinforcement Learning (**DRL**) to play Atari games (Mnih et al., 2013) and to master the game of Go (Silver et al., 2016), researchers have in recent years made a lot of progress towards designing algorithms capable of learning and solving, *without human knowledge*, the Rubik's Cube (**RC**) - as well as similar single player puzzles - by using Deep Q-Learning (**DQL**) (McAleer et al., 2018a) or search and (**DRL**) value iteration (McAleer et al., 2018b).

In this project, I will attempt to implement a variety of solvers combining $A^*$ search and heuristics, some of which will be handcrafted, others which I will train on randomly generated sequences of puzzles using **DL**, **DRL** or **DQL**, to solve the 15-puzzle (and variations of different dimensions), as well as the Rubik's cube.

**Organisation of this thesis** – In the first section, I describe what I hope to get out of this project, both in terms of personal learning, as well as in terms of tangible results (solving some puzzles!). In section 2, I will do a recap of the different methods used in the project. Section 3 is dedicated to discussing the mathematics of the sliding puzzle **SP** and the **RC**. I might make interesting observations in there and give some references for the keen reader. I give then an overview in section 4 of the code base I have developed (see my github page Berrier, 2022) - for this project. Finally, sections 6 and 7 present my results on respectively the **SP** and the **RC** and section 8 concludes the thesis.

A couple of appendix sections complement the main text. The first one details how to use the code base, from constructing puzzles, to learning and solving them using the various solvers I have developed. The second one describes a limitation I bumped into while using the kociemba library (a well-known open source 3x3x3 **RC** solver), and how I circumvented it.

**Acknowledgements** – I am grateful to my employer Bank of America for sponsoring my part time 2-year MSc in Artificial Intelligence at Royal Holloway. I entered the study of AI with a heavy dose of skepticism and am delighted to have learnt so much and revised my judgment of this field. In particular I would like to thank my managers Mitrajit Dutta and Stephen Thompson for supporting me in pursuing this MSc.

I have been fortunate to have had the company of my colleague Saurabh Kumar, as he decided to follow me in this MSc journey. We have had countless opportunities to debate about all the new cool stuff we learnt during the MSc, and that has definitely made the whole process much more enjoyable.

I would also like to thank Professor Chris Watkins, for agreeing to supervise my project. It was an honour to attend his very lively lectures on Deep Learning during the first year of the MSc, as well as to absorb some of his wisdom and enthusiasm at our meetings during my work on this project. I am also glad to have followed his advice at our last meeting: I stopped shaving for a month, which did free enough time for me to implement DQL (joint policy and value learning), as well as a Monte Carlo Tree Search algorithm, to nicely complement my assortment of sliding-puzzle and Rubik's cube solvers.

Last but not least, my wife Thanh Nhã is my biggest supporter in everything I do, and her continued encouragement in my pursuit of this MSc has made it so much easier to juggle between a demanding banking job, running 50 to 70 miles a week in preparation for the Chicago marathon, and the coursework, lectures and exam revisions.

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# 1 Objectives

## 1.1 Learning Objectives

Back when I studied Financial Mathematics, almost 2 decades ago, it was all about probability theory, stochastic calculus and asset pricing. These skills were sought after in the field of derivatives trading, and often enough to get a job in algorithmic or systematic trading. By the middle of the 2010s, with the constant advances in computing power and storage, the better availability of off-the-shelves libraries and data sets, I witnessed a first revolution: machine learning (**ML**) became more prominent and started overshadowing more traditional maths skills. In recent years, a second revolution has taken not only the world of finance, but that of every science and industry, by storm: we are now in the artificial intelligence (**AI**) age. In 2019, I decided to see by myself what this was all about, and if the hype was justified. What better way to do that than embark on a proper MSc in Artificial Intelligence?

Of the modules I have studied over the last two years, I have been most impressed by **DL**, Natural Language Processing (**NLP**) and particularly interested in AI Principles & Techniques (**AIPnT**), especially our excursion in graphs search. I have totally changed my mind around the potential of **DL**, **DRL** and **NLP** and think they are incredibly promising. I have been astonished to see by myself, through several of the MSc courseworks, how incredibly efficient sophisticated **ML**, **DL** and **DRL** algorithms can be, when applied well on the right problems, often vastly outperforming more naive and traditional approaches.

For the project component of the MSc, I thought it would be interesting (and fun) for me to apply some of the **DL**, **DRL** and search techniques from **AIPnT** to the sliding puzzle (**SP**) and of course the famous Rubik's cube (**RC**). I am in particular looking to solidify my understanding of **DRL** and **DQL** by implementing and experimenting with concrete (though arguably of limited practical use) problems.

## 1.2 Project's Objectives

I am hoping to try a mix of simple searches such as depth first search (**DFS**), breadth first search (**BFS**) and A* with simple admissible heuristics, then move to more advanced ones such as A* informed by heuristics learnt via **DL** and **DRL**, as well as try different network architectures. Time permitting I would like to give a go at **DQL**, and maybe also compare things with some open-source domain-specific implementations (for instance a Kociemba Rubik's algorithm implementation, see e.g. Tsoy, 2019).

Along the way, I am also hoping to learn a bit about the mathematics of the **SP** and the **RC**.

# 2 Deep Reinforcement Learning Search

In this chapter, I succinctly go through the different techniques underlying the algorithms I have implemented for this project and present them in simplified pseudo-code. Along the way, I will give some references for the interested reader.

## 2.1 Graphs Search & Heuristics

It is fruitful to think of single-player, deterministic, fully-observable puzzles such as the **SP** and **RC** as unit-cost graphs. We start from an initial *node* (usually some scrambled configuration of the **SP** or **RC**), and via legal moves, we transition to new nodes, until hopefully we manage to get to the goal in the shortest number of moves possible.

Graphs search (or graphs traversal) is a rather large, sophisticated and mature branch of **CS** that studies strategies to find *optimal* paths from initial to goal node in a graph. What is meant by *optimal* can vary, but usually is concerned with one or several of minimizing the run-time of the strategies, their memory complexity/usage or the total cost/length of the solutions they come up with. In the general theory, different transitions can have different costs associated with them. In this project however, we can reasonably consider that each move of a tile in the **SP** or each rotation of a face in the **RC** are taking a constant and identical amount of time and effort to perform, and I will therefore consider all the graphs to be unit-cost (i.e. all moves have cost 1).

Search strategies typically maintain a frontier, which is the collection of unexpanded nodes. They keep expanding the frontier, by choosing the next node to process (by adding all of its children nodes - i.e. those which are reachable via legal transitions - to the frontier for future evaluation) until a solution is found. The question is how to choose the next node to expand! Some graphs search strategies are said to be *blind*, in the sense that they do not exploit any domain-specific knowledge or insight about what the graphs represent to choose the next node to expand. In that category fall Breadth First Search (**BFS**) and Depth First Search (**DFS**), which as their name suggest expand nodes from the frontier based on, respectively, a **FIFO** and **LIFO** policy (see pseudo-code 1). **BFS** and **DFS** will only work for modest problems where the number of transitions and states are reasonably small; they can however work in a wide variety of situations as they make no assumptions and require no knowledge. It is quite easy to see that **BFS** is an *optimal* search strategy, in that when it does find a solution, that solution is of smallest possible cost (i.e. optimal). **DFS** is obvisouly not optimal as it could very well find a solution very deep in the graph while expanding the very first branch, not realising that a solution was one level away from the root on the next branch!

*Informed* strategies (see pseudo-code 2) on the other hand exploit domain-specific knowledge. One popular algorithm is $\mathbf{A}^*$ (see Dechter and Pearl, 1985), which first examines the node of smallest expected total cost (**f**), itself the sum of the cost-so-far

from initial to current node (**g**) plus the expected cost-to-go from current node to goal (**h**). The expected cost-to-go **h** is called a *heuristic*. The better the heuristic, the better **A**$^*$ performs. An important property of heuristics is *admissibility*: admissible heuristics never over-estimate the real cost-to-go, and can easily be shown to render **A**$^*$ optimal.

**Algorithm 1** Blind Graphs Search – BFS & DFS

```
function BlindSearch(root, time_out, search_type = Search.BFS)
    InitialiseTimeOut(time_out)
    if IsGoal(root) then return root
    explored ← {}
    frontier ← [root]
    while true do
        CheckTimeOut(void)
        if Empty(frontier) then return failure
        if Equal(search_type, Search.BFS) then
            node ← PopFront(frontier)
        else
            node ← PopBack(frontier)                    ▷ Search.DFS
        Add(explored, node)
        for child ∈ Children(node) do
            if IsGoal(child) then return child
            Add(frontier, child)
```

**Algorithm 2** Informed Graphs Search – A$^*$

```
function A*(root, time_out, H)                          ▷ H – cost-to-go heuristic
    InitialiseTimeOut(time_out)
    f ← 0 + H(node)
    explored ← {}
    frontier ← SortedMultiMap({cost : node})
    while true do
        CheckTimeOut(void)
        if Empty(frontier) then return failure
        (cost, node) = PopSmallest(frontier)
        if IsGoal(node) then return node
        Add(explored, node)
        for transition, child ∈ Children(node) do
            child_cost ← Cost(transition) + H(child)
            if child ∈ frontier and child_cost ≤ cost then
                UpdateCost(frontier, child, child_cost)
            else if child ∉ explored then Add(frontier, child, child_cost)
```

## 2.2 Reinforcement Learning

**RL** (see Sutton and Barto, 2018 for a brilliant exposition of the basic concepts and theory) has known a bit of false start in the 1950s and 1960s but recently been extremely successfully applied to a variety of problems (from Atari to board games and puzzles, robotics, ...). **RL** is concerned with how intelligent agents can learn optimal decisions from experiencing rewards while interacting in their environment. One of the fundamental concept in the field is that of value function $s \rightarrow \mathbf{V}(s)$, which tells us the maximum expected reward - or equivalently and better suited to our puzzle solving task, the minimum cost - the agent can obtain from a given state $s$ (assuming optimal decisions). In finite state and transitions spaces, the value function can be remarkably computed by a mechanical, rather magic-like procedure called value-iteration (equivalent to Optimal Control's Bellman equation, see pseudo-code below 3), where each state $s$'s value is iteratively refined by combining the value of $s$'s reachable children states.

**Algorithm 3** Reinforcement Learning – Value Iteration

```
function ValueIteration(states)                    ▷ states – generator of states
    V ← {state : ∞ for state ∈ states}
    change ← true
    while change do
        change ← False
        for state, cost ∈ states do
            V[state] ← ∞
            for child, t_cost ∈ Children(state) do
                V[state] ← Min(V[state], V[child] + t_cost)
            if V[state] ≠ cost then
                change ← true
    return V
```

## 2.3 Deep Learning

Similarly to **RL**, **DL** has not initially had the success the **AI** community was hoping it would. Marvin Minsky, who often took the blame for having *killed* funding into the field, even regretted writing his 1969 book (Minsky and Papert, 1969) in which he had proved that three-layer feed forward perceptrons were not quite the universal functions approximators some had hypothesized them to be. Since around 2006 (see Goodfellow, Bengio, and Courville, 2016 for more history of the recent burgeoning of **DL**), the field has known a rebirth, probably due to a combination of factors, from ever more powerful computers and larger storage, the availability of data sets large and small on the internet, the advances in many techniques and heuristics (backward propagation, normalisation, drop-outs, different optimisation schemes, etc ...) and the huge amount of experimentation with different architectures (from very deep feed forward fully connected networks, to convolutional, recurrent and more exoctic networks). It is not an

exageration to say that **DL** has revolutionized entire fields of research such as computer vision, robotics, computational biology and **NLP**. **DL** has often become the method of choice to learn or approximate highly dimensional functions or random processes. The beauty of it is that the relevant features are autodiscovered during the training of the network, via back-ward propagation and trial-and-error, rather than having to be postulated or handcrafted as is often the case with other **ML** techniques.

### 2.4 DL and DLR Heuristics

So what is the link between all of these: A$^*$'s heuristics, **DL**, **RL**'s value iteration? Sometimes we have ways of computing good solutions/heuristics to our puzzles, but cannot computationally do this for all states (the state space might be too large!). One approach in that case is to compute solutions for *some manageable number of* states, and let a **DL** model learn how to extrapolate to the whole state space. This is a case of *supervised* learning, since we need a teacher-solver to tell us good solutions or heuristics to extrapolate from. Pseudo-code is provided below, see 4:

**Algorithm 4** Deep Learning – Heuristic

```
function DeepLearningHeuristic(**args)
    puzzle_type ← FromParams(**args)
    n_puzzles ← FromParams(**args)
    H ← FromParams(**args)          ▷ H – teacher heuristic to extrapolate via DL
    loss_function ← FromParams(**args)
    net_architecture ← FromParams(**args)
    V = {state : H(state) for state ∈ GenerateRandomStates(puzzle_type, n_puzzles)}
return TrainNeuralNetwork(V, loss_function, net_architecture)
```

An alternative approach to compute the cost-to-go is via **RL** value-iteration as described in the previous section (2.2). The state space is often so large however - and this certainly is the case for pretty much all **SP** and **RC**, except maybe the smallest dimensional **SP**s - that we cannot practically perform the value iteration procedure for all states. This is where **DL** comes again to the rescue to act as function approximator, combining with **RL** into what has become known as **DRL**. The subtlety is that both the left-hand-side and right hand side in the value-iteration procedure are given by a **DL** network which we are constantly tweaking. For my implementation of **DRL**, I followed the same approach as in Mnih et al., 2013, utilising two loops. During iteration over the first (inner) loop, the right hand-side $V$ of the value-function update equation is computed using a fixed *target-network*. The left hand side $V$ is using another *current-network* which alone is modified by the **DL** learning (backward propagation and optimization), until convergence is deemed reached. When convergence in the inner loop is deemed obtained, we break out of it, and run the outer loop, which updates the *target-network* via a copy of the *current-network*. The outer loop is itself broken out of when deemed appropriate (some kind of convergence criteria). See pseudo-code 5 below:

**Algorithm 5** Deep Reinforcement Learning – Heuristic

```
function DeepReinforcementLearningHeuristic(**args)
    puzzle_type ← FromParams(**args)
    puzzles_gen_params ← FromParams(**args)
    puzzles_generation_criteria ← FromParams(**args)
    n_puzzles ←← FromParams(**args)
    target_network_update_params ← FromParams(**args)
    max_epochs ← FromParams(**args)
    loss_function ← FromParams(**args)
    net_architecture ← FromParams(**args)
                                        ▷ initial network and target network
    net ← GetNetwork(puzzle_type, network_architecture)
    target_net ← GetNetwork(puzzle_type, network_architecture)
    epoch ← 0
    puzzles ← null
    while epoch < max_epochs && other_convergence_criteria(network) do
        epoch ← epoch + 1
                                        ▷ generate training puzzles if criteria met
        if puzzles_generation_criteria(puzzles) then
            puzzles ← generate_random_states(puzzle_type)
        V ← dict()
        for puzzle ∈ puzzles do
            V[puzzle] ← ∞
            if  (then)IsGoalpuzzle:
                V[puzzle] ← 0
            else:
                for transition, child ∈ Children(puzzle) do
                                                    ▷ perform value iteration
                    child_cost ← Cost(transition) + target_net(child)
                    V[puzzle] ← Min(V[puzzle], child_cost)
        ▷ iterate through network training running feed-forward and backward-prop
        net ← TrainNeuralNet(V, loss_function, net_architecture)
                                        ▷ update target network if criteria met
        if target_network_update_criteria(net, target_net) then
            target_net ← Copy(net)
        return net
```

### 2.5 Deep Q-Learning

Another fundamental concept of **RL** is that of the Q-function $Q(s, a)$, the maximum expected reward the agent can obtain from state $s$, taking action $a$ and acting optimally afterwards. Notice that the knowledge of $V$ everywhere is equivalent to that of $Q$, since obviously:

$$V(s) = max_{a \in \mathcal{A}(s)} Q(s, a) \tag{1}$$

where $\mathcal{A}(s)$ are the actions from state $s$. Conversely, we can recover $Q$ from $V$ since:

$$Q(s, a) = R(a) + V(a(s)) \tag{2}$$

where $R(a)$ is the reward of performing action $a$ and $a(s)$ is the state we reach by performing action $a$ from state $s$. Similarly to the way one can compute $V$ via value-iteration (at least in finite state and action spaces), $Q$ can also be computed by iteration (See Watkins and Dayan, 1992 for details of convergence of that procedure).

Similarly to our discussion about **DRL**, in cases where the state space is large, it can be useful to approximate $Q$, or a somewhat related quantity (such as e.g. a probability distribution over the actions that can be taken from $s$) by a neural network, and use a similar procedure to that of the previous section to update the right-hand-side and left-hand-side of the iterations. That becomes **DQL**!

I have for this project followed the exact same procedure described in McAleer et al., 2018b (and also used by alpha-go Silver et al., 2016): the output of the neural network that is learnt by **DQL**, which actually is surprisingly similar to the approach and pseudo code shown for **DRL** earlier. The only 3 differences are that:

- the networks (target and current) now output a vector of size $a + 1$, where $a$ is the number of possible actions/moves. That is, one dimension for each of the possible actions, representing the probability/desirability of that action, and one dimension for the value-function's value.
- the target update by Q-iteration now needs to update both the value-function and the optimal decision ($a$-dimensional vector of 0s, with a 1 for the optimal decision only)
- the loss function used need to be compatible with the size of the output and target vectors. I have used as loss the average of the mean square error of the value function difference (current network and target) and the cross entropy loss of the actions probability versus the actual optimal move.

Since in my **DRL** pseudo-code above (as well as in my actual code), the loss function is abstracted, and the network architecture (including the size of the output) configurable, the only modification to get **DQL** in lieu of **DRL** are extremely minimal, and essentially only to do with the Q-iteration-update section:

**Algorithm 6** Deep Q Learning – Heuristic

```
function DeepReinforcementLearningHeuristic(**args)
                                        ▷ ... same params and init as for DRL ...
    nb_actions ← GetNbActions(puzzle_type)
    while epoch ... do
                                        ▷ ... same while epoch loop as for DRL ...
                                        ▷ ... update cost and actions via V & Q iteration ...
        Q_and_V ← dict()
        for puzzle ∈ puzzles do
            value ← target_network(puzzle).value
            actions = [0] * nb_actions
            best_action_id ← 0
            if IsGoal(puzzle) then
                value ← 0
            else:
                for action_id, child ∈ Children(puzzle) do
                    child_value ← target_network(child).value
                    if child_value ≤ value then:
                        value ← child_value
                        best_action_id ← action_id
                                        ▷ ... update cost and best action ...
            actions[best_action_id] ← 1
            Q_and_V[puzzle] ← actions + [value]
```

## 2.6 Monte Carlo Tree Search

The **DQL** heuristics from 6 no longer only produce cost-to-go estimates as **DRL**, but rather a joint cost-to-go and distribution over actions (i.e. a 5-dimensional vector for the **SP** and a 13-dimensional vector for the **RC**). This leaves us with the question of how can we use the output of such a network to search for a solution. One simple answer (which I have tried, see e.g. subsection 5.2.3) is that we could disregard the distribution and only take into account the cost-to-go by simply using $A^*$. The rationale for doing so is that we might hope that jointly learning the cost-to-go and the actions via a combination of MSE and cross-entropy-loss produces a better network and leads to better heuristics, since we use more information during the learning and iterations.

Another possibility is to use an algorithm combining the actions distribution and the value function to inform its search. The Monte Carlo Tree Search (**MCTS**) is such an algorithm. It generates at each iteration (possibly in a distributed or multithreaded manner) paths to a *leaf* on the frontier of unexpanded nodes, expands that node and checks if it is a goal state (and keeps going until the goal is found). The paths followed from initial state to leaves are decided via a combination of the probability distribution

over actions (allowing exploration) and value function (exploitation), according to a trade-off which can be tuned via a hyper-parameter $c$. To prevent following the same paths (which might lead the search far from the goal), the **MCTS** keeps track of actions already followed and downweight their probability so that subsequent paths explore different actions. Let me first present in pseudo-code the paths generation, in particular the trade-off between actions-values (exploration-exploitation):

**Algorithm 7** Monte Carlo Tree Search – Child Node Choice

```
function ChooseChildNode(node, actions_probas, actions_values, actions_count, c)
                                    ▷ c is the actions-values trade-off hyper-parameter
    N ← √(Σ_{n∈actions_count} n)
    ▷ ... frequent actions penalized as denominator grows faster than numerator N ...
    Q ← N.(actions_probas / actions_count)
    V ← actions_values
                                    ▷ ... high c gives weight to actions to favour exploration ...
                                    ▷ ... return child for which cQ + V is maximized ...
    action_id ← IndexMax(c.Q + V)
return Child(node, action_id)
```

The actual **MCTS** algorithm is simply generating a new path from root to a new leaf at each iteration, until the goal is found:

**Algorithm 8** Monte Carlo Tree Search

```
function MCTS(root, time_out, q_v_network, c)
    InitialiseTimeOut(time_out)
    tree ← Tree(root)
    if IsGoal(root) then return root
    while true do
        CheckTimeOut(void)
        leaf ← root
        while leaf.expanded do
            actions_probas, actions_values ← q_v_network(leaf)
            leaf ← ChooseChildNode(leaf, actions_probas, actions_values, leaf.actions_count, c)
            Expand(leaf, tree)
        IncrementActionsFromLeafToRoot(leaf)
        ▷ path to leaf can usually be improved by re-running BFS on the resulting tree
        if IsGoal(leaf) then return BlindSearch(tree, search_type = Search.BFS)
```

Note that for this project, I have implemented all the above algorithms in Python (BFS, DFS, A*, DeepLearner, DeepReinforcementLearner, DeepQLearner, MonteCarloTreeSearch), and more details can be found in section (4).

# 3 Puzzles

## 3.1 Sliding Puzzle

### 3.1.1 History - the 15-Puzzle

The first puzzle I will focus on in this thesis is the sliding puzzle (see Wikipedia, 2022b) whose most common variant is the 15-puzzle, seemingly invented in the late 19th century by Noyes Chapman (see WolframMathWorld, 2022), who applied in 1880 for a patent on what was then called "Block Solitaire Puzzle". In 1879, a couple of interesting notes (Johnson and Story, 1879), published in the American Journal of Mathematics proved that exactly half of the 16! possible ways of setting up the 16 tiles on the board lead to solvable puzzles. A more modern proof can be found in Archer, 1999.

Since then, several variations of the 15-puzzle have become popular, such as the 24-puzzle. A rather contrived but interesting one is the coiled 15-puzzle (Segerman, 2022), where the bottom-right and the top-left compartments are adjascent; the additional move that this allows renders all 16! configurations solvable.

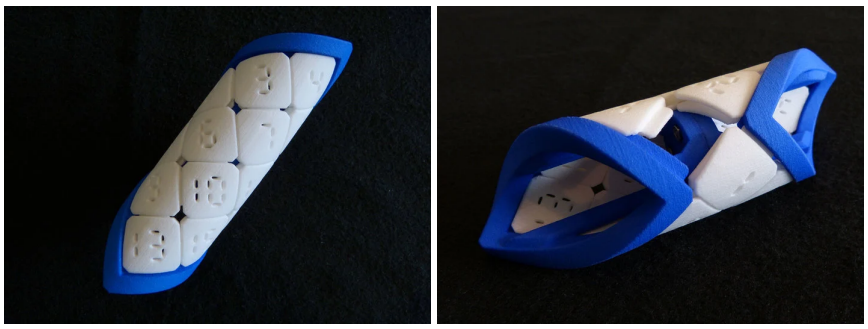

Figure 1: Coiled 15-puzzle

It is easy to see why this is the case, let me discuss why: given a configuration $c$ of the tiles, let us define the permutation $p(c)$ corresponding to enumerating the tiles row by row (top to bottom), left to right for odd rows and right to left for the even rows, ignoring the empty compartment. For the following left-hand-side15-puzzle $c_l$ we have $p(c_l) = (1, 6, 2, 3, 4, 7, 10, 5, 9, 15, 14, 11, 8, 12, 13)$:

| | | | |
|---|---|---|---|
| 1 | 6 | 2 | 3 |
| 5 | 10 | 7 | 4 |
| 9 | 15 | 14 | 11 |
| 13 | 12 | | 8 |

| | | | |
|---|---|---|---|
| 1 | 6 | 2 | 3 |
| 5 | 10 | 7 | 4 |
| 9 | 15 | | 11 |
| 13 | 12 | 14 | 8 |

The parity $p(c)$ of a configuration $c$ cannot change via a legal move. Indeed, p(c) is clearly invariant by lateral move of a tile, so its parity is invariant too. A vertical move of a tile will displace a number in $p(c)$ by an even number of positions right or left. For instance, moving tile 14 above in $c_l$ into the empty compartment below it results in a new configuration $c_r$ with $p(c_r)$ = (1, 6, 2, 3, 4, 7, 10, 5, 9, 15, 11, 8, 14, 12, 13), which is equivalent to moving 14 by 2 positions on the right. This obviously cannot change the parity since exactly 2 pairs of numbers are now in a different order, that is (14, 11) and (14, 8) now appear in the respective opposite orders as (11, 14) and (8, 14). This is the crux of the proof of the well known necessary condition (even parity of p(c)) for a configuration c to be solvable (see part I of Johnson and Story, 1879). In the case of the coiled puzzle, we can solve all configurations of even parity, since all the legal moves of the normal puzzle are allowed. In addition, we can for instance transition between the following 2 configurations, which clearly have respectively even and odd parities:

| | | | |
|---|---|---|---|
| 1 | 2 | 3 | 4 |
| 5 | 6 | 7 | 8 |
| 9 | 10 | 11 | 12 |
| 13 | 14 | 15 | |

| | | | |
|---|---|---|---|
| | 2 | 3 | 4 |
| 5 | 6 | 7 | 8 |
| 9 | 10 | 11 | 12 |
| 13 | 14 | 15 | 1 |

Since it is possible to reach an odd parity configuration, we conclude by invoking symmetry arguments that we can solve all 16! configurations.

### 3.1.2 Search Space & Solvability

In this thesis, as well as in the code base (Berrier, 2022) I have written to do this project, we will consider the general case of a board with n columns and m rows, where $(n, m) \in \mathbb{N}^{+2}$, forming $n * m$ compartments. $n * m - 1$ tiles, numbered 1 to $n * m - 1$ are placed in all the compartments but one (which is left empty), and we can slide a tile directly adjascent to the empty compartment into it. Notice from a programming and mathematical analysis perspective, it is often easier to equivalently think of the empty compartment being moved into (or swapped with) an adjacent tile. Starting from a given shuffling of the tiles on the board, our goal will be to execute moves until the are tiles in ascending order: left to right, top to bottom (in the usual western reading order), the empty tile being at the very bottom right.

Note that the case where either n or m is 1 is uninteresting since we can only solve the puzzle if the tiles are in order to start with. For instance, in the (n, 1) case, we can only solve n of the $\frac{n!}{2}$ possible configurations. We will therefore only consider the case where both n and m are strictly greater than 1.

As hinted in the previous section when discussing the coiled 15-puzzle, we can note that the parity argument used there implies that in general, out of the $(n * m)!$ possible permutations of all tiles, only half are attainable and solvable. This gives us a neat way to generate *perfectly shuffled* puzzles, and we make use of this in the code. When comparing various algorithms in later sections, I will compare them on a same set of shuffled puzzles, where the shuffling is either done via a fixed number of random moves from goal position, or via what I call *perfect shuffle*, which means I give equal probability to each attainable configuration of the tiles. A simple way to achieve this is therefore to start with one randomly selected among the $(n * m)!$ permutations, and then to verify that the parity of that permutation is the same as that of the goal (for the given choice of n and m), and simply swap the first two (non-empty) tiles if it is not.

### 3.1.3 Optimal Cost & God's Number

Let us fix n and m, integers strictly greater than 1 and call $\mathcal{C}_{(n,m)}$ the set of all $\frac{(n*m)!}{2}$ solvable configurations of the n by m sliding-puzzle. For any $c \in \mathcal{C}_{(n,m)}$ we define the optimal cost $\mathcal{O}(c)$ to be the minimum number of moves among all solutions for c. Finally we define $\mathcal{G}(n,m)$, God's number for the n by m puzzle as $\mathcal{G}(n,m) = \max_{c \in \mathcal{C}_{(n,m)}} \mathcal{O}(c)$. Note that since $\frac{(n*m)!}{2}$ grows rather quickly with n and m, it is impossible to compute $\mathcal{G}$ except in rather trivial cases.

A favourite past time among computer scientists around the globe is therefore to search for more refined lower and upper bounds for $\mathcal{G}(n,m)$, for ever increasing values of n and m. For moderate n and m, we can actually solve optimally all possible configurations of the puzzle and compute exactly $\mathcal{G}(n,m)$ (using for instance $A^*$ and an admissible heuristic (recall 2.1, and we shall see modest examples of that in the results section later). For larger values of n and m (say 5 by 5), we do not know what the God number is. Usually, looking for a lower bound is done by *guessing* hard configurations and computing their optimal path via an optimal search. Looking for upper bounds is done via smart decomposition of the puzzle into disjoint nested regions and for which we can compute an upper bound easily (either by combinatorial analysis or via exhaustive search). See for instance Karlemo and Ostergaard, 2000 for an upper bound of 210 on $\mathcal{G}(5,5)$.

A very poor lower bound can be always obtained by the following reasoning: each move can at best explore three new configurations (4 possible moves at best if the empty tile is not on a border of the board (less if it is): left, right, up, down but one of which is just going back to an already visited configuration). Therefore, after $p$ moves, we would span at best $\mathcal{S}(p) = \frac{3^{p+1}-1}{2}$ configurations. A lower bound can thus be obtained for $\mathcal{G}(n,m)$ by computing the smallest integer $p$ for which $\mathcal{S}(p) \geq \frac{(n*m)!}{2}$

## 3.2 Rubik's Cube

### 3.2.1 History – from Erno Rubik to speed cubing competitions

The second puzzle I will focus on is the Rubik's Cube (**RC**), invented in 1974 by Erno Rubik, originally known as *Magic Cube* (see Wikipedia, 2022a). Since it was commercialised in 1980, it has kown a worldwide success: countless people are playing with the original 3x3x3 cube, as well as with variants of it of all shapes and sizes. Competitions bring together *speedcubers* who have trained for years and memorized algorithms to solve the Rubik's in astonishly fast times (seconds for the best ones). Some of the principles used by speedcubers generalise to different dimensions. As an example, it is quite impressive to watch *Cubastic* solve a 15x15x15 cube in (only) two and a half hours! (see Cubastic, 2022). The key insight to solving high dimensional **RC**s (short obviously of coming up with specific strategies) is the following: if we manage to group all the inside (i.e. not located on a corner or an edge) cubies by colour, and then all the non-corner edges on a given tranche of a face by colour, we are essentially reducing the cube to a 3x3x3, since no face rotation will ever undo these groupings. The picture below (2) shows my own 4x4x4 and 3x3x3 cubes arranged to be in identical configurations.

Figure 2: Reducing a 4x4x4 **RC** to a 3x3x3 – home made picture

If we can bring the 4x4x4 cube to such a configuration on all faces (which is not very hard), and if we know how to solve a 3x3x3, we are essentially done. (The additional degrees of freedom on the 4x4x4 complicate slightly the story since certain arrange-

ments of colors which are possible on the 4x4x4 are not on the 3x3x3, e.g. red an and white on opposite faces). Overall, the difficuly of hand-solving cubes does not grow as much with dimensionality as one would think, and the time difference comes mostly from the difficulty of handling and manipulating larger cubes.

### 3.2.2 Conventions: faces, moves and configurations

I follow the conventions and notations of the **RC** community and refer to the faces as F (front), B (back), U (up), D (down), L (left) and R (right). It is common in **RC** jargon to refer to moves by the name of the face that is rotated clock-wise (when facing it), and by adding a ′ for counter-clock-wise rotations. Sometimes numbers are used to indicate repeated moves, though I will count that as multiple moves, since obviously e.g. U2 = U U = U′ U′. As another example: F B′ F2 means rotating the front face clock-wise, the back face counter-clock-wise, followed by the front face twice. The convention I follow is called the *quarter-turn-metric*, and obvioulsy the length of solutions is affected by which metric we use.
Since I am interested in experimenting with *no-human-knowledge* methods such as **DRL** and **DQL**, I will consider cubes which are identical up to full cube rotation such as the *flattened* cubes on figure 3 ) to be different. They will be represented by different tensors in my code, and this is up to the solvers to make sense of things.

Figure 3: Two equivalent configurations by full-cube-rotation

The **RC** has, as one would expect, an extremely large state space. I will compute the state space size for the 3x3x3 and 2x2x2 cubes in the next two subsections and discuss conditions under which a cube is solvable.

### 3.2.3 3x3x3 Rubik's – search space, solvability & God's number

A good strategy to compute the state space size of a the Rubik's of a given dimension is to compute:

- $N$: the number of possible arrangements of the *cubies* (individual small cubes that constitute the Rubik's) in space, taking into account physical constraints and some invariants.
- $D$: the number of possible configurations which are equivalent via full cube rotation in space.

The state space can then be considered to be either $\frac{N}{D}$ or $N$, depending on our representation (as mentioned earlier my code will treat each rotation of the cube in space as a different representation, so I shall not be dividing by $D$ below).

In order to compute $D$, we just need to realise that each configuration can be arranged in (only) 24 different ways via full cube rotation in space. In particular that means that there are 24 possible goal states (and not 6! as we might naively think at first), so for instance in figure 3 I could only have picked 2 out of 24 different configurations. Why is this?
Any of the six colors can be placed on the F face, and then any of the four adjacent colors can be placed on the U face (say). Once these two colors are chosen, the remaining faces are determined. This is not immediately obvious, but not difficult to convince oneself that this is the case with the following two observations about the structure of corner *cubies*: first observation is that they have 3 determined colors, which are fixed once and for all. In particular, the fact that there is no corner with colors F and B, means that once the cube is in solved state, we have to have colors F and B on opposite faces, and similarly for colors U and D as well as colors L and R. Hence, having fixed the color on face F, the color on face B is fixed too. The second observation is that when facing a corner cubie, the order of its three color (e.g. enumerated clock-wise) is invariant. For instance, consider the corner cubie with colors (F, R, U). No scrambling of the cube will ever produce clock-wise order of e.g. (F, U, R). This is obvious once you consider that there is no move of the Rubik's cube you could not perform while holding a given corner fixed in space (e.g. by pinching that corner cubie with your fingers and never letting go of it).

Computing $N$ is a bit tricker. For the 3x3x3 Rubik's, each of the 8 corner cubies could be placed at one of the physical corner locations and oriented three different ways (rather than six, since as discussed earlier, the clock-wise orientation of a given corner cubie can never be changed). We have therefore $8!.3^8$ corner arrangements. Similarly, the 12 edge cubies can be placed at 12 physical edge locations and oriented 2 different ways, so we have another multiplicative factor of $12!.2^{12}$. There are however some well know parities (see Martin Schoenert, 2022 for details) which are invariant under legal moves of the Rubik's cube and which reduce the number of arrangements that are physically attainable via face rotations. The *corner orientation parity* (**COP**) for

instance sums over the corner cubies the number of $120^o$ rotations it would take to bring a given cubie to its standard orientation (i.e. compared to the top cube in figure 3). It is easy to observe that the **COP** is invariant (% 3) since any face rotation will displace four corner cubies, two of which see their individual **COP** increase by 2, and the other two by 1 (so a total increase of 6). Similarly, there are two additional parities called *edge orientation parity* (**EOP**) and *total permutation parity* (**TPP**) which are both invariant (% 2) under face rotation. Overall, these three parities mean that only 1/12 of the $8!.3^8.12!.2^{12}$ arrangements are physically attainable, leaving us with a grand total of $43,252,003,274,489,856,000$ different cubes (still a rather staggeringly large number!).

Finally, let me mention that there is a long history of research into finding tighter and tighter bounds on the 3x3x3 God's number (usually, proofs of upper bounds were obtained and refined by decomposing the Rubik's moves group into subgroups, then finding upper bounds of distance between two elements of a given subgroup, and finally summing these upper bounds over the different subgroups). See e.g. Alexander Chuang, 2022 for an exposition of this type of approach. In 2007, an upper bound of 34 in the quarter turn metric was published (Silviu Radu, 2007) but the question got properly settled in Tomas Rokicki and Morley Davidson, 2022 by Google's researchers which used clever symmetry arguments to reduce the search space to the maximum, followed by Google's vast computing power capabilities to brute force solve all of the configurations they were left with. They concluded that the 3x3x3 Rubik's God number is in fact a mere 26.

#### 3.2.4 2x2x2 Rubik's – search space, solvability

For the 2x2x2 cube, there are eight possible ways of choosing the physical position of the eight corner cubies (and since there are known algorithms, such as R' U R' D2 R U' R' D2 R2, to swap exactly two and only two adjacent corners we know all can indeed be obtained). Each corner cubie can be oriented in 3 different ways, so we get a total of $8!.3^8$ configurations. However, due to the **COP** parity discussed in the previous section, we conclude that only one third of these are attainable (namely those for which the **COP** is equal to 0 % 3). Overall, this gives $8! * 3^7$ = 88,179,840 possible configurations (probably a larger number than most people would expect for a mere 2x2x2 cube).
The insight and knowledge of this section has been useful for me to implement *perfect scrambling* for the 2x2x2 **RC**. Indeed, the way I generate perfectly shuffled cubes is by randomly placing the 8 corners, then randomly choosing the orientation of the first 7, and finally fixing the $8^{th}$ corner's orientation to make sure COP is equal to 0 % 3.
Some quick googling suggests the 2x2x2 Rubik's God number to be 11 in the quarter turn metric, but I could not find any clear and definitive paper on this.

#### 3.2.5 Rubik's – multi-stage search

Modern Rubik's domain-specific solvers (such as the Kociemba solver which I have used in this project as a comparison point) make use of a multi-stage search approach.

Essentially, they just do what speedcubers do by hand, just much faster and better. The general idea is as follows: let us suppose we have a puzzle with a state space $\mathcal{S}$ of size $N$ (some large number) and one goal state $g$. Now imagine that we have discovered a much smaller subset of configurations $\mathcal{S}_1 \in \mathcal{S}$ (say of size $n \ll N$) such that $g \in \mathcal{S}_1$ and such that it is *easy* to check whether or not a given configuration $p \in \mathcal{S}$ belongs to $\mathcal{S}_1$. In addition, suppose we also have discovered a set of algorithms $\mathcal{A}_1$ (sequence of actions) under which elements of $\mathcal{S}_1$ are stable and which spans $\mathcal{S}_1$. Finally, suppose that we have a set of algorithms $\mathcal{A}_2$ which allow us to (provably) take any given configuration $p \in \mathcal{S}$ into $\mathcal{S}_1$ in a bounded number of steps. A viable strategy to solve any puzzle then becomes:

**Multi-stage search**

1. If $p \in \mathcal{S}_1$, set $a_2$ to be the identity move in $\mathcal{S}$, and jump to step 3.
2. Apply a search algorithm (e.g. A$^*$ - or some variant such as IDA$^*$ (Wikipedia, 2022c) - restricting eligible actions to $\mathcal{A}_2$, until we find a sequence of actions $a_2$ such that $a_2(p) \in \mathcal{S}_1$
3. Apply our search algorithm to $a_2(p)$, restricting eligible actions to $\mathcal{A}_1$, until we find a sequence of actions $a_1$ such that $a_1(a_2(p)) = g$.
4. $a_1 \circ a_2$ is our multi-stage solution

Notice that this is exactly how beginners and advanced speedcubers solve the Rubik's cube, except they usually have more than 2 stages as described above. $S_1$ might for instance be the set of cubes where both lower layers are solved, the cross on the top layer as well as all corners are in their respective places (but maybe not oriented as expected), and then they search within a well known and small set of algorithms how to get to the goal state. A previous stage might consist in $S_2$, the set of configurations where the two layers are solved, but the top layer is random, and then they will search for a sequence of moves to get into $S_1$, etc ...

## 3.3 Solving puzzles without human knowledge

In the upcoming implementation (4) and results (5, 6) sections, I will be discussing various solvers. I would put them broadly in four different categories, by decreasing level of human knowledge that has been assumed and handcrafted in them. Notice that my human-knowledge-required scale is obviously somewhat arbitrary, but good to keep in mind in later (and in particular results) sections.

**Domain-specific solvers** At 4 on the human-knowledge-required scale, I would put my NaiveSolver (handcrafted to solve the **SP**) as well as the hkociemba (2x2x2) and kociemba (3x3x3) open source implementations which I have integrated in my KociembaSolver. They make heavy use of specific knowledge about the two puzzles (see 3.2.5),

not only about their mechanics, but also about how to actually (and provably) solve them.

**Domain-specific heuristics** At 3 on the human-knowledge-required scale, I put A*-with-handcrafted-heuristics (e.g. Manhattan heuristic for the **SP**) algorithms. Constructing the heuristics usually require some knowledge about the puzzle's mechanics, but not necessarily about how to solve them efficiently (though of course knowing the latter might help come up with more efficient heuristics).

**Supervised learning** At 2 on the human-knowledge-required scale, I put my DeepLearner solver (also using A* but whose heuristic is learnt via **DL**). This solver does not require any knowledge of the structure or mechanics of the puzzle, nor of how to solve them, but just need a teacher algorithm to learn/extrapolate from.

**Blind search& unsupervised learning** Finally at 1 on the human-knowledge-required scale, I put the blind solvers such as **BFS** and **DFS**. Also in that group I put A* with heuristics learnt using my DeepReinforcementLearner and DeepQLearner, and my MonteCarloSearchTree which all know (almost) nothing about the puzzles and do totally work from generic interfaces alone (states, transitions, etc ...) and are operating in an unsupervised way.

One important comment I would make to end this section is that it is easy to inject, without realising or acknowledging it, specific knowledge into the solvers, or in the tensor representation of the puzzles that the solvers take as input. Pretty much all the papers about **RC** that I have surveyed chose a more compact representation for the cube than I have. They remove the center cubies of the 3x3x3 cube since, they argue, those never move via face-turns. Some of them go much further and make use of various symmetry arguments to reduce the search space and reduce the **RC** to having one goal state (instead of 24). One of the main papers I have taken inspiration from for this project, McAleer et al., 2018a, reduces the representation of the Rubik's considerably more, by making use of arguments about the physical structure of the edge and corner cubies: knowing the color of one of their face allows you do deduct the other faces, and therefore, they only need to track one face. I of course understand that they do that for the sake of reducing the size of the tensors representing the cube, and in order to remove redundant information. This is still *cheating* a bit in my opinion, especially if you are claiming to solve these puzzles *without-human-knowledge*, as we can only perform these dimensionality reduction tricks if we have external world knowledge about the physical structure of the puzzles. In this project, I have chosen as pure an approach as I could, and not only did not reduce the dimensionality of the tensor representation of the puzzles, but also, specifically for the Rubik's cube, I did not make use of invariance by spacial rotation of the full cube.

# 4 Implementation

The code I have developed for this project is all publicly available on my github page (Berrier, 2022). It can easily be installed using the setup file provided, which makes it easy to then use Python's customary import command to play with the code. The code is organised in several sub modules and makes use of factories in plenty of places so that I can easily try out different puzzles, dimensions, search techniques, heuristics, network architecture, etc... without having to change anything except the parameters passed in the command line. Here is a visual overview of the code base with the main dependencies between the main submodules and classes. Solid arrows indicate inheritance (e.g. AStar inherits from SearchStrategy), while dotted lines indicate usage (e.g. AStar uses Heuristic, DeepReinforcementLearner uses DeepLearning, etc..).

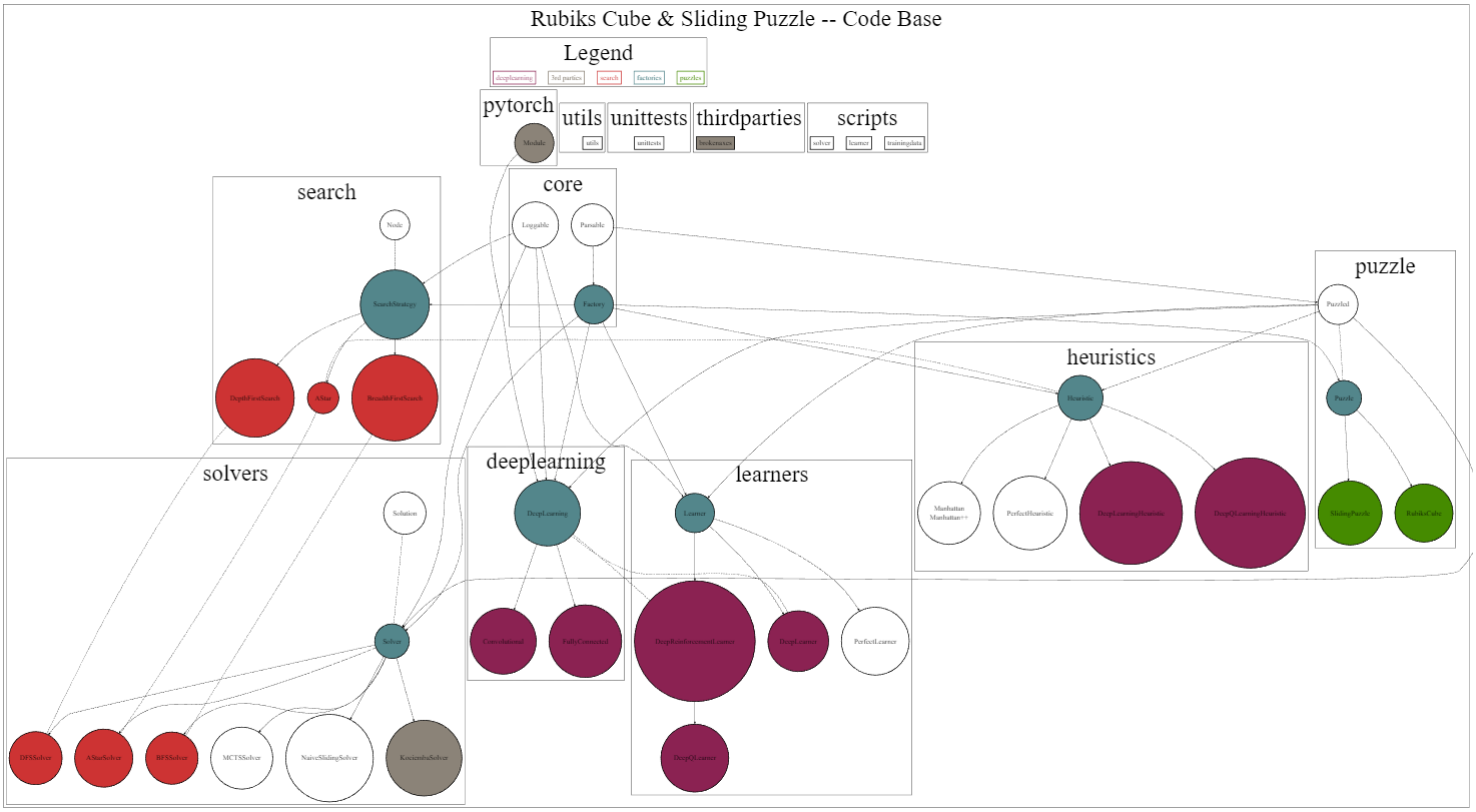


Figure 4: Code base

Let me now describe what each submodule does in more details:

## 4.1 rubiks.core

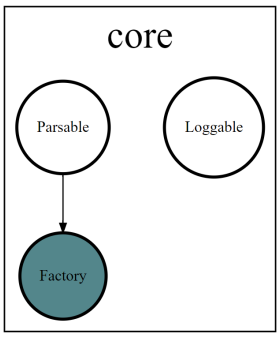


Figure 5: rubiks.core

This submodule contains base classes that make the code base easier to use, debug, and extend. It contains the following:

- **Loggable**: a wrapper around Python's logger to automatically picks up classes' names at init and format things nicely (dict, series and dataframes in particular).
- **Parsable**: a wrapper around ArgumentParser, which allows to construct objects in the project from command line, to define dependencies between object's configurations and to help a bit with typing of configs. The end result is that you can pretty much pass **kw_args everywhere and it just works.
- **Factory**: a typical factory pattern. Concrete factories can just define what widget they produce and the factory will help construct them from **kw_args (or command line, since Factory inherits from Parsable)

## 4.2 rubiks.puzzle

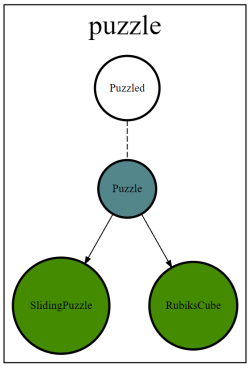


Figure 6: rubiks.puzzle

This submodule contains:

- **Puzzle**: a Factory of puzzles. It defines states and actions in the abstract, and provides useful functions to apply moves, shuffle, generate training sets, tell if a state is the goal, etc. Puzzle can manufacture the two following types of puzzles:
- **SlidingPuzzle**. Implements the states and moves of the sliding puzzle.
- **RubiksCube**. Implements the states and moves of the Rubik's cube.

  A **Puzzled** base class which most classes below inherit from. It allows e.g. heuristics, search algorithms, solvers and learners to know what puzzle and dimension they operate on, without having to reimplement these facts in each of them.

### 4.3 rubiks.search

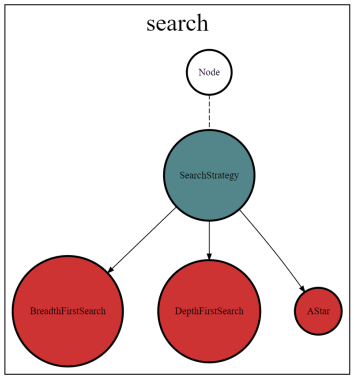


Figure 7: rubiks.search

This modules contains graph search strategies. I have actually reused the code I implemented for one of the AIPnT assignments here. It contains the following classes:

- **Node**: which contains the state of a graph, as well as link to the previous (parent) state, action that leads from the latter to the former and the cost of the path so far.
- **SearchStrategy**, a Factory class which can instantiate the following three types of search strategies to find a path to a goal:
- **BreadthFirstSearch**, which is obviously an optimal strategy, but not particularly efficient.
- **DepthFirstSearch**, which is not an optimal strategy, and also generally not particularly efficient.
- **AStar**, which is optimal, and as efficient as the heuristic it makes use of is.

## 4.4 rubiks.heuristics

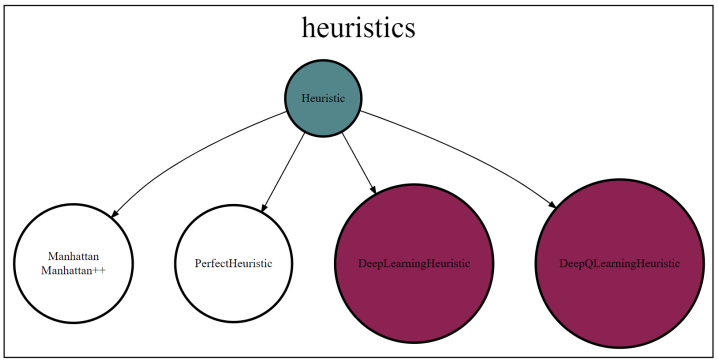


Figure 8: rubiks.heuristics

This module contains base class Heuristic, also a Factory. Heuristic can instantiate the following heuristics, which we can use in the AStar strategy from the previous section:

- **Manhattan**: This heuristic is specific to the **SP**. It adds over non-empty tiles the $L_1$ distance between their current and their target position. This heuristic is admissible: indeeed, each move displaces one (and one only) tile by one position (notice that in other puzzles such as the **RC**, a move might affect multiple tiles). Therefore, if tiles could somehow freely move on top of one-another, the number of moves necessary to solve the **SP** would exactly be the Manhattan distance. Having an admissible heuristic will be useful to ascertain the optimality (or not) of other heuristics based on **DL**, **DRL** and **DQL**.

  I have also implemented an improvement which I call Manhattan++. It can be activated by passing *plus=True* to the Manhattan Heuristic (see example 8.3.4 as well as the 2x5 **SP** performance comparison in 5.1.2). It is based on the concept of linear constraints (see lecture notes from Washington University Richard Korf and Larry Taylor, 2022): when tiles are already placed on their target row or column, but not in the expected order, we need to get them out of the way of one another to reach the goal, which the Manhattan distance does not account for. For instance, in the following 2x3 puzzle, tile 3 needs to get out of the way for tiles 1 and 2 to move left, and then needs to get back in its row, adding 2 to the total cost.

| | | |
|---|---|---|
| 3 | 1 | 2 |
| 4 | 5 | 0 |

Linear constraints across rows and columns (which I generically refer to as *lines*) can be added without breaking admissibility. This is because a tile involved in two linear constraints needs to get out of the way both horizontally and vertically. Also notice that when several pairs on a line are out-of-order, we cannot naively add 2 for each. The right penalty to add needs to be computed recursively. The following configuration for instance with all pairs (1, 2), (1, 3) and (2, 3) out-of-order only inccurs an extra penalty of 4, not 6.

| | | |
|---|---|---|
| 3 | 2 | 1 |
| 4 | 5 | 0 |

It would indeed be enough to get tile 3 out of the way above the puzzle, and tile 2 under the puzzle to let tile 1 pass across. My recursive implementation takes the minimum additional cost of moving either the left-most or the right-most tile of the line under consideration out of the way (that additional cost being 2 or 0, depending on whether or not the tile in question is currently in place) plus the penalty of reordering the rest of the line.

Finally, as suggested in the rather vagues details of Richard Korf and Larry Taylor, 2022, I have precomputed and stored all the penalties for all possible rows, columns and tiles ordering. For memory efficiency, I only saved non-zero panalties. The very first time a call to Manhattan++ is made, for a given dimension nxm, the appropriate linear constraint penalties are computed and saved. For an nxm **SP**, each of the n rows can have $\frac{(n*m)!}{(n*m-m)!}$ different tiles orderings and each of the m columns $\frac{(n*m)!}{(n*m-n)!}$. As a result, my Manhattan++ pre-computations and data-bases are quite manageable, as they grow with n and m much slower than the state space. The number of penalties to compute for $nxm \leq 5x5$ are:

| n | m | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 2 | | 48 | 330 | 3,584 | 60,930 |
| 3 | | | 3,024 | 40,920 | 1,094,730 |
| 4 | | | | 349,440 | 8,023,320 |
| 5 | | | | | 63,756,000 |

Removing 0 penalties, we get the following (quite smaller) data base sizes:

| n | m | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 2 | | 2 | 46 | 1,238 | 32,888 |
| 3 | | | 278 | 7,122 | 328,894 |
| 4 | | | | 40,546 | 1,456,680 |
| 5 | | | | | 8,215,382 |

- **PerfectHeuristic**: this reads from a data base the optimal costs, pre-computed by the PerfectLearner (see below 4.6)
- **DeepLearningHeuristic**: this uses a network which has been trained using **DL** (DeepLearner) **DRL** (DeepReinforcementLearner) or **DQL** (DeepQLearner). See 4.6 for a discussion of these three learners.
- **DeepQLearningHeuristic**: this uses a network which has been trained using **DQL** by the DeepQLearner (see below 4.6). The DeepQLearningHeuristic follows the same interface as the other heuristics, and therefore can be used by A* for instance. It also has an additional method *optimal_actions* that returns the learnt probability distribution over actions for a given puzzle, for use in search algorithms (e.g. **MCTS**) which make use of this to inform their search.

## 4.5 rubiks.deeplearning

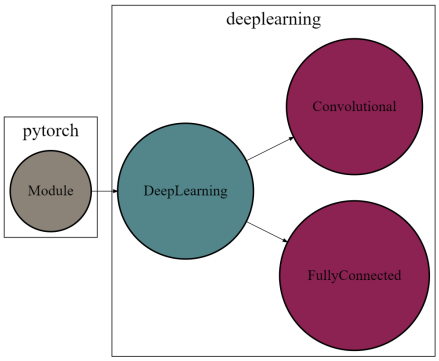


Figure 9: rubiks.deeplearning

This module is a wrapper around Pytorch. It contains:

- **DeepLearning**: a Puzzled Loggable Factory that can instantiate some configurable deep networks, and provide the necessary glue with the rest of the code base so that puzzles be seemlessly passed to the networks and trained on.
- **FullyConnected**: wrapper around a Pytorch fully connected network, with configurable hidden layers and size. Parameters allow to add drop out, to indicate whether or not the inputs are one hot encoding (in which case the first layer is automatically adjusted in size, using information from the puzzle dimension). There is also importantly a *joint_policy* parameter to indicate whether we want the output to be 1 dimensional (e.g. for value function learning) or $a + 1$-dimensional, where $a$ is the size of the actions space (for joint policy-value learning).
- **Convolutional**: similar wrapper to FullyConnected, but with the ability to add some parallel convolutional layers to complement fully connected layers.

## 4.6 rubiks.learners

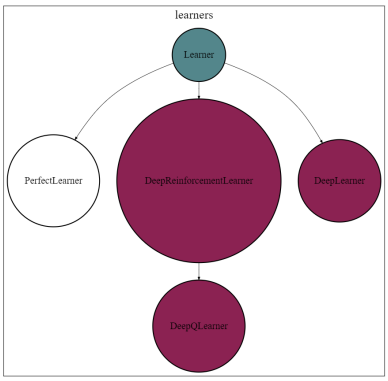


Figure 10: rubiks.learners

This module implements learners, which learn something from a puzzle, store what they learnt, and can display interesting things about what they learnt.

- **Learner** is a Puzzled Loggable Factory. It provides some common code to learners (to save or purge what they learnt), kick off learning and plot results. Concrete derived implementation define what and how they learn, and what interesting they can display about this learning process. The four implemented learners are:

- **PerfectLearner**: It instantiates an optimal solver ($A^*$ with a configurable heuristic - but will only accept heuristic that advertise themselves as optimal. The learning consists in generating all the possible configuration of the considered puzzle, solve them with the optimal solver, and save the optimal cost of it as well as those of the whole solution path. The code allows for parallelization, stop and restart so that we can run on several different occasions and keep completing a database of solutions if necessary or desired. Once the PerfectLearner has completed its job, it can display some interesting information, such as the puzzle's God's number, the distribution of number of puzzles versus optimal cost, the hardest configuration it came across, and how long it took it to come up with the full knowledge of that puzzle. I will show in section 8.2.1 how to run an example. Notice that for puzzles of too high dimension, where my computing resources will not allow to solve exhaustively all the configurations of a given dimension, this class can still be used to populate a data base of optimal costs, which can then be used by DeepLearner. If it is to be used this way, the PerfectLearner can be configured to use perfectly random configurations to learn from, rather than going through the configurations one by one in a well defined order.

- **DeepLearner** DeepLearner instanciates a DeepLarning (neural network), and trains it on training data by minimizing the mean square error between the cost-

to-go from the target solver versus the neural network. The main parameters driving this learner are:

- *training_data_from_data_base* which controls whether the training samples are generated on the fly via another solver (defaults to $A^*[Manhattan++]$ for **SP** and $A^*[Kociemba]$ for **RC**) or read from a data base (similarly constructed from other solvers, but has the advantage of being done offline)
- *nb_epochs* and *threshold* which control exit criteria for the network training.
- *nb_sequences*, *nb_shuffles_min*, *nb_shuffles_max*, *training_data_freq* and *training_data_every_epoch* which control how often we regenerate new training data, how many sequences of puzzles it contais, how scrambled the puzzles should be.
- *learning_rate*, *scheduler*, *optimizer* and assorted parameters which control the optimisation at each backward propagation.

Once it has completed (or on a regular basis), DeepLearner saves the trained network, which can then be used with DeepLearningHeuristic to guide $A^*$.

- **DeepReinforcementLearner**: It instantiates a DeepLearning (network), and trains it using **DRL** essentially following the pseudo-code from 2.4. Unlike DeepLearner, the targets are here generated via value iteration rather than via another solver (teacher). It has very similar parameters to the DeepLearner, in particular some parameters to control exit criteria (same as DeepLearner's plus a few that help it exit early when the value function's range has not been increasing anymore for a while), some parameters to control and configure the optimiser, some to control the training puzzles (how many, how often, how scrambled).

- **DeepQLearner**: The implementation of the DeepQLearner is actually only a few lines of code, for it inherits pretty much all of its behaviour from the DeepReinforcementLearner. The only overwritten functions are:

  - *get_loss_function* which constructs the loss function to be used by the network's training. Instead of returning a simple torch.nn.MSELoss, it returns a function which computes the average of torch.nn.MSELoss on the value-function and torch.nn.CrossEntropyLoss on the actions.
  - *__construct_target__* which performs the the Q-V-iteration to update the targets, as described in pseudo code form in 2.5. This function updates not only the value function of a node given its children nodes, but also updates the optimal action vector (0 for non optimal actions, 1 for the optimal action leading to the child node of highest value function).

### 4.7 rubiks.solvers

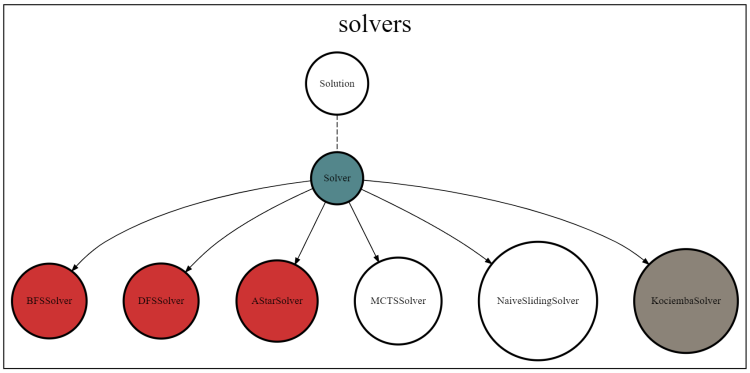


Figure 11: rubiks.solvers

This module implements the actual puzzles solvers. The base class Solver is a Factory, and in addition to being able to instantiating the following types of solvers, can run different solvers through a similal sequences of random puzzles (for various increasing degrees of difficulty (scrambling), and/or perfectly shuffled ones) and display a comparison of how they perform in a number of metrics (configurable from percentage of puzzles solved before time out, percentage of optimal puzzle (if optimality can be ascertained), mean-median-maximum run time, mean-median-maximum expanded nodes (for solvers where it makes sense), mean-median-max cost, and an optimality score which compares the total sum of cost over all puzzles versus a benchmark solver). Ideally the benchmark solver to compute the optimality score should provably optimal, but in the case of the **RC** that was not possible so I used A* with KociembaHeuristic as my benchmark. For the **SP** I used the optimal A* with Manhattan++ heuristic.

- **DFSSolver** This solver is literally a few lines of code, extremely close to the pseudo code detailed in 1
- **BFSSolver** Ditto, see 1
- **AStarSolver** Ditto, see 2
- **NaiveSlidingSolver** The NaiveSolver is conceptually simple, but was far from trivial to implement and debug. Its functioning is detailed in the appendix section 8. Basically, it does what a beginner player would do, certainly what I do when I play the sliding puzzle: solving the top row first, then the left column, hence reducing the puzzle to a smaller dimensional one, and keep iterating until done.
- **KociembaSolver** This solver is a wrapper around two libraries. The first one, hkociemba (see Herbert Kociemba, 2022) is a 2x2x2 implementation written by Kociemba himself, the second one is a Python pip-installable library which solves

the 3x3x3 Rubik's. My wrapper simply translates my cube representation in that accepted by these 2 solvers, and their result string into moves usable by my code. I also do some additional massaging for the 3x3x3 case, due to a shortcoming/bug in the 3x3x3 Python library, as I have detailed in appendix 9.

- **MonteCarloSearchTreeSolver** My implementation follows McAleer & Agostilenni et al McAleer et al., 2018b but is however single-threaded. As a consequence, I dropped the $v$ parameter from their implementation, since it only introduces a penalty to discourage parallel threads from generating the same paths (in single threaded mode, this parameter is inconsequential).
  This solver basically generates *pseudo-random* paths from initial node to a new leaf at each iteration (see 8), until we obtain a goal leaf.Paths are, despite the name, completely deterministic: they indeed result from a trade-off between the probability of actions (penalised for repeated use) and the value function, but there are no random draws being performed.
  As per McAleer & Agostilenni's paper, I have implemented a final pruning via **BFS** of the tree resulting from the above *Monte-Carlo* process.It is inded clear that the paths generated by this **MCTS** algorithm have little chance of being optimal since there is no correction mechanism to favour shortcuts over long loops. I have however made this **BFS** trimming optional via a *trim_tree* parameter to study its effect on solutions' optimality and run time (see results section 5.2.2).
  I will study and report on the effect of the trade-off hyper-parameter $c$, and confirm how it affects solutions' quality and run time in section 5.2.2.

### 4.8 data

The code generates a fair amount of data, in particular:

- Manhattan++ generates databases of linear constraint penalties (see 4.4)
- TrainingData: (see e.g. 8.2.2) generates databases of puzzles and their associated costs for later training of a DeepLearner.
- Learners: DeepLearner, DeepReinforcementLearner, DeepQLearner generate models as well as some convergence data useful to understand how the networks learn. Similarly PerfectLearner saves its results for later reuse (in e.g. PerfectHeuristic) or display.
- Solver: Generates sequences of scrambled puzzles used to make the performance test (comparing different solvers) fair.
- Solver.performance_test: Generates a data frame containing the metrics discussed earlier in 4.7, for each solver and each level of difficulty.

That data is saved under a tree following the schema below:

$$\$RUBIKSDATA/data_type/puzzle_type/dimension/file_name.pkl$$

# 5 Results - Sliding Puzzle

I now discuss results on the **SP**, going from *small* dimensions (which I can reasonably *fully* solve given my computing resources, the finite time I have to complete this project, and the choice of programming language), then I move to studying in detail the 3x3 **SP**, and finally move to higher 3x4 and 4x4 dimensions. Table 1 shows which solvers I have run on each dimension. The reader is referred to the theory (2) and implementation (4) sections for details on each solver, and to the appendix section 8 for code examples.

| **solver** | **Sliding Puzzle** | **2x2** | **2x3** | **2x4** | **2x5** | **3x3** | **3x4** | **4x4** |
|---|---|---|---|---|---|---|---|---|
| BFS | | | | | | x | | |
| A*[Manhattan] | | | | | x | x | x | |
| A*[Manhattan++] | | | | | x | x | x | x |
| A*[Perfect] | | x | x | x | x | x | | |
| Naive | | | | | | x | x | x |
| A*[DL[FullyConnected]] | | | | | | x | x | x |
| A*[DL[Convolutional]] | | | | | | x | | |
| A*[DRL] | | | | | | x | x | x |
| A*[DQL] | | | | | | x | | |
| MCTS[DQL] | | | | | | x | | |

Table 1: Solvers used vs **SP** dimension

I am not making claims of depth (each solver could be tuned and optimized much further) nor breadth (I have not run all solvers versus all dimensions). These experiments take a lot of computing time, so I had to be somewhat selective. I wanted however to run all of the solvers on at least one particular dimension (3x3 seemed appropriate) to try and answer, even if not in generality, as many of the following interesting questions:

- How hard is too hard for **BFS** to complete in *reasonable* time?
- How much, if any, improvement do we get with Manhattan++ over Manhattan?
- Does **DL** perform much better than **DRL** due to supervision?
- Is **DQL**, all things being equal, able to learn a better value-heuristic than **DRL**?
- How does **MCTS** perform? How important is it to tune the hyper-parameter $c$? How much improvement does the final **BFS** tree-trimming bring?
- Are the **D*L** heuristics competitive versus Manhattan++ or the perfect heuristic?

## 5.1 Low dimension

### 5.1.1 God numbers and hardest puzzles

As mentioned in chapter 3, the state space cardinality for the **SP** grows quickly with n and m. The only dimensions which have less than 239.5 millions states are shown in table 2.

| n | m | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 2 | | 12 | 360 | 20,160 | 1,814,400 |
| 3 | | | 181,440 | | |

Table 2: # puzzles for *small* dimensions

Using my PerfectLearner with A* and Manhattan heuristic (see 8.2.1 for example of how to run this), I obtained the following God numbers (table 3) for these dimensions:

| n | m | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 2 | | 6 | 21 | 36 | 55* |
| 3 | | | 31 | | |

* provisional result

Table 3: God numbers for *small* dimensions

Among those dimensions, 2x5 has the largest state space and my result for it is still provisional, as I have only solved about 1.2 out of 1.8 million puzzles at the time of writing, despite running a combined 600 hours (mostly over 16 cores, except for a full week-end run on a 72-core c5.18xlarge Amazon EC2 instance). It is well possible that I haven't yet bumped into the hardest 2x5 configuration! The perfectLearner also keeps track of the hardest puzzle it has encountered (i.e. a configuration whose optimal solution has a cost equal to the God number). I obtained the following hardest puzzles for each of the 5 *small* dimensions:

| | |
|---|---|
| | 3 |
| 2 | 1 |

| | | | | |
|---|---|---|---|---|
| | 9 | 3 | 7 | 1 |
| 5 | 4 | 8 | 2 | 6 |

| | | |
|---|---|---|
| 4 | 5 | |
| 1 | 2 | 3 |

| | | |
|---|---|---|
| 8 | 6 | 7 |
| 2 | 5 | 4 |
| 3 | | 1 |

| | | | |
|---|---|---|---|
| | 7 | 2 | 1 |
| 4 | 3 | 6 | 5 |

### 5.1.2 Manhattan heuristic

Next, I verify empirically that, as expected, the overhead of adding penalty in Manhattan++ for the linear constraint is compensated for by the reduction in nodes expansion. I have run my solver script for 2x5 in performance test mode, for both Manhattan and Manhattan++, with 250 randomly shuffled puzzles with *nb_shuffles* from 0 to 60 by increment of 5, as well as with *nb_shuffles* = inf. The resulting run time and nodes expansions are shown in table 12:

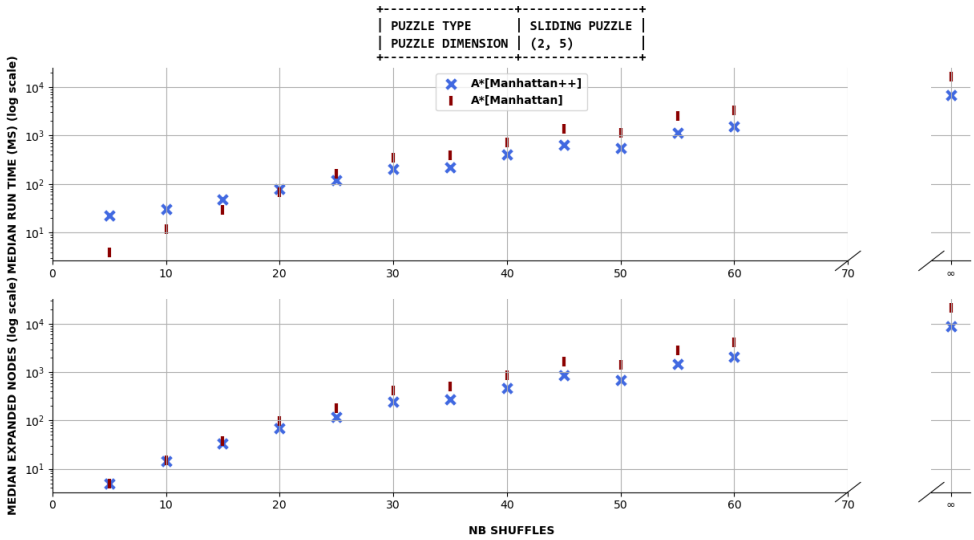


Figure 12: Manhattan vs Manhattan++ for the 2x5 **SP**

For low difficulty (*nb_shuffles* $\leq$ 20), the node expansions are about the same in both cases, and the overhead of adding the linear constraints penalty increases the run time. However, for harder puzzles, Manhattan++ considerably outperforms, by a factor of 2.5+. Table 4 below summarizes the results for the 250 *perfectly* shuffled configurations:

| | avg cost | max cost | avg nodes | max nodes | avg run time (ms) | max run time (ms) |
|---|---|---|---|---|---|---|
| Manhattan | 34.6 | 49 | 46,483 | 575,050 | 36,088 | 428,887 |
| Manhattan++ | 34.6 | 49 | 18,780 | 213,557 | 14,665 | 165,830 |
| Improvement | n/a | n/a | **x2.5** | **x2.7** | **x2.5** | **x2.6** |

Table 4: Manhattan++ outperformance on perfectly scrambled 2x5 **SP**

## 5.2 Intermediary case - 3x3

In this section, which focusses on the 3x3 **SP**, I detail some results from the PerfectLearner (5.2.1) before moving to a discussion of the **DQL MCTS** solver and the effect of its trade-off hyper-parameter $c$ and of its optional **BFS** tree-trimming on the

quality of the solutions (5.2.2). I then run a comprehensive comparison of my 10 different solvers on the 3x3 **SP** in 5.2.3 including **DL**, **DRL** and **DQL**. Finally, I end the section by running a few select solvers on one of the two hardest 3x3 puzzle in 5.2.4

### 5.2.1 Perfect learner

As discussed in the previous section section 5.1, the 3x3 **SP** is one of the cases I have been able to solve perfectly, since it only has 181,440 possible configurations. Its God number is only 31, which definitely makes it manageable. However, this is already an intermediary size, large enough that it is worth trying and comparing a few different methods, including **DL**, **DRL** and **DQL**. To start with, I ran the PerfectLearner and the results are shown below in figure 13. It is interesting to note that there are only two hardest configurations (of cost 31) and 221 configurations of cost 30.

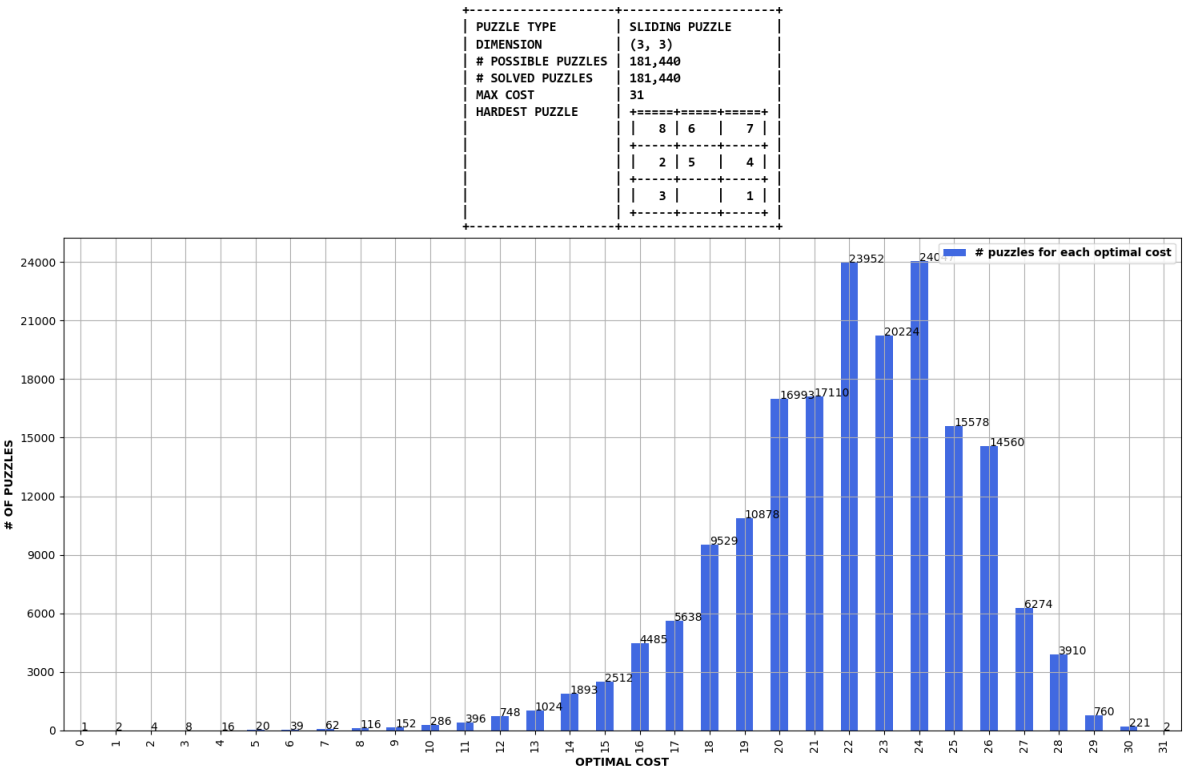


Figure 13: Perfect Learning of the 3x3 **SP**

### 5.2.2 MCTS DQL

In this subsection I explore the effect on **MCTS** of the trade-off hyper-parameter $c$ as well as of trimming the resulting tree via **BFS**. (see the threory section 2.6 as well as the implementation section 4.7 for more details). To that effect, I have run my Solver

performance test with four different values of $c$ (0, 1, 10 and 100), and in each case, with and without **BFS** trimming. $A^*[Manhattan++]$ is also presented to have an optimal solver benchmark. For each level of difficulty, the test present the solvers with the same 150 random configurations (for fairness and to increase the significance of the results). The levels of difficulty (number of scrambles from goal) used here go from 5 to 50 in step of 5. The tests were also run with perfect shuffling (difficulty = $\infty$ on the graphs), corresponding to taking scrambling to $\infty$ as explained in 3.1.2). I used a *time_out* of 5 minutes, which none of the solvers hit on any of the (1,650) configurations they were presented with. The detailed results (percentage of configurations solved, optimality score, median and max cost, run time and expanded nodes) are shown on the next page 14, but let me make here some remarks on those results:

- $c = 0$ makes no exploration as it simply follows the path of lowest cost-to-go. As $c$ increases, we expect more exploration, and therefore higher run time, more expanded nodes, and higher quality solutions. This is what we observe, where $c = 0$ converges (for difficulty=$\infty$) to solutions on average three times longer than the optimal solver but take not much longer to obtain. At the other extreme, $c = 100$ takes almost 2 orders of magnitude more time to obtain a solution, but these solutions are only 20-25% longer than that of the optimal solver

- trimming via **BFS** takes hardly any time, and improves solutions' lengths by about 10% at high values of $c$. At low value of $c$ there is little benefit as expected (since the trees are deep but not bushy at all and have much fewer leaves and branches).

- The quality of solutions is not amazing, but then given the algorithm has not really any mechanism to guarantee optimality this is not very surprising.

- Notice that the number of expanded nodes can be compared within **MCTS** but given the algorithm is totally different to $A^*$ it makes little sense to compare between the different families of solvers. Also one point to note is that **MCTS** would be fairly easy to multithread (within the same process) using an appropriate language such as C++, and this is what McAleer et al., 2018b have done, and probably why they get considerably faster and better results.

- Despite the name *Monte Carlo*, there is no randomness (or even peudo-randomness) in this algorithm, since the paths generated at each iteration are really just a deterministic function of the output of the **DQL** network (or QHeuristic in my code-jargon).

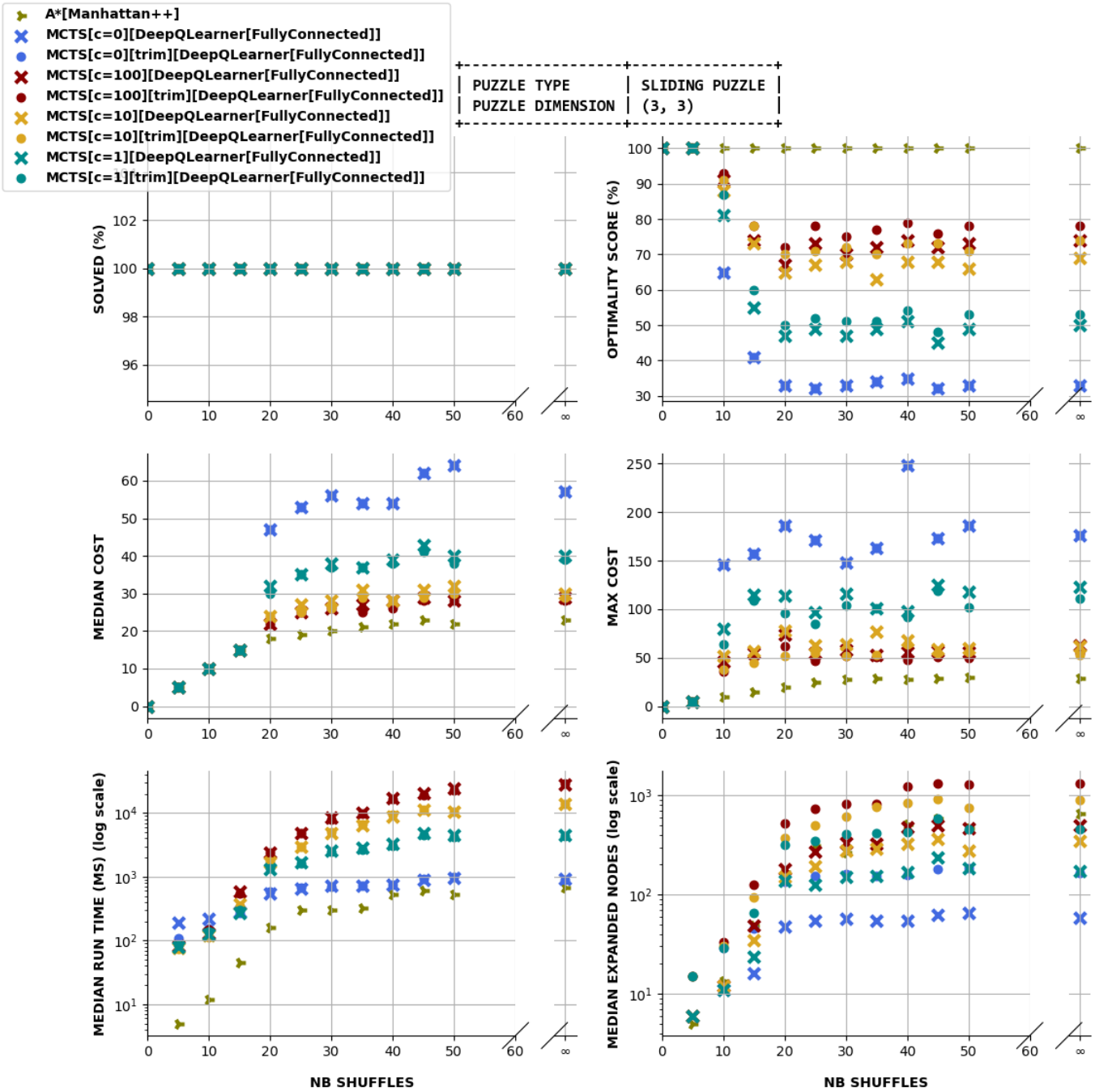


Figure 14: **MCTS** tuning 3x3 **SP**

### 5.2.3 Solvers' comparison

As promised earlier in table 1, I have run the Solver's comparison test with 10 different solvers (Naive, **MCTS**, **BFS**, A* with the following heuristics: Manhattan, Manhattan++, Perfect, **DRL**, DQL and DL), to get an idea of their respective success rate, strengths and weaknesses. The **DRL** and **DQL** heuristics were trained with the exact same parameters and a fully connected network of 3 hidden layers with 600, 300 and 100 nodes. For the **DL** heuristic (trained on perfect solutions from A*[Perfect]) I tried with the same fully connected network as well as with a combination of parallel fully connected and convolutional layers (see figure 15 for the exact architecture I used). The detailed results (percentage of configurations solved, optimality score, median and max cost, run time and expanded nodes) can be found on the next page in figure 16. Each solver had to solve 1,000 random puzzles for each level of difficulty (scrambling from goal) going from 5 to 50 in step of 5, as well as for perfect shuffling. Let me list some of the important findings from this rather comprehensive experiment:

- As expected, **BFS** becomes quickly hopeless.
- The naive solver is obvioulsy by far the fastest but finds poor solutions (about 2.5 longer on average than optimal).
- As discussed in the previous section, **MCTS** is slow, and even with much exploration and **BFS** tree trimming found solution about 25% longer than optimal.
- I originally was naively hoping a pure convolutional network would do well but did not manage to get the loss to converge. I later realized that this is quite different from the typical image patterns recognition as there is less direct translation and scale invariants at play here, and decided instead to try combining convolutional with fully connected layers in parallel in order to appropriately value 2x2 patterns together with their position on the sliding-puzzle. That did improve things, but overall I saw little difference in performance from my simpler 3-hidden-layer fully connected network.
- **DRL** and **DQL** heuristics, though not as efficient in terms node-expansion as the perfect and the **DL** heuristics, were rather surprisingly doing better than Manhattan++. They ended up *seeing* around 25% of all the possible configurations during training (in an *unsupervised* way though) so did show some reasonable amount of out-of-sample generalization. Their optimality score was an impressive 99%+ at all levels of difficuly for **DRL** and 98%+ for **DQL**. Even more interestingly, the **DQL** heuristic expanded almost 4 times less nodes than **DRL**, suggesting some benefit from the joint learning of the policy and value function.
- The **DL** heuristics (fully connected and convolutional) performed almost on par with the perfect heuristic (optimality score of 99%+ at all levels of difficulty and nodes expansion only increased by about 12%), despite seeing only 8% of the configurations by the end of their training.

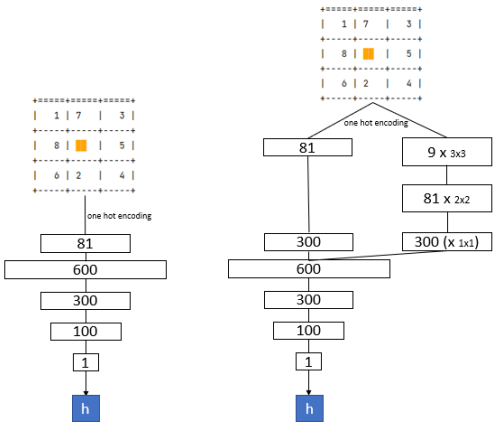


Figure 15: Architecture I used for the **DL** heuristics training on the 3x3 **SP**

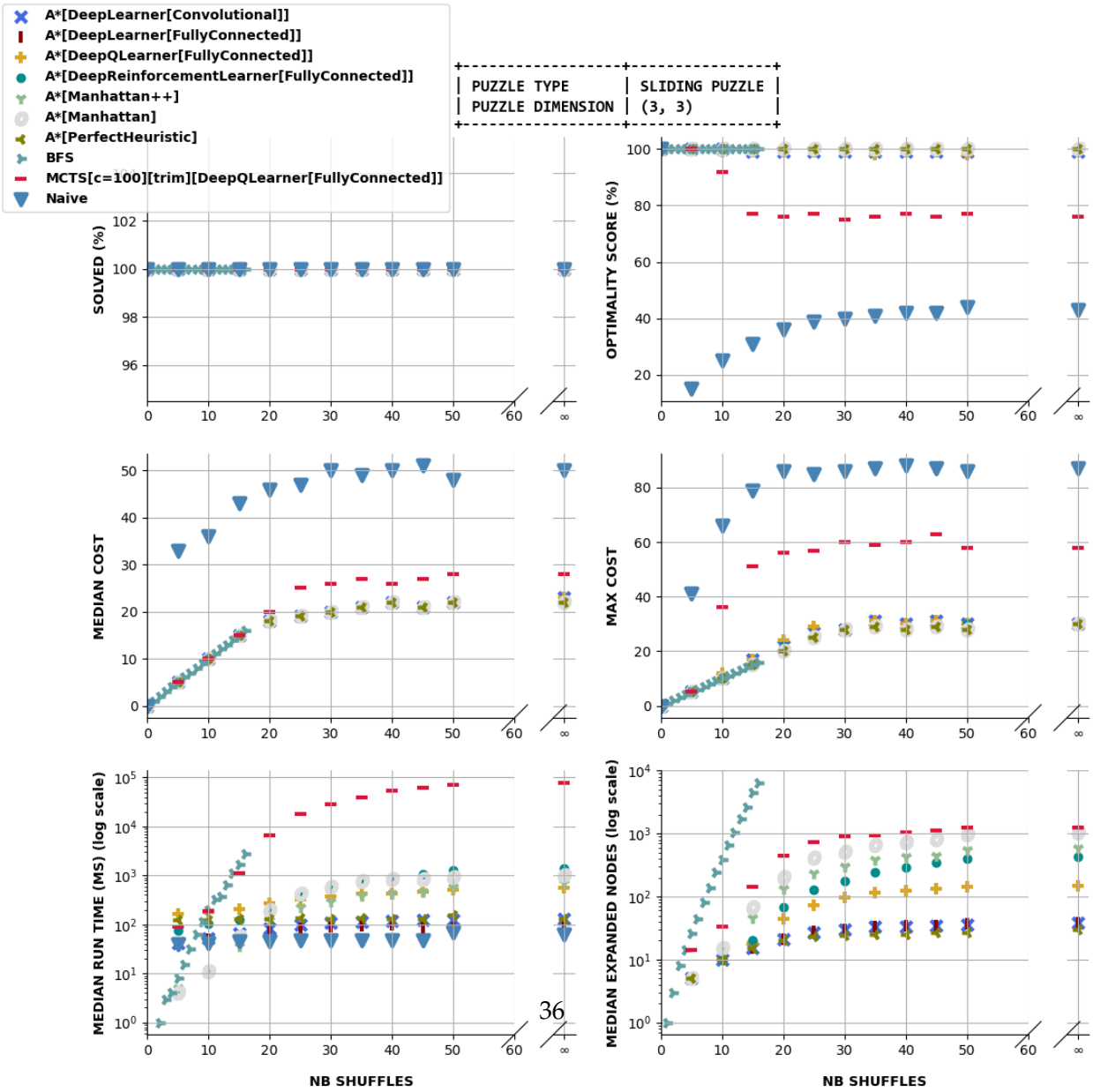


Figure 16: Solvers' performance comparison 3x3 **SP**

### 5.2.4 Solving the hardest 3x3 problem

To finish with the 3x3 SP, let me try to throw one of the two hardest 3x3 configurations (see subsection 5.1) at the different solvers to see how they fare. The results are shown here

| solver | cost | # expanded nodes | run time (ms) |
|---|---|---|---|
| AStarSolver[Manhattan] | 31 | 58,859 | 11,327 |
| AStarSolver[Manhattan++] | 31 | 34,224 | 7,080 |
| AStarSolver[PerfectHeuristic] | 31 | 1,585 | 202 |
| AStarSolver[DRLHeuristic] | 31 | 101 | 58 |
| MCTSSolver[DQLHeuristic][c=0] | 101 | 103 | 456 |
| MCTSSolver[DQLHeuristic][c=69] | 35 | 2,244 | 8,873 |
| BFS | - | - | time out |
| NaiveSlidingSolver | 61 | n/a | 18 |

On this specific configuration, **BFS** was unable to complete before the time-out of sixty seconds. In an implementation without duplicate pruning, **BFS** would time out no matter what the bound is set. Indeed, it would need to explore in the order of $3^{31}$ - roughly 617 trillions - nodes to reach the goal! Even with my implementation which does pruning, it would need to pretty much traverse the entire 3x3 **SP** tree.
Rather interestingly, the **DRL** heuristic performs much better than the Manhattan heuristic (not super suprising), but also outperforms the perfect heuristic quite significantly both in terms of run time and of nodes expansion. Obviously there is no guarantee that the perfect heuristic will not be outperformed on some random configuration, and it does on this occasion. However, as we have seen in the previous subection 5.2.3, it is not the case on average.
**MCTS** with $c = 0$ performs rather poorly, finding the longest solution (even than my Naive solver). It does behave a bit like **DFS** when $c$ is very small, expect the direction of travel is a bit more informed. I increased $c$, and for values over 69, it always gave me a solution of cost 35, which is not bad at all.
Finally, the naive solver outperforms every other solver in terms of run time, but finds a rather poor solution of 61 moves.

## 5.3 3x4

For the 3x4 **SP**, I ran the performance test (100 random puzzles for difficulty going from 1 to 45 as well as $\infty$ shuffling) on the Naive solver and A* with Manhattan, Manhattan++, **DRL**, **DQL** and **DL** heuristics. Given the 239,500,800 total possible configurations there was no chance for me to compute the perfect heuristic as I did with smaller dimensions, so **DL** got trained on randomly generated configurations solved by A*[Manhattan++]. The network architecture for all **DxL** was the fully-connected (left-hand-side of figure 15), mutatis-mutandis for the input size, which in the general case is $(n.m)^2$ when using one-hot-encoding (I always did after a few unsuccessful attempts without it). Detailed results can be found at 17. Key take-aways are that all **DxL**

outperformed A*[Manhattan++] in terms of node expansion and got optimality scores of 99%+ for all levels of difficulty, despite only seeing 0.009% of all configurations for **DL**, and 0.27% for **DRL** and **DQL**. Again this shows very impressive generalisation and performance from the**DxL** methods.

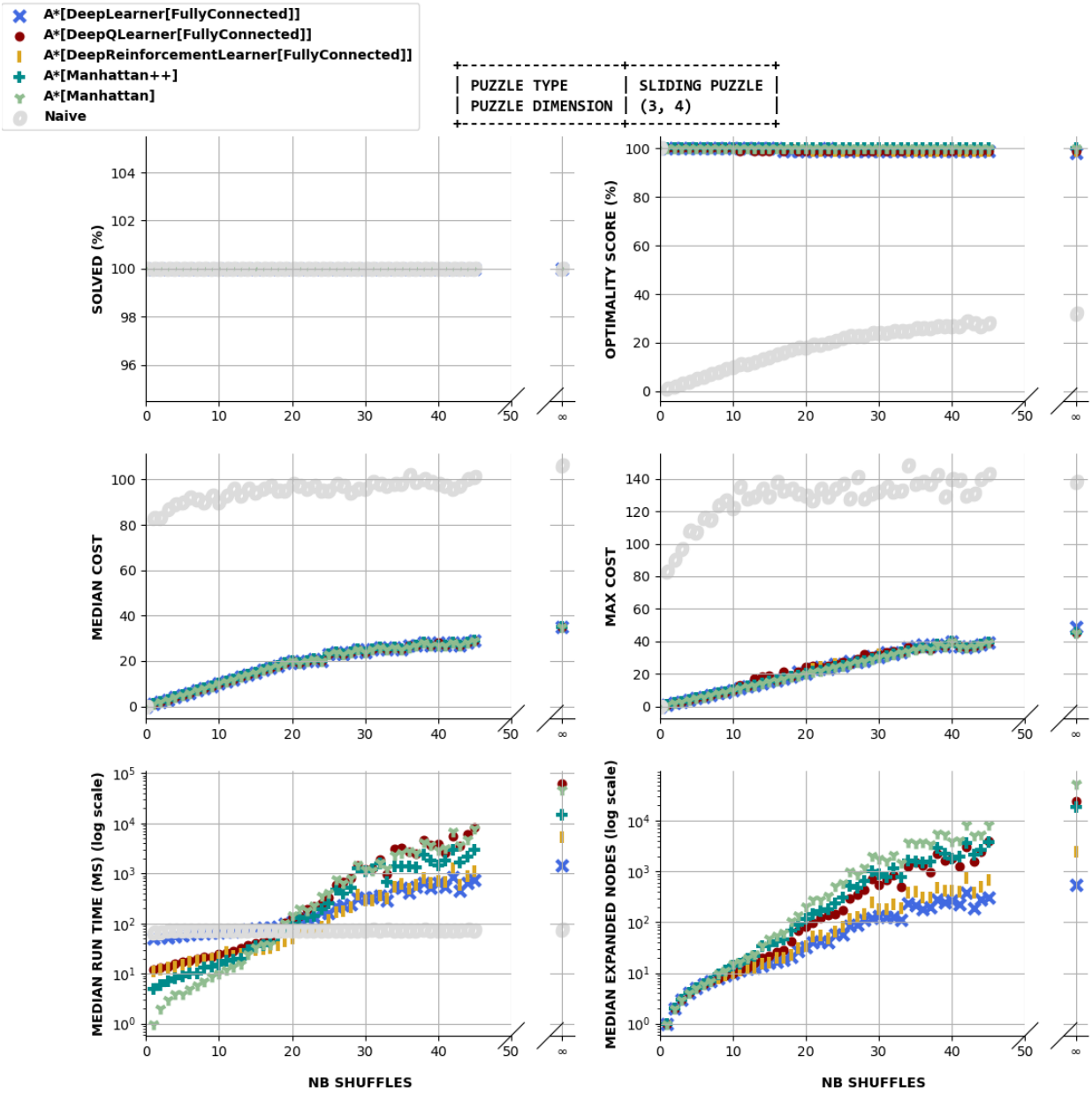


Figure 17: Solvers' performance comparison 3x4 **SP**

### 5.4 4x4

In the 4x4 case, due to time constraints, I ran the performance test with 100 random puzzles for difficulty going from 5 to 60 except for ∞ shuffling where I only ran a handful of configurations (5). I ran the Naive solver as well as A* with Manhattan++, **DRL** and **DL** heuristics, again using the same fully-connected network architecture (left-hand-side of figure 15). The 4x4 **SP** has 10,461,394,944,000 total possible configurations so it does start being quite a large state space! Again **DL** got trained on randomly generated configurations solved by A*[Manhattan++]. **DL** obtained an optimality scores of 97%+ across all levels of difficulty and **DRL** managed 99%+. **DL** and **DRL** saw of the order of respectively $10^{-7}$% and $10^{-5}$% of all configurations during training, so again showed impressive performance and generalization!

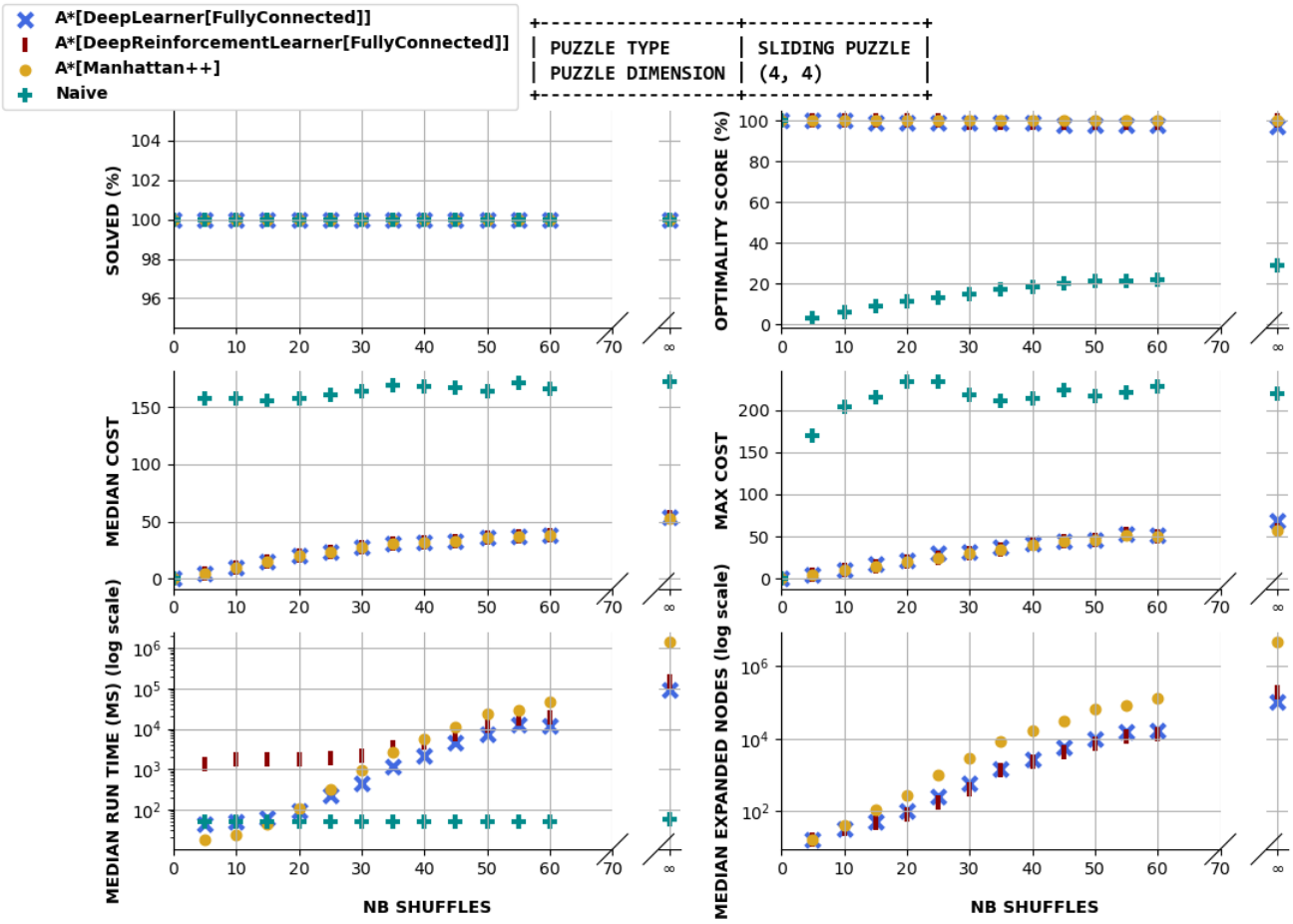


Figure 18: Solvers' performance comparison 4x4 **SP**

# 6 Results - Rubik's Cube

I now discuss my experiments on the Rubik's cube. I have run reasonably comprehensive trial on the 2x2x2, throwing 6 of my solvers at the problem. As mentioned in 3, the 2x2x2 **RC**, in spite of its deceivingly simple physical appearance, is actually not that much easier to solve (by hand) than the 3x3x3. For instance, it takes me usually just under one minute, versus two minutes for the 3x3x3. I am obviously no *speedcuber*, but my time-to-solve and perceived difficulty ratios are in line with that of experienced players who might take 2-3 seconds for the 2x2x2 and 10 seconds for the 3x3x3. Computing wise, the 2x2x2 was of decent size for my purpose, with its 88 million configurations. Table 5 summarizes which solvers I have attempted to run on the 2 dimensions:

| **solver** | **Rubik's** | **2x2x2** | **3x3x3** |
|---|---|---|---|
| BFS | | x | x |
| Kociemba | | x | x |
| A*[Kociemba] | | x | x |
| A*[DL[A*[Kociemba]]] | | x | x |
| A*[DRL] | | x | |
| A*[DQL] | | x | |

Table 5: Solvers used vs **RC** dimension

## 6.1 2x2x2

All the following experiments on the 2x2x2 **RC** have been run using my Solver's *performance_test* (see 4.7): for each level of difficulty, the test present the solvers with the same 100 random configurations (for fairness and to increase the significance of the results). The levels of difficulty (number of scrambles from goal) used here go from 2 to 20 in step of 2. The tests were also run with perfect shuffling (difficulty = $\infty$ on the graphs), corresponding to taking scrambling to $\infty$ as explained in 3.2.4).

### 6.1.1 BFS

For **BFS** I used a step of 1 on the difficuly and stopped at 5 as it was clear it would not go much further. Its run time and expanded nodes are increasing linearly with difficulty, and it was already taking an average close to a minute for 5 shuffles from goal.

### 6.1.2 Kociemba, A*[Kociemba], A*[DL[A*[Kociemba]]]

I obviously expected Kociemba (see Herbert Kociemba, 2022 and Tsoy, 2019) to be by far the fastest solver since it is handcrafted with much specific knowledge about the **RC** group theory and multi-stage solving (see section 3.2.5). Contrary to its claims, I found the 2x2x2 library to not be optimal, running A* with Kociemba's cost as a heuristic indeed resulted in shorter solutions. I did however set Kociemba as my benchmark

in the *performance_test* since I had no admissible heuristic to guarantee optimality otherwise. The optimality scores (top-right graph of figure 22) therefore do reach more than 100%, as all other solvers found shorter solutions than Kociemba. I used the solutions of A*[Kociemba] on perfectly randomly generated configurations to train the **DL** heuristic. Since Kociemba is itself using a two-stage IDA* solver, I end-up here with 3 levels of nested A* algorithms: A*[DL[A*[IDA*[2-stage-subgroups]]]]!

### 6.1.3 Deep Reinforcement Learner & Deep Q Learner

To get my **DRL** and **DQL** heuristics, I have run the DeepReinforcementLearner and DeepQLearner with the following main parameters:

- Update the target network every 1,000 epochs (*update_target_network_frequency*) or when $\frac{MSE}{maxtarget}$ falls below 0.1% (*update_target_network_threshold=1e-3*)
- Stop at *nb_epochs*=11,000 or if the max target has not increased more than 1% (*max_target_uptick*) in the last 5,500 epochs (*max_target_not_increasing_epochs_pct*=0.5)
- At each target net update (*training_data_every_epoch*=False), generate *nb_sequences*=10,000 sequences of puzzles comprised of a 15-scramble puzzle along with its path to goal (*nb_shuffles*=15).
- Fully connected network (*network_type=fully_connected_net*) with three hidden layers (*layers_description*=(600,300,100)), an RMSProp optimiser (*optimiser=rms_prop*), *scheduler=exponential_scheduler* with *gamma_scheduler*=0.9999 and *learning_rate*=0.1%. The networks architecture are shown in figure 19.

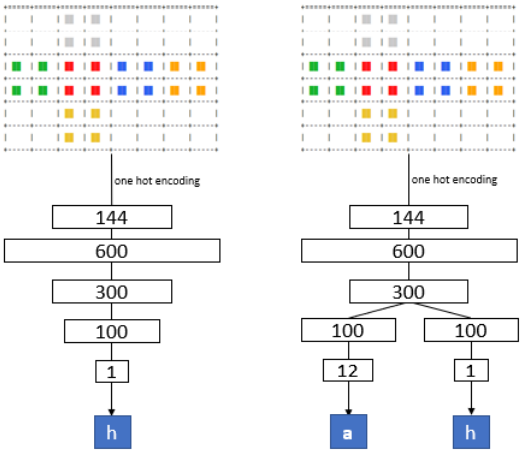


Figure 19: 2x2x2 **RC** architecture for **DRL** (left) & **DQL** (right) heuristics training

Graphs 20 and 21 show both learners' following metrics tracked over the epochs:

- learning rate: decreasing due to the scheduler and reset at each network update.
- max target: an interesting dynamic during learning is that since targets are constructed using value-iteration update, starting from an all 0 network, the max target increases by at most about 1 at every network update, until we reach God's number. The first network only learns to differentiate goal from non-goal, the second one learns how to differentiate goals, cost 1 and cost 2+ .... This is why I introduced *update_target_network_threshold* discussed above, to makes sure we do not spend time initially training the left-hand-side network when it is easy. *max_target_uptick* and *max_target_not_increasing_epochs_pct* make sure that we stop training when the max target does not grow anymore.
- loss: MSE for **DRL**, MSE + CrossEntropyLoss for **DQL**
- loss divided by max target: the exit criterion *update_target_network_threshold* is based on that quantity, since a loss of e.g. 1% means little if the we do not compare it to the possible range of the cost-to-go.
- The percentage of all the possible puzzles of that dimension *seen* by the learner. This is an interesting quantity, as it tells us how well the solvers are able to generalise. From both graphs (20 & 21) we can see that the learners saw less than 1% of all puzzles. It is good to keep in mind however that *seen* does not mean really much here, since the learning is *unsupervised*. This is quite in contrast to the DeepLearner, whose traiing data consist of puzzles with their cost-to-go computed by a *teacher* (optimal or other efficient solver).

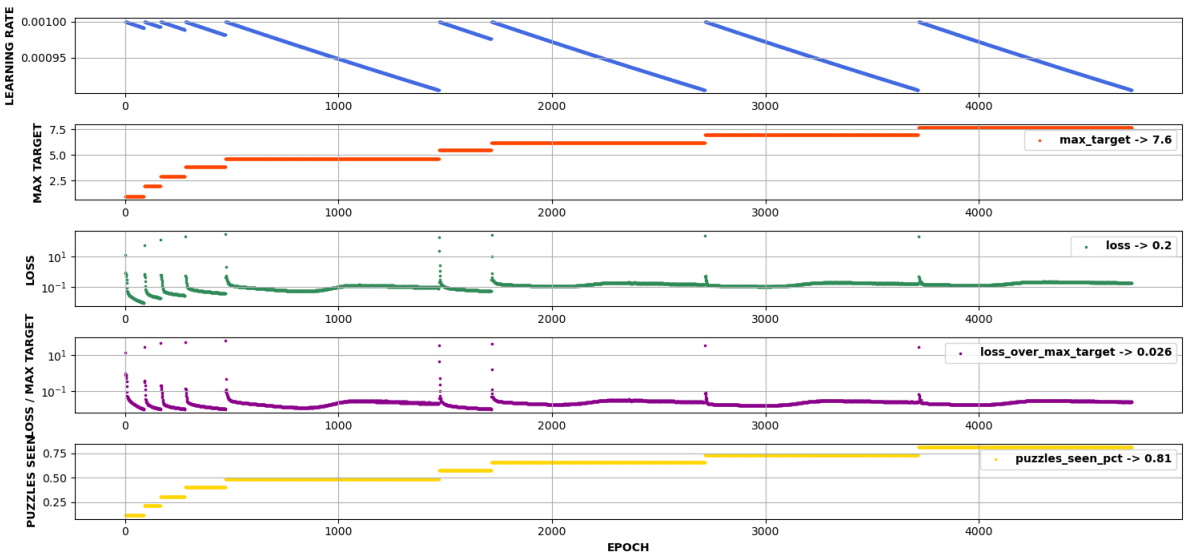


Figure 20: **DRL** of the 2x2x2 **RC**

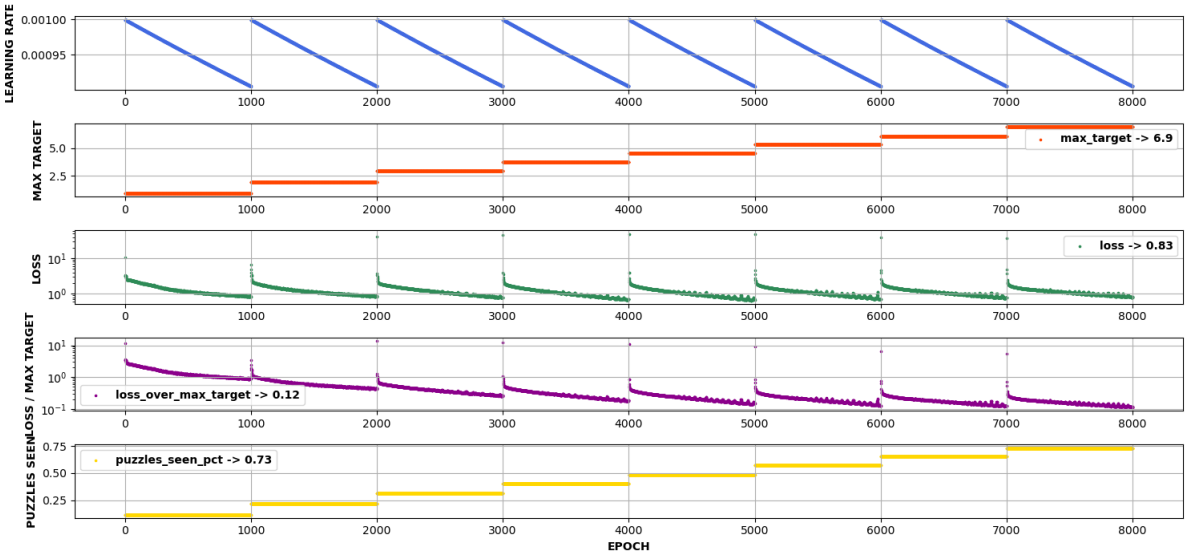


Figure 21: **DQL** of the 2x2x2 **RC**

### 6.1.4 Solvers' comparison

I summarize as usual the 2x2x2 **RC** performance tests with my usual metrics in figure 22. Overall, the **DL** and **DRL** managed to solve all cubes (though **DL** took over an hour and **DRL** 6 hours for their slowest cube. Both methods outperformed Kociemba in terms of optimality-score and got on par with A*[*Kociemba*]. Their max cost over all cubes encountered was 12 for up to 20 shuffles, and 13 for $\infty$ shuffling. Considering God's number for the 2x2x2 **RC** of 11, this is rather impressive!

Quite remarkably we can see (second graph of 20) that the **DRL** heuristic only ever assigned a cost-to-go of 7.6 at most. Despite that, it was still able to solve cubes requiring up to 13 moves (likely to have been among the hardest 2x2x2 cubes). How is that possible? Notice that the loss of 0.2 towards which the network converged at the end of its training is misleading, since this is in-sample loss versus the target network. My theory is that while the value the **DRL** assigned to hard-to-solve cubes can be off (by at least 4 or 5), it is likely that the network gets the relative value of neighbouring cubes right (not that surprising given the value-iteration), and this is sufficient to guide A* extremely well. If both the absolute value of the cost-to-go and the relative (among neighbouring cubes) was totally off, we would indeed not expect the heuristic to make A* any better than, say, **BFS** and we would therefore not expect it to be able to solve *costly* cubes requiring 10+ moves.

Finally, we can see that **DQL**, despite showing visually cleaner and more monotonic loss convergence than **DRL** (see 21 versus 20), struggled a lot more to solve difficult cubes (above 10 shuffles). This shows that my earlier findings on the 3x3 **SP** are likely

not universal, and very much depend on the parameters set during training, as well as on the problem at hand.

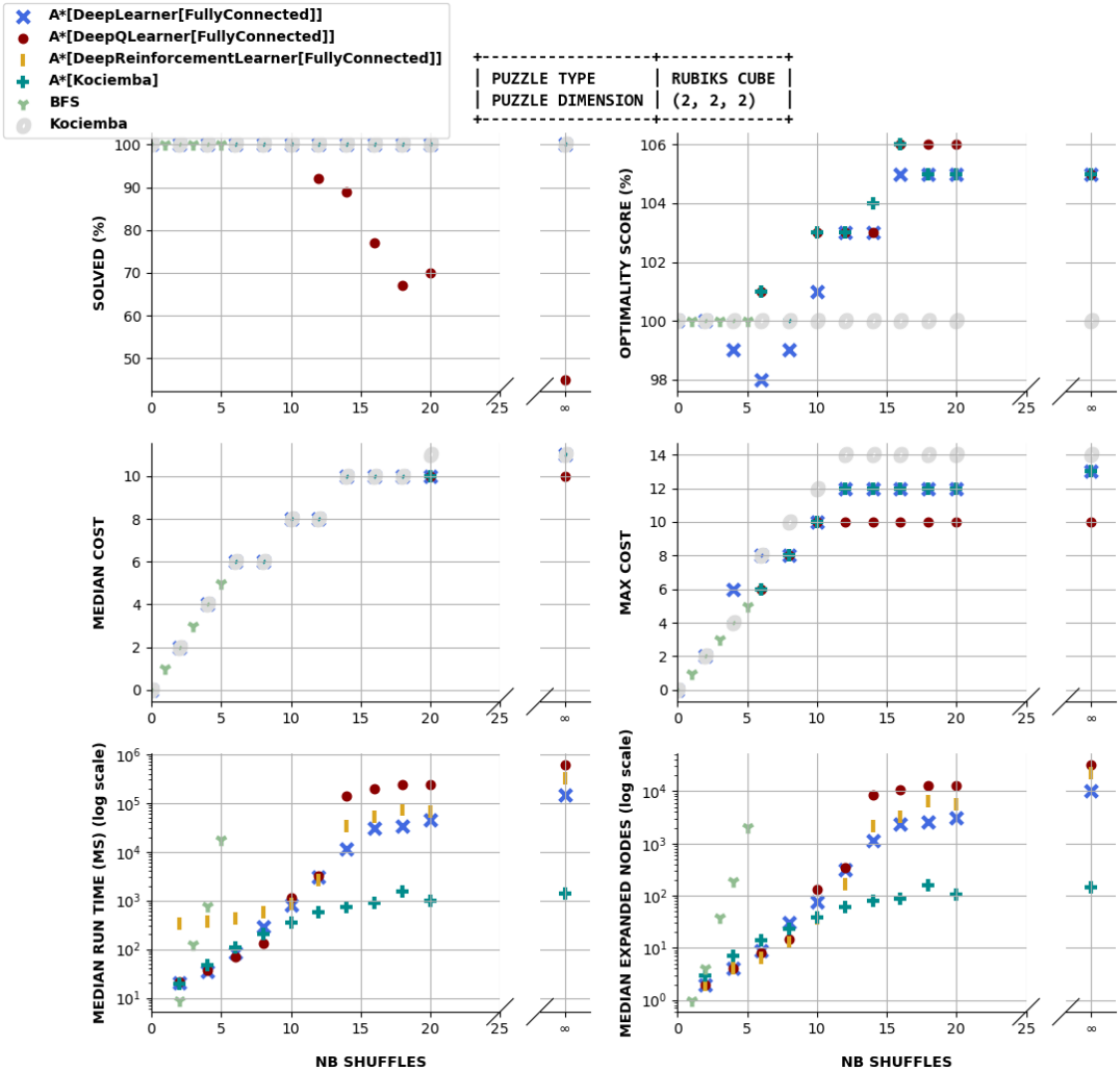


Figure 22: Solvers' performance comparison 2x2x2 **RC**

## 6.2 3x3x3

I did not get to run very many experiments on the 3x3x3 **RC**. The results of the performance test (50 random configurations for levels of difficulty from 2 to 40 by increment of 2 as well as ∞ shuffling) can be found on figure 23.

- Here again, Kociemba does not show optimality, since we can see that my A*[*Kociemba*], that is A* using Kociemba as a heuristic, performs much better

than Kociemba (solutions about 20% shorter at ∞ shuffling). This is not surprising though since Kociemba 3x3x3 does not claim to be optimal and is meant to find solution in the 40 moves at most (which is what I have observed indeed). A*[*Kociemba*] never took more than 30 moves on any of the cubes presented to it, which is not bad given the known God number of 26 in the quarter-turn-metric (as discussed earlier in 3.2.3)

- A*[**DL**] managed to solve all puzzles scrambled less than 10 times, and found shorter worst case solutions than even A*[*Kociemba*] on which it was trained. Within the 2 hours time out, it failed to solve one of the 50 cubes for difficulty 10, and two of the 50 cubes of difficulty 12, so i did not try further than that.
- A*[**DRL**] only managed to solve all puzzles of difficulty less than 6 but at least did find only optimal solutions (compared with **BFS**).

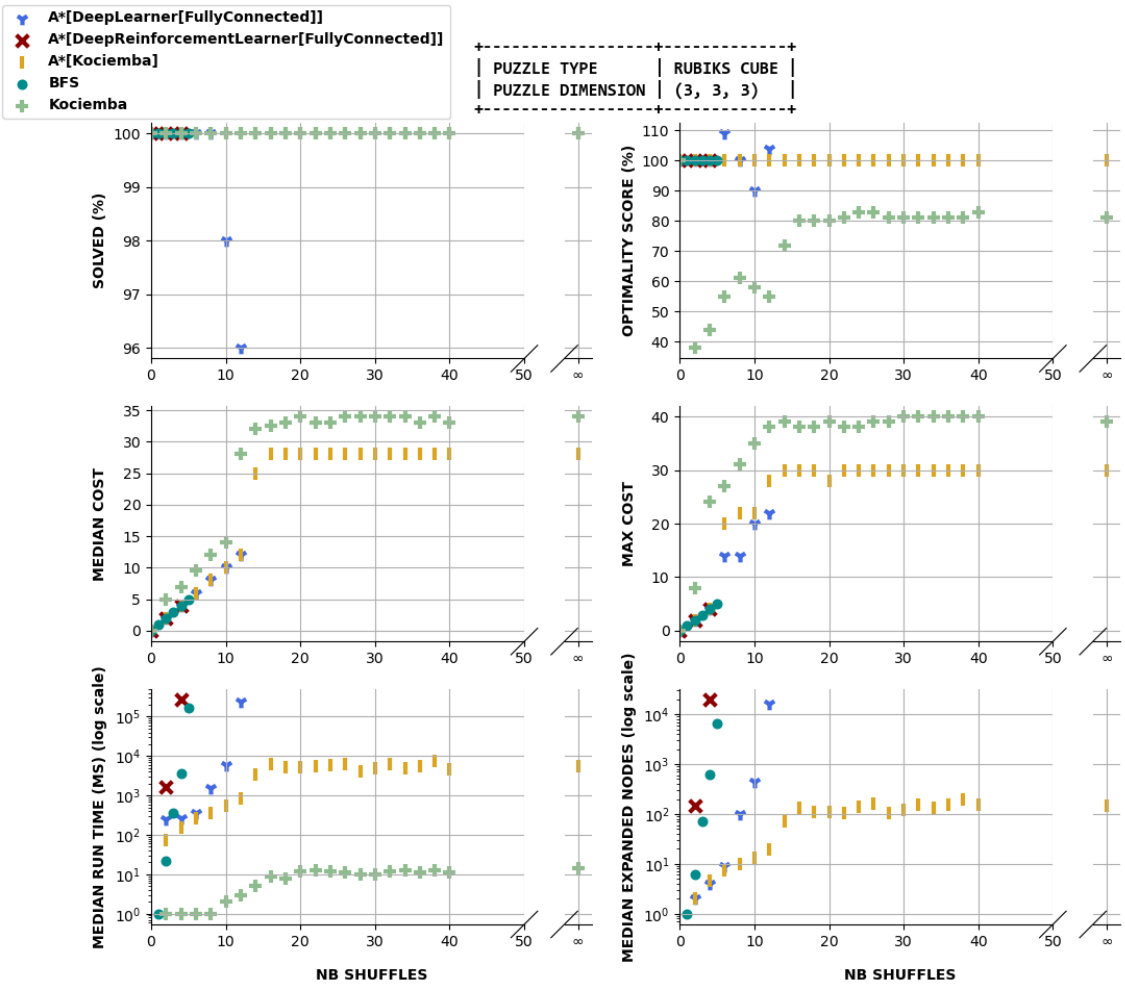


Figure 23: Solvers' performance comparison 3x3x3 **RC**

# 7 Conclusion & Professional Issues

## 7.1 Learning

Working on this project has been overall a lot of fun. Even setting aside implementation and computer-experimentation for a moment, I have learnt a great deal about puzzles in general and how to approach thinking about them in a more structured fashion. Specifically about the Rubik's cube, I have even spent the time to learn a few algorithms that are sufficient to solve them by hand. I am now able to solve the 2x2x2 under one minute, 3x3x3 usually around 2 minutes and the 4x4x4 in about 5 minutes. More specifically regarding the techniques discussed in this project, the principles that underly uninformed and informed search, $A^*$ and heuristics, multi-stage solvers, and of course the various deep learning methods I have played with (**DL**, **DRL** and **DQL**) all extend to many other puzzles and dimensions and are a great new addition to my tool-set and knowledge.

## 7.2 Implementation

I am quite satistified to have had the time to implement and play with so many solvers and methods, spanning so many different **CS** and **AI** paradigms, from handcrafting my own **SP** *naive* solver, playing with Kociemba, to implementing **BFS**, **DFS**, $A^*$, admissible heuristics such as Manhattan for the **SP** and improving on it via linear constraints penalty, and of course all the machinery necessary to fit, train and exploit some **DL**, **DRL** and **DQL** heuristics to guide search algorithms such as $A^*$ and **MCTS**. Ideally I would have liked to implement things in C++ for speed and multithreading (especially for **MCTS**) but time was limited so I decided to prioritize breadth and ease of experimentation over depth and efficiency of implementation. The choice of Python definitely made it much easier to integrate with many of the ecosystem's libraries (matplotlib, pandas and pytorch in particular).

## 7.3 Deep Reinforcement-Q Learning

It will not come as a surprise to anyone who has played with them that Deep Reinforcement Learning and Deep Q Learning models can be quite capricious to train: choosing the convergence mechanisms and criteria, the interplay of generation of new training data with the inner and outer loop of the **DRL** and **DQL** algorithms (see 2.4 and 2.5) seemed more of an art than a sicence at times. Obviously a lot more tuning, as well as much longer training time and computing resources would have been necessary to make these techniques more competitive at higher dimensions, but overall I remain extremely impressed by how, all things considered - and given how daunting the project seemed at first - it took me little effort to train successful **DRL** and **DQL** models capable of solving puzzles with such large state and action spaces.

### 7.4 Professional issues

My favourite principle within the BCS code of conduct (BCS, 2022) is to 'show what you know, learn what you don't'. The whole point of this MSc in AI, after a 20 year career, most of which spent in quantitative trading, was indeed for me to revise old skills, learn some new ones and further my knowledge in **ML** and **AI**. That has the 'learn what you don't' covered. As for the 'show what you know', I have endeavoured to show honest, and therefore in some cases modest, results. Ideally I would have liked to be able to try more methods and go further with the **DxL** methods on the 3x3x3 **RC** as well as higher dimensional **SP** like the 5x5, but this was sadly not possible within the time imparted.

As for issues related to ethics and safety, some of which are outined in the ACM code of ethics (ACM, 2022), anyone working in **AI** should in my opinion be acutely aware of them. There is clearly some divide in the community regarding the dangers of **AI**, but I myself stand firmly in the Bostrom camp (see in particular Bostrom, 2019 and Bostrom, 2014). His paper-clip-maximiser is one of the most thought provoking ideas and does show that the most benign looking **AI** agent, if sufficiently capable, could create disproportionate harm. To conclude on a humorous (?) note, we probably would not want either to see a Rubik's solver engulf all of the earth's and galaxy's resources in order to compute the nxnxn Rubik's God number for ever growing values of n.

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# 8 Appendix - Examples

In this appendix, I will go through many examples, illustrating how to use the code base to create, learn and solve various puzzles. For each section, a snippet of code will be indicated in **python code** paragraphs, and can easily be run from command line or copied into a script and run from your favourite Python IDE.

## 8.1 Puzzles

Let me start by showing how to construct puzzles, using the Puzzle factory. Notice that in order to run a learner or solver of any kind (assuming of course that they are meant to work on the puzzle type in question), we can just use the exact same code, simply specifying *puzzle_type* and the expected parameters to construct a puzzle. The factories will just pick up the relevant parameters indicating the puzzle type and dimension and everything should work seamlessly.

For instance, let us create a 5x6 **SP**, shuffle it a thousand times, and print it:

**python code – sliding puzzle construction**

```
#####################################################################
from rubiks.puzzle.puzzle import Puzzle
#####################################################################
puzzle_type=Puzzle.sliding_puzzle
n=5
m=6
nb_moves=1000
print(Puzzle.factory(**globals()).apply_random_moves(nb_moves))
#####################################################################
```

The output from the above code snippet will look like (subject to randomness):

```
+=====+=====+=====+=====+=====+=====+
|  16 |  28 |   1 | 7   |   6 |   5 |
+-----+-----+-----+-----+-----+-----+
|  24 |   9 |   2 | 20  |  13 |  10 |
+-----+-----+-----+-----+-----+-----+
|   3 |  22 |  17 | 15  |  21 |  27 |
+-----+-----+-----+-----+-----+-----+
|  12 |   8 |  11 | 14  |  18 |  23 |
+-----+-----+-----+-----+-----+-----+
|  26 |   4 |  19 |     |  25 |  29 |
+-----+-----+-----+-----+-----+-----+
```

Figure 24: scrambled 5x6 **SP** example

.. similarly to construct a perfectly scrambled 2x2x2 **RC**:

python code – Rubik's cube construction

```
#################################################################
from math import inf
from rubiks.puzzle.puzzle import Puzzle
#################################################################
puzzle_type=Puzzle.rubiks_cube
n=2
""" Here we use perfect shuffle by spcifying infinite number of shuffles
                                        """
nb_moves=inf
print(Puzzle.factory(**globals()).apply_random_moves(nb_moves))
#################################################################
```

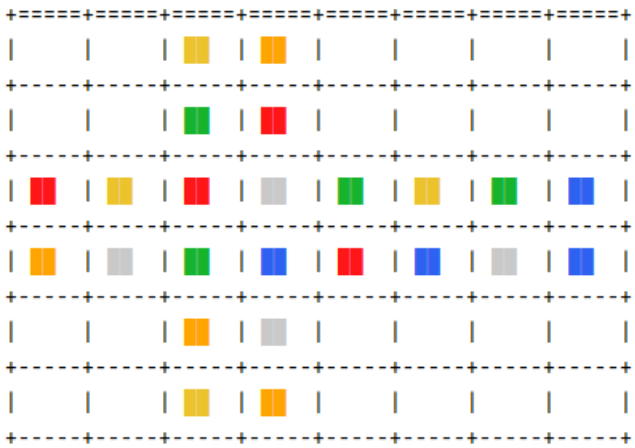

Figure 25: rubiks cube construction example

## 8.2 Learners

### 8.2.1 Perfect Learner

The perfect learner has been discussed in details in 4.6. We simply show here how to run it to learn the value function for the 2x3 **SP**, that is, to solve all 360 possible configurations via an optimal solver (A* with Manhattan heuristic).

python code – perfect learner

```
#################################################################
from rubiks.heuristics.heuristic import Heuristic
from rubiks.puzzle.puzzle import Puzzle
from rubiks.learners.learner import Learner
from rubiks.utils.utils import get_model_file_name
#################################################################
action_type=Learner.do_learn
n=2
```

```
m=3
puzzle_type=Puzzle.sliding_puzzle
learner_type=Learner.perfect_learner
heuristic_type=Heuristic.manhattan
nb_cpus=4
learning_file_name=get_model_file_name(puzzle_type=puzzle_type,
                                       dimension=(n, m),
                                       model_name=Learner.perfect)
if __name__ == '__main__':
    # we fully solve the 2 x 3 SP ... should take ~5s
    Learner.factory(**globals()).action()
#################################################################
action_type=Learner.do_plot
if __name__ == '__main__':
    # we display the results
    Learner.factory(**globals()).action()
#################################################################
```

The above snippet of code solves the 2x3 **SP** and then displays the results, showing the distribution of optimal costs, as well as the most difficult puzzle:

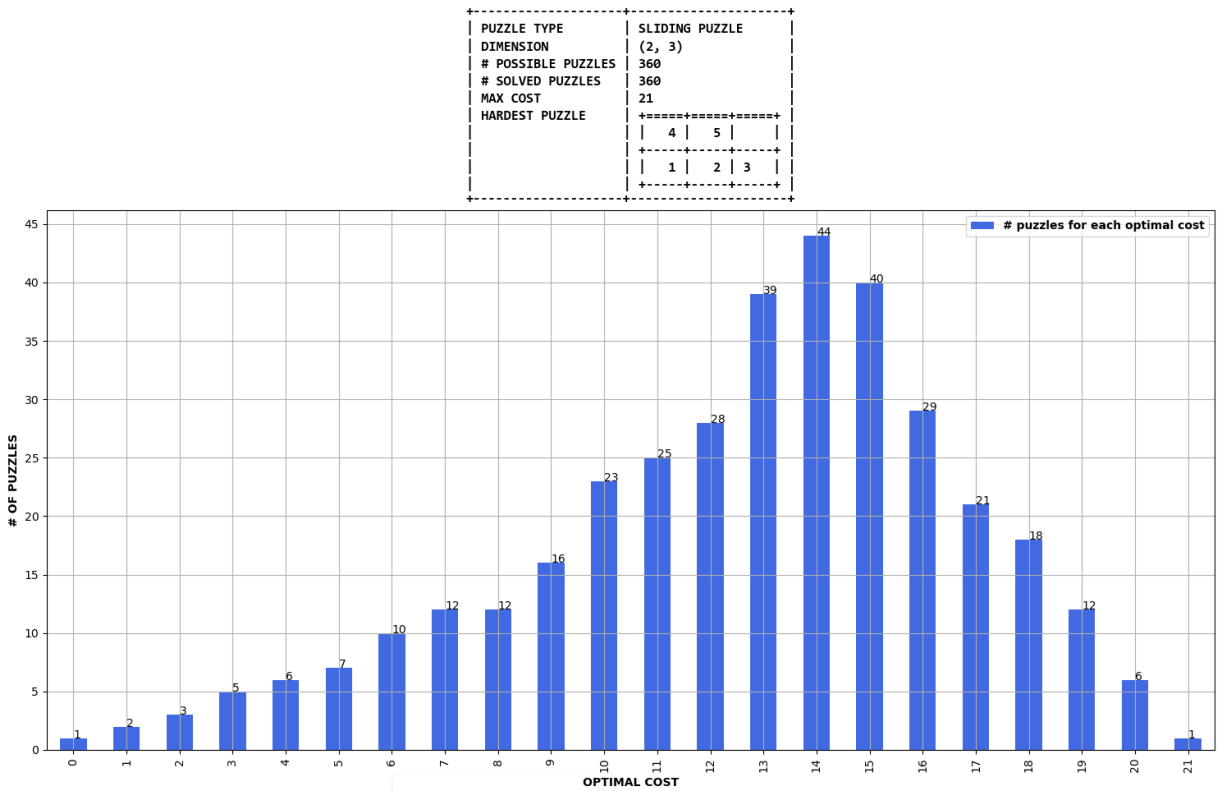


Figure 26: perfect learner example

### 8.2.2 Deep Learner

The DeepLearner, also discussed in details in 4.6, needs some training data. It could in principle of course be trained on any data, not necessarily optimal data (i.e. generated by an optimal solver). Here however, I make use of the TrainingData class to generate 100 sequences of fully solved 5x2 **SP** via A* with Manhattan++.

**python code – deep learner**

```
#####################################################################
from math import inf
#####################################################################
from rubiks.deeplearning.deeplearning import DeepLearning
from rubiks.learners.learner import Learner
from rubiks.learners.deeplearner import DeepLearner
from rubiks.puzzle.puzzle import Puzzle
from rubiks.puzzle.trainingdata import TrainingData
#####################################################################
if '__main__' == __name__:
    puzzle_type=Puzzle.sliding_puzzle
    n=5
    m=2
    """ Generate training data - 100 sequences of fully
    solved perfectly shuffled puzzles.
    """
    nb_cpus=4
    time_out=600
    nb_shuffles=inf
    nb_sequences=100
    TrainingData(**globals()).generate(**globals())
    """ DL learner """
    action_type=Learner.do_learn
    learner_type=Learner.deep_learner
    nb_epochs=999
    learning_rate=1e-3
    optimiser=DeepLearner.rms_prop
    scheduler=DeepLearner.exponential_scheduler
    gamma_scheduler=0.9999
    save_at_each_epoch=False
    threshold=0.01
    training_data_freq=100
    high_target=nb_shuffles + 1
    training_data_from_data_base=True
    nb_shuffles_min=20
    nb_shuffles_max=50
    nb_sequences=50
    """ ... and its network config """
    network_type=DeepLearning.fully_connected_net
    layers_description=(100, 50, 10)
    one_hot_encoding=True
    """ Kick-off the Deep Learner """
    learning_file_name=Learner.factory(**globals()).get_model_name()
```

```
    Learner.factory(**globals()).action()
    """ Plot its learning """
    action_type=Learner.do_plot
    Learner.factory(**globals()).action()
#####################################################################
```

As can be seen in the code snippet, this example will generate 100 perfectly shuffled (n=5, m=2) SPs and solve them. Once done, a summary of the training data is printed, indicating, for each optimal cost, how many sequences have been generated.

| 16 | 20 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3 | 3 | 4 | 5 | 2 | 2 | 5 | 2 | 4 | 6 | 4 | 8 | 11 | 8 | 7 | 7 | 5 | 3 | 3 | 2 | 2 | 1 | 1 |

Figure 27: deep learner training example

Then the Deep Learner will get trained on this data for 999 epochs. In the above example, I have chosen to fetch, every 100 epochs, 50 random sequences of puzzles from the training data. Each sequence is composed of a random puzzle of cost between 20 and 50, fetched from the training data, along with its optimal path to the solution. The default optimiser (rms_prop) is used, together with an exponential scheduler starting with a learning rate of 0.001 and a gamma of 0.9999. We can see that the (MSE) loss on the value function decreases rapidly, and jumps back up every time we change the training data (since it has not yet seen some of it). By the end of the training, the in-sample MSE loss has dropped to 1.5 and the Deep Learner has seen 0.14% of the possible (n=5, m=2) puzzles.

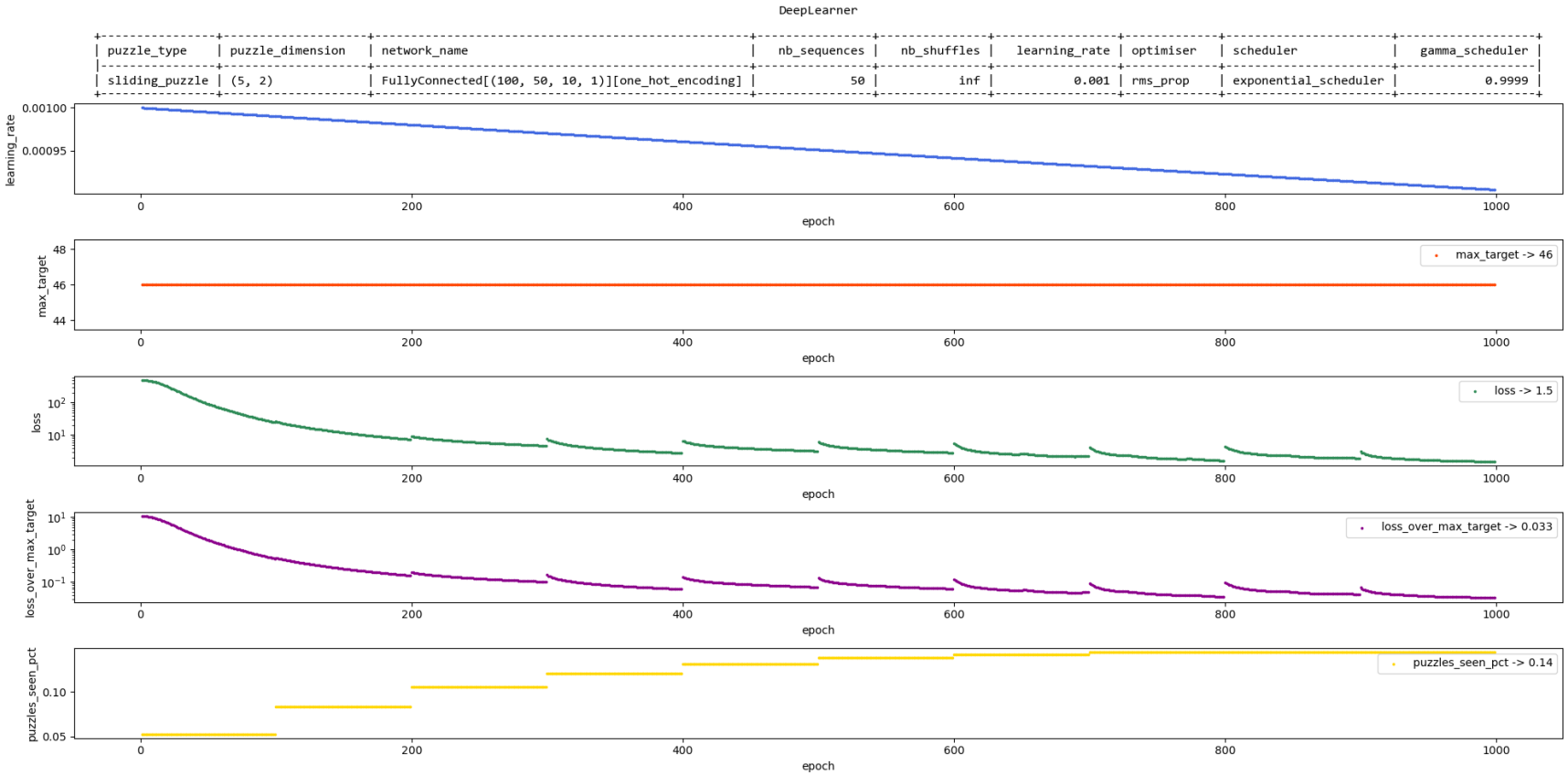


Figure 28: deep learner learning data example

### 8.2.3 Deep Reinforcement Learner

Unlike the Deep Learner, the Deep Reinforcement Learner learns unsupervised (in the sense that there is no need to pre-solve puzzles to tell if what the actual (target) costs are), since it generates its own target using a combination of a target network and the simple min rule described in 4.6. Let us see here how to run it on the (n=4, m=2) SP for instance. The following code snippet will run a Deep Reinforcement Learner for a maximum of 25,000 epochs, generating randomly 10 sequences of puzzles shuffled 50 times from goal state every time it updates the target network. That update will happen either after 500 epochs or when the (MSE) loss on the value function gets under one thousands of the max target value. The learner will stop if it reaches 25,000 epochs or if the target network updates 40 times. The network trained is a fully connected network with 3 hidden layers and the puzzles are one-hot encoded. We use the same optimiser and scheduler as in the previous subsection.

**python code – deep reinforcement learner**

```
#####################################################################
from rubiks.deeplearning.deeplearning import DeepLearning
from rubiks.learners.learner import Learner
from rubiks.learners.deepreinforcementlearner import
                                    DeepReinforcementLearner
from rubiks.puzzle.puzzle import Puzzle
#####################################################################
if '__main__' == __name__:
    puzzle_type=Puzzle.sliding_puzzle
    n=4
    m=2
    """ Generate training data - 100 sequences of fully
    solved perfectly shuffled puzzles.
    """
    nb_cpus=4
    """ DRL learner """
    action_type=Learner.do_learn
    learner_type=Learner.deep_reinforcement_learner
    nb_epochs=25000
    nb_shuffles=50
    nb_sequences=10
    training_data_every_epoch=False
    cap_target_at_network_count=True
    update_target_network_frequency=500
    update_target_network_threshold=1e-3
    max_nb_target_network_update=40
    max_target_not_increasing_epochs_pct=0.5
    max_target_uptick=0.01
    learning_rate=1e-3
    scheduler=DeepReinforcementLearner.exponential_scheduler
    gamma_scheduler=0.9999
    """ ... and its network config """
    network_type=DeepLearning.fully_connected_net
    layers_description=(128, 64, 32)
```

```
    one_hot_encoding=True
    """ Kick-off the Deep Reinforcement Learner ... """
    learning_file_name=Learner.factory(**globals()).get_model_name()
    Learner.factory(**globals()).action()
    """ ... and plot its learning data """
    action_type=Learner.do_plot
    Learner.factory(**globals()).action()
#####################################################################
```

As can be seen on the next page, which I obtained from running the above code snippet (keep in mind that every run is going to be slightly different due to the random puzzles being generated), the training stopped after about 17,100 epochs as the 40 target network updates had been reached. By that point, the DRL learner had seen 40% of the possible puzzles, and the very last MSE loss (after update, so out-of-sample) was around 0.4, corresponding to 2% of the max target cost. It is interesting to notice that since I have shuffled the sequences only 50 times, and since the (n=4, m=2) SP is quite constrained in terms of possible moves, the max target ever produced by the network was only around 25, whereas we know the God number for this dimension is 36 (see later section 5.1). It is therefore likely that the resulting network would not produce very optimal solutions for puzzles whose cost is in the region [25, 36].

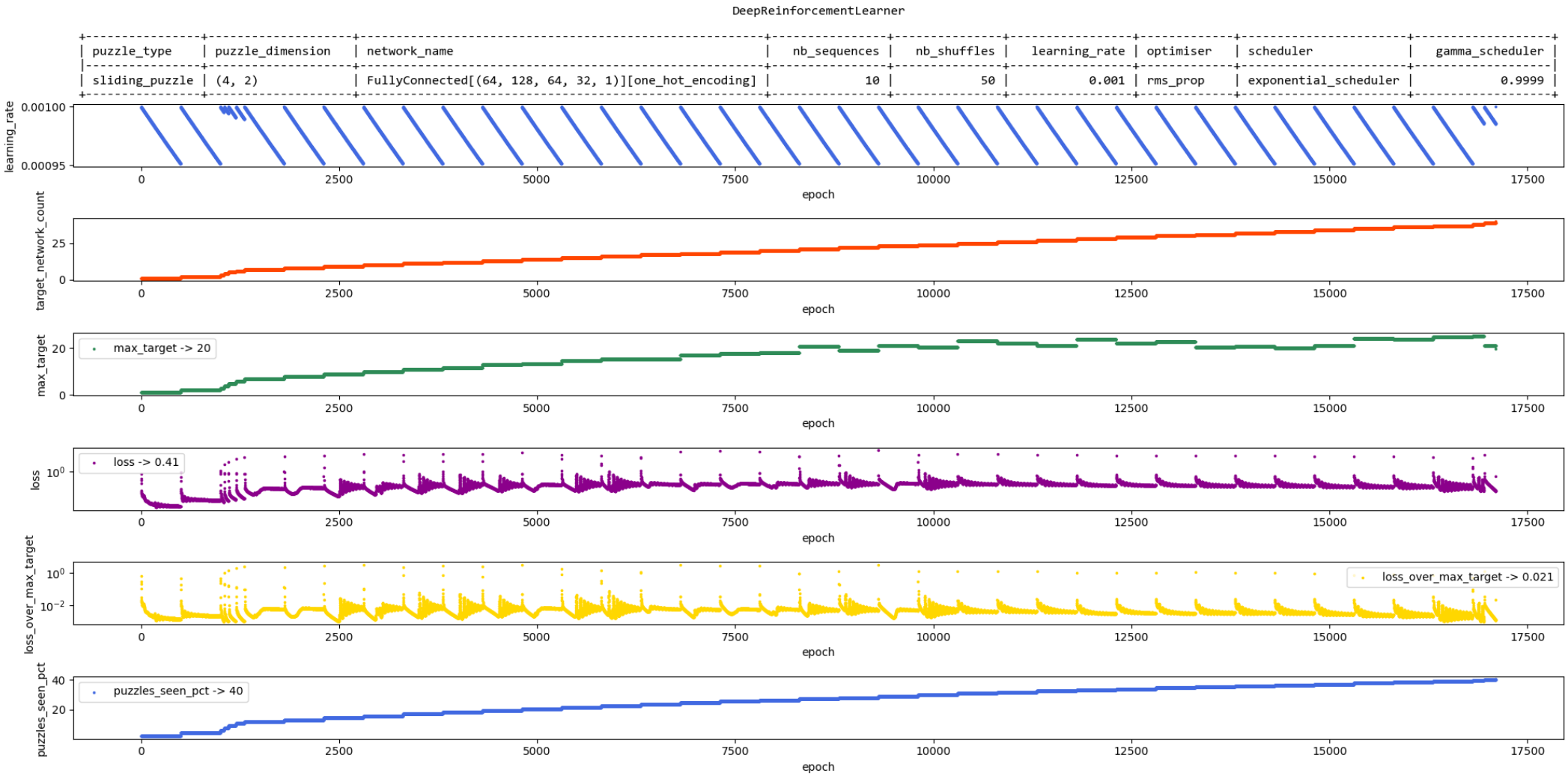


Figure 29: deep reinforcement learner learning data example

## 8.3 Solvers

### 8.3.1 Blind search

First let me start with some of the blind search algorithms, which I only have been able to use on small dimension SP. They quickly become too memory hungry to be practical on anything but the smallest puzzles.

**BFS** The following example shows how to use Breadth First Search to solve a (n=3, m=3) SP which we do not *shuffle* too much.

**python code – breadth first search solver**

```
#####################################################################
from rubiks.solvers.solver import Solver
from rubiks.puzzle.puzzle import Puzzle
#####################################################################
if '__main__' == __name__:
    puzzle_type = Puzzle.sliding_puzzle
    n=3
    m=3
    nb_shuffles=10
    solver_type=Solver.bfs
    check_optimal=True
    action_type=Solver.do_solve
    print(Solver.factory(**globals()).action())
#####################################################################
```

As expected (since BFS is optimal), the solution found, printed by the snippet of code above, is optimal. The check_optimal flag in the code snippet indicates that the solver should let us know if solution is optimal. Since BFS advertises itself (via the Solver base class API) as an optimal solver, the solution is deemed optimal.

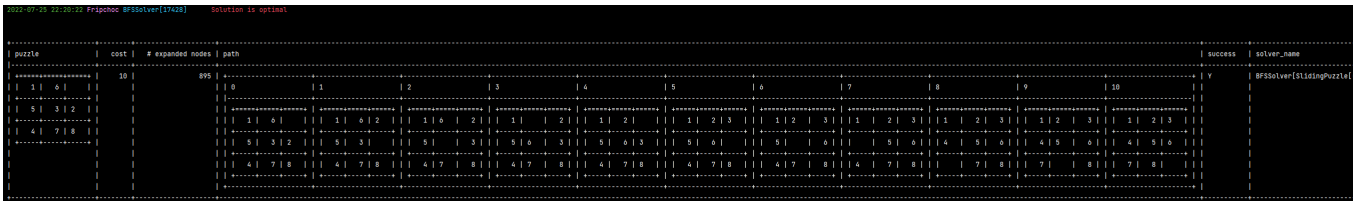


Figure 30: breadth first search solver example

**DFS**

**python code – depth first search solver**

```
#####################################################################
from rubiks.solvers.solver import Solver
```

```
from rubiks.puzzle.puzzle import Puzzle
#####################################################################
if '__main__' == __name__:
    puzzle_type = Puzzle.sliding_puzzle
    n=3
    m=3
    nb_shuffles=8
    limit=15
    time_out=60
    solver_type=Solver.dfs
    check_optimal=True
    log_solution=True
    action_type=Solver.do_solve
    Solver.factory(**globals()).action()
#####################################################################
```

Here we can see, in contrast with the previous example, that the solution obtained by DFS is not optimal. The Solver indicates it and shows an optimal solution. Clearly since we shuffled 8 times from goal configuration, the optimal path cannot have a cost higher than 8 (it could be lower though of course).

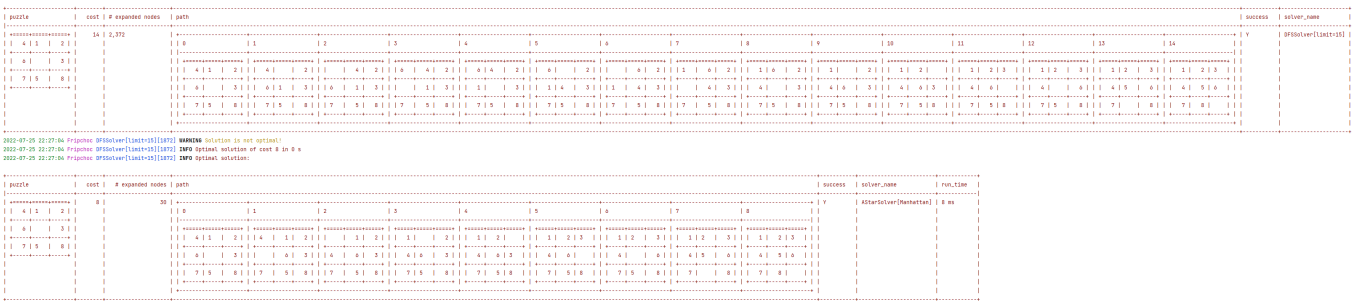

Figure 31: depth first search solver example

### 8.3.2 Naive Sliding Puzzle Solver

As a comparison point for otherSP solvers, I have implemented a naive sliding puzzle solver, which does what most beginner players would intuitively do when solving the sliding puzzle by hand: solve the top row, then the left column, and keep iterating until done. Notice that once either the top row or left column is solved, there is no longer any need to modify it, we have simply reduced the problem to a sub-problem of reduced dimension. For the interested reader, the details of the algorithm are as follows:

- if n and m are both equal to 2, we just keep moving the empty tile clock-wise until the puzzle is solved. Notice that this is bound to work, since moving clock-wise or counter-clock-wise are the two ony possible moves, and one of them is just undoing the other one, therefore the only possible sequence of move in a (n=2, m=2) puzzle is to either keep moving clock-wise or counter-clock-wise.

- if n $\geq$ m, we solve the top row
- otherwise we solve the left column

Solving the top row of a n by m puzzle (left column is similar, mutatis mutandis, so I will not detail it) is accomplished as follows:
**naive algorithm - top-row solver**

1. we sort the tiles (which since we are potentially dealing with a sub-problem, are not necessarily 1 to $m * n - 1$), and select the m smaller ones $t_1, ..., t_{m-1}, t_m$.
2. we place $t_m$ in the bottom-left corner
3. we place $t_1, ..., t_{m-2}$ to their respective positions (in that order, and making sure not to undo any previous steps as we do so)
4. we place $t_{m-1}$ in the top-right corner
5. we then move $t_m$ just under $t_{m-1}$
6. we move the empty tile to the left of $t_{m-1}$
7. finally we move the empty tile right and then down to put $t_{m-1}$ and $t_m$ in place.

In order to move the tiles, we have written a few simple routines which can move the empty tile from its current position next to (above, below, left or right) any tile, and then can move that tile to another position, all the while avoiding to go through previously moved tiles (hence the particular order in which we move the different tiles above). The only case where the above algorithm can get stuck is when both n and m are equal to 3 and that by step 6 we end up with $t_3$ under the empty tile. We have handcrafted a sequence of moves to solve this particular position. Other than this one particular case, the above naive algorithm is guaranteed to succeed (and is obviously quite fast in terms of run time, though not elegant).

As a concrete example, let us assume we started with the following (n=6, m=6) puzzle:

| | | | | | |
|---|---|---|---|---|---|
| 14 | 27 | 6 | 2 | 5 | 18 |
| 21 | 29 | 13 | 23 | 35 | 30 |
| 26 | 3 | 7 | 9 | 24 | 19 |
| 22 | 12 | 11 | 17 | 16 | 33 |
| 32 | 10 | 20 | 25 | 34 | 28 |
| 8 | 4 | 15 | 31 | | 1 |

After one call to solve the top row and the left column, we are left with solving the (n=5,m=5) sub-puzzle in blue:

| | | | | | |
|---|---|---|---|---|---|
| 1 | 2 | 3 | 4 | 5 | 6 |
| 7 | 9 | 17 | 27 | 18 | 35 |
| 8 | 23 | 11 | 15 | 24 | 21 |
| 9 | 20 | 8 | 29 | 33 | 10 |
| 10 | 22 | 30 | 14 | 32 | 16 |
| 11 | | 12 | 26 | 34 | 28 |

Let us now detail how the **naive algorithm** will solve the top row if that sub-puzzle:

| | | | | |
|---|---|---|---|---|
| 9 | 17 | 27 | 18 | 35 |
| 23 | 11 | 15 | 24 | 21 |
| 20 | 8 | 29 | 33 | 10 |
| 22 | 30 | 14 | 32 | 16 |
| | 12 | 26 | 34 | 28 |

step 1 above will decide to solve the top row by placing $t_1, ..., t_5 = 8, 9, 10, 11, 12$ in that order as the top row. Steps 2 to 7 will yield in order:

| | | | | |
|---|---|---|---|---|
| 9 | 17 | 27 | 18 | 35 |
| 23 | 11 | 15 | 24 | 21 |
| 20 | 8 | 29 | 33 | 10 |
| 22 | 30 | 14 | 32 | 16 |
| | 12 | 26 | 34 | 28 |

| | | | | |
|---|---|---|---|---|
| 9 | 17 | 27 | 18 | 35 |
| 23 | 11 | 15 | 24 | 21 |
| 20 | 8 | 29 | 33 | 10 |
| 22 | 30 | 14 | 32 | 16 |
| 12 | | 26 | 34 | 28 |

| | | | | |
|---|---|---|---|---|
| 8 | 9 | 10 | | 18 |
| 17 | 15 | 27 | 24 | 35 |
| 11 | 23 | 29 | 21 | 33 |
| 20 | 22 | 14 | 32 | 16 |
| 12 | 30 | 26 | 34 | 28 |

| | | | | |
|---|---|---|---|---|
| 8 | 9 | 10 | | 11 |
| 23 | 29 | 21 | 18 | 24 |
| 17 | 15 | 27 | 33 | 35 |
| 20 | 22 | 14 | 32 | 16 |
| 12 | 30 | 26 | 34 | 28 |

| | | | | |
|---|---|---|---|---|
| 8 | 9 | 10 | 18 | 11 |
| 29 | 27 | 32 | | 12 |
| 23 | 21 | 33 | 35 | 24 |
| 15 | 17 | 22 | 14 | 16 |
| 30 | 20 | 26 | 34 | 28 |

| | | | | |
|---|---|---|---|---|
| 8 | 9 | 10 | 11 | 12 |
| 29 | 27 | 32 | 18 | |
| 23 | 21 | 33 | 35 | 24 |
| 15 | 17 | 22 | 14 | 16 |
| 30 | 20 | 26 | 34 | 28 |

and we are left with solving the bottom sub-puzzle (n=4,m=5):

| | | | | |
|---|---|---|---|---|
| 29 | 27 | 32 | 18 | |
| 23 | 21 | 33 | 35 | 24 |
| 15 | 17 | 22 | 14 | 16 |
| 30 | 20 | 26 | 34 | 28 |

which the naive solver can keep solving iteratively by taking care of the left-most column, etc...

Below is a simple code snippet to run the naive solver on a randomly generated (n=2, m=2) SP:

**python code – naive solver**

```
##################################################
from math import inf
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.solver import Solver
##################################################
action_type=Solver.do_solve
n=2
puzzle_type=Puzzle.sliding_puzzle
solver_type=Solver.naive
nb_shuffles=inf
##################################################
print(Solver.factory(**globals()).action())
##################################################
```

```
+--------------+-------+--------------------+-------------------------------------------------------------------------------------------------------------------------------------------+-----------+-----------------------------------------------------------------------------------------------------------------------
```

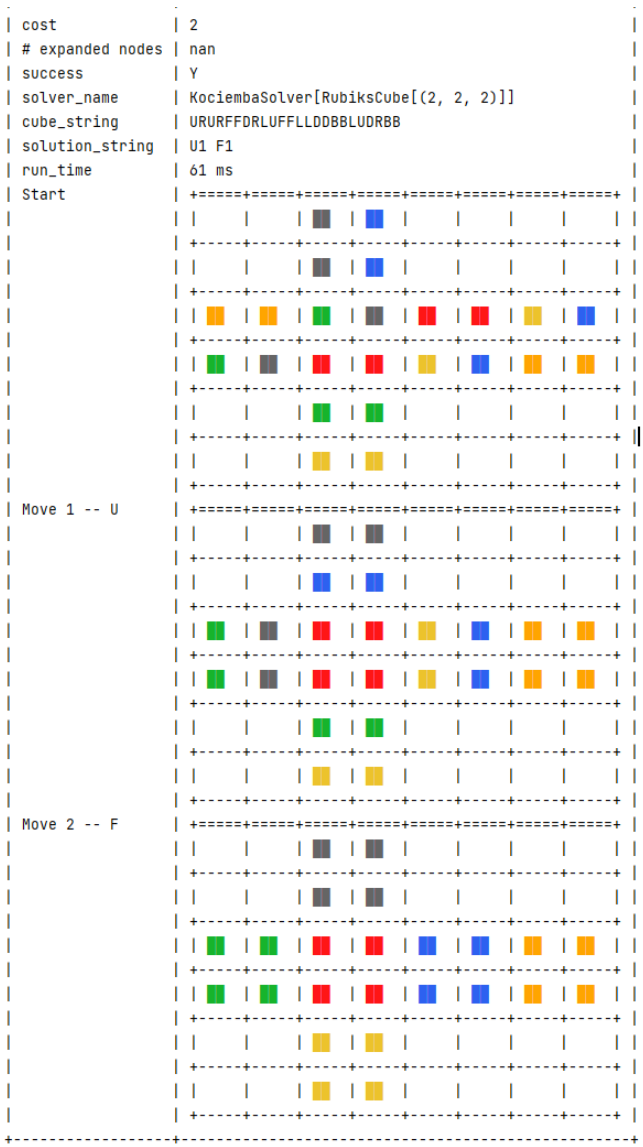


Figure 33: Kociemba solver example

### 8.3.4 A*

#### Manhattan heuristic

#### python code – depth first search solver

```
##################################################################
from rubiks.heuristics.heuristic import Heuristic
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.solver import Solver
```

```
#####################################################################
if '__main__' == __name__:
    puzzle_type = Puzzle.sliding_puzzle
    tiles=[[3, 8, 6], [4, 1, 5], [0, 7, 2]]
    solver_type=Solver.astar
    heuristic_type=Heuristic.manhattan
    plus=False
    action_type=Solver.do_solve
    print(Solver.factory(**globals()).action().to_str_light())
#####################################################################
```

We run this example twice, one with simple Manhattan and one with Manhattan++. As can be seen from the output below, the Manhattan++ improves on the number of expanded nodes (as expected, since the heuristic is less optimistic while retaining its optimality property). See a more detailed analysis in the SP results section **??**

```
+---------------------+--------+--------------------+-----------+-------------------------+------------+
| puzzle              |   cost |   # expanded nodes | success   | solver_name             | run_time   |
|---------------------+--------+--------------------+-----------+-------------------------+------------|
| +=====+=====+=====+ |     18 |                472 | Y         | AStarSolver[Manhattan]  | 95 ms      |
| | 3   |   8 |   6 | |        |                    |           |                         |            |
| +-----+-----+-----+ |        |                    |           |                         |            |
| | 4   |   1 |   5 | |        |                    |           |                         |            |
| +-----+-----+-----+ |        |                    |           |                         |            |
| |     |   7 |   2 | |        |                    |           |                         |            |
| +-----+-----+-----+ |        |                    |           |                         |            |
+---------------------+--------+--------------------+-----------+-------------------------+------------+
```

Figure 34: a* manhattan solver example

```
+---------------------+--------+--------------------+-----------+--------------------------+------------+
| puzzle              |   cost |   # expanded nodes | success   | solver_name              | run_time   |
|---------------------+--------+--------------------+-----------+--------------------------+------------|
| +=====+=====+=====+ |     18 |                340 | Y         | AStarSolver[Manhattan++] | 76 ms      |
| | 3   |   8 |   6 | |        |                    |           |                          |            |
| +-----+-----+-----+ |        |                    |           |                          |            |
| | 4   |   1 |   5 | |        |                    |           |                          |            |
| +-----+-----+-----+ |        |                    |           |                          |            |
| |     |   7 |   2 | |        |                    |           |                          |            |
| +-----+-----+-----+ |        |                    |           |                          |            |
+---------------------+--------+--------------------+-----------+--------------------------+------------+
```

Figure 35: a* manhattan++ solver example

**Perfect Heuristic** To run A* with a perfect heuristic, we just need to specify the heuristic type as such, and set the parameter *model_file_name* to point to a pre-recorded database populated by the PerfectLearner (see earlier section 8.2.1).

### python code – depth first search solver

```
#####################################################################
from rubiks.heuristics.heuristic import Heuristic
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.solver import Solver
```

```
from rubiks.utils.utils import get_model_file_name
#####################################################################
if '__main__' == __name__:
    puzzle_type = Puzzle.sliding_puzzle
    n=3
    nb_shuffles=40
    solver_type=Solver.astar
    heuristic_type=Heuristic.perfect
    model_file_name = get_model_file_name(puzzle_type=puzzle_type,
                                          dimension=(n, n),
                                          model_name=Heuristic.perfect)
    action_type=Solver.do_solve
    print(Solver.factory(**globals()).action().to_str_light())
#####################################################################
```

Running this code snippet will output something like (the shuffle is random obviously):

```
+--------------------+--------+-------------------+-----------+-----------------------------+------------+
| puzzle             |   cost |   # expanded nodes | success   | solver_name                 | run_time   |
|--------------------+--------+-------------------+-----------+-----------------------------+------------|
| +=====+=====+=====+ |     24 |                84 | Y         | AStarSolver[PerfectHeuristic] | 51 ms      |
| | 2   |   8 |   7 | |        |                   |           |                             |            |
| +-----+-----+-----+ |        |                   |           |                             |            |
| | 6   |   4 |   5 | |        |                   |           |                             |            |
| +-----+-----+-----+ |        |                   |           |                             |            |
| |     |   1 |   3 | |        |                   |           |                             |            |
| +-----+-----+-----+ |        |                   |           |                             |            |
+--------------------+--------+-------------------+-----------+-----------------------------+------------+
```

Figure 36: a* perfect solver example

### Deep Learning Heuristic

### Deep Reinforcement Learning Heuristic

### Deep Q Learning Heuristic

# 9 Appendix - Kociemba Bug

Let me discuss in this appendix in more details the issue I mentioned in section 6.2 regarding the *poor* interface of the kociemba (3x3x3) library.

I personally like to follow the great Scott Meyers' advice (see item 18 of Meyers, 2005), which is to not merely make interfaces easy to use, but also difficult to misuse. In that instance, I would argue they have made it very easy to shoot oneself in the foot with their interface which assumes the cubes passed to the solver are in *standard* form (my terminology), not only without making that explicit anywhere, but worse than that: sometimes non standard initial configuration raise an exception, sometimes not and returning a solution which is not really one! So what is the problem exactly?

To start with, let us remember from chapter 3 that each **RC** configuration has 24 equivalent configurations under invariance by full rotation of the cube in space. Out of 24 equivalent configurations, and for an observer facing the cube, there is only one whose center front (F) cubie is red and center up (U) cubie is white.

In hkociemba (the third parties 2x2x2 implementation which I used under the hood of my KociembaSolver), the problem of these equivalent puzzles is irrelevant (since full cube rotation can always be achieved by 2 rotations of 2 opposite faces in opposite directions, e.g. FB' is equivalent to full cube rotation around F (CF in my jargon)). That being said, the hkociemba is smarter than just using the equivalence between full cube rotation and two faces' rotations. It does automatic color scheme recognition when passed a *cube string*, and gets a smart solution given that coloring scheme. For instance, if we pass it a solved configuration, but not in standard form, it knows there is no need to do anything. In the general case of a scrambled cube, it will also endeavour to find solutions to the closest among the 24 equivalent solved configurations. Let's look at the following concerete example:

**Kociemba bug – 2x2x2 RC – example of good interface design**

```
#####################################################################
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.solver import Solver
from rubiks.solvers.kociembasolver import KociembaSolver
from_kociemba = KociembaSolver.from_kociemba
to_kociemba = KociembaSolver.to_kociemba
#####################################################################
puzzle_type = Puzzle.rubiks_cube
n=2
init_from_random_goal=False
cube = Puzzle.factory(**globals()).get_equivalent()[-1].
                                    apply_random_moves(nb_moves=1)
solver_type = Solver.kociemba
solver = Solver.factory(**globals())
print(solver.solve(cube))
```

```
#######################################################################
```

which, subject to randomness, gave me the following scrambled cube and solution:

```
| success          | Y                                                |
| solver_name      | KociembaSolver[RubiksCube[(2, 2, 2)]]            |
| cube_string      | URURFFFFLULUDLDLBBBBDRDR                         |
| solution_string  | R1                                               |
| run_time         | 65 ms                                            |
| Start            | +=====+=====+=====+=====+=====+=====+=====+=====+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | | ■   | ■   | ■   | ■   | ■   | ■   | ■   | ■   | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | | ■   | ■   | ■   | ■   | ■   | ■   | ■   | ■   | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
| Move 1 -- R      | +=====+=====+=====+=====+=====+=====+=====+=====+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | | ■   | ■   | ■   | ■   | ■   | ■   | ■   | ■   | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | | ■   | ■   | ■   | ■   | ■   | ■   | ■   | ■   | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
|                  | |     |     | ■   | ■   |     |     |     |     | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+ |
+------------------+--------------------------------------------------+
```

Figure 37: 2x2x2 **RC** – hkociemba finds path to closest of the 24 equivalent goals

As we can see, hkociemba happily returned a 1-move solution R to green F, white U, instead of the costlier solution it would have taken to get to *standard* form red F white U (clearly at a cost of 3 with solution RUD').

In the 3x3x3 case, things are not quite that simple. There is no way to reproduce full cube rotation from faces rotations alone, since the center cubies will never move via the latter, but do via the former. If we run the equivalent of the above problem with the (3x3x3) kociemba library, we silently get to a false solution as is apparent from printing the resulting cube.

### Kociemba bug – 3x3x3 RC – example of bad interface design

```
#######################################################################
from kociemba import solve
```

```
#################################################################
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.kociembasolver import KociembaSolver
from_kociemba = KociembaSolver.from_kociemba
to_kociemba = KociembaSolver.to_kociemba
#################################################################
puzzle_type = Puzzle.rubiks_cube
n=3
init_from_random_goal=False
cube = Puzzle.factory(**globals()).get_equivalent()[-1].
                                    apply_random_moves(nb_moves=1)
print(cube)
cube_string = to_kociemba(cube)
solution = solve(cube_string)
print('Kociemba Solution:', solution)
print(cube.apply_moves(from_kociemba(solution)))
################################################################
```

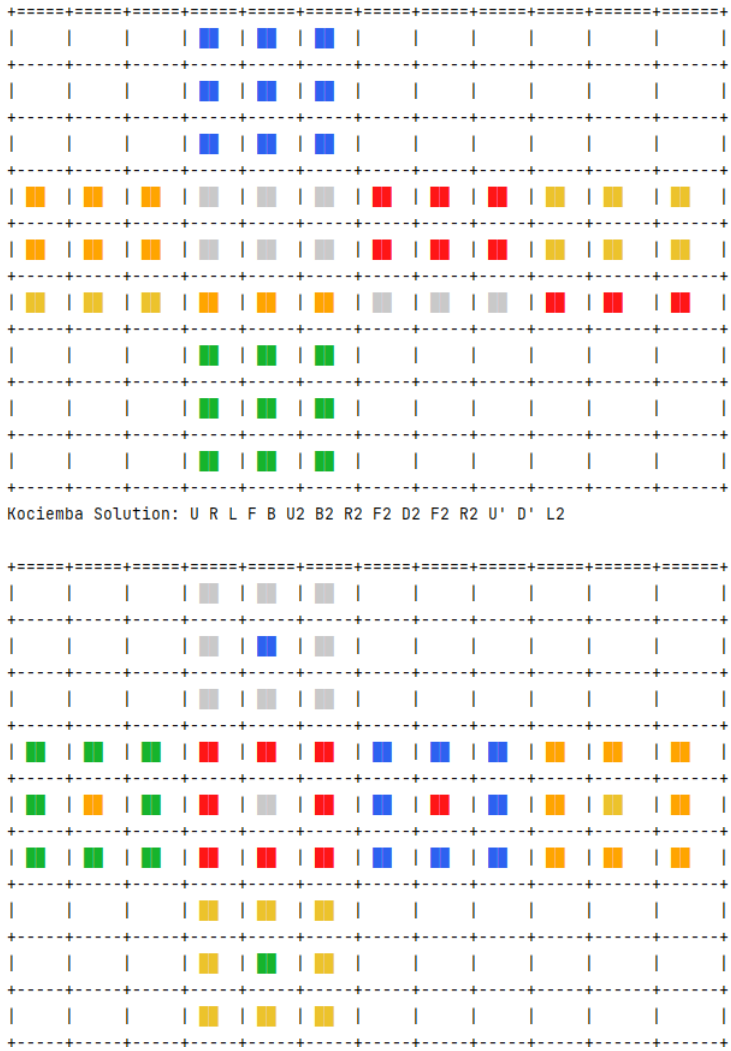


Figure 38: 3x3x3 **RC** – kociemba does not check center cubies and returns wrong solution

In order to counteract that, and make the comparisons between Kociemba 3x3x3 and other solvers and methods fairer, I have had to implement a layer on top of kociemba. My Kociemba solver basically will check if a cube is in *standard* form, and if not, it will find the sequence of full cube rotations that bring us to an equivalent configuration in *standard* form, pass that to equivalent *standard* cube to kociemba, and stich the cube rotation to the kociemba solution (treating cube rotation as 0 cost everywhere in the code). That way, we seamlessly get to an answer that makes sense from kociemba, without the user having to worry about whether or not the cube they are passing as input is in *standard* form or not! Running the same example as above via my KociembaSolver, we get the expected result, composed of 3 cube rotations to bring it to *standard* form, followed by one face rotation to solve it:

### Kociemba bug – 3x3x3 RC – massage to fix the broken interface

```
#####################################################################
from rubiks.puzzle.puzzle import Puzzle
from rubiks.solvers.solver import Solver
from rubiks.solvers.kociembasolver import KociembaSolver
from_kociemba = KociembaSolver.from_kociemba
to_kociemba = KociembaSolver.to_kociemba
#####################################################################
puzzle_type = Puzzle.rubiks_cube
n=3
init_from_random_goal=False
cube = Puzzle.factory(**globals()).get_equivalent()[-1].
                                    apply_random_moves(nb_moves=1)
solver_type = Solver.kociemba
solver = Solver.factory(**globals())
print(solver.solve(cube))
#####################################################################
```

```
| success          | Y                                                                    |
| solver_name      | KociembaSolver[RubiksCube[(3, 3, 3)]]                                |
| cube_string      | UUUUUURRRDRRDRRDRRFFFFFFFFFLLLDDDDDDLLULLULLUBBBBBBBBB               |
| solution_string  | F                                                                    |
| run_time         | 62 ms                                                                |
| Start            | +======+=====+=====+=====+=====+======+=====+======+=====+=====+======+======+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
| Move 1 -- CU     | +======+=====+=====+=====+=====+======+=====+======+=====+=====+======+======+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | ■  | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
|                  | |    |    |    | ■  | ■  | ■  |    |    |    |    |    |    | |
|                  | +-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+------+------+ |
```

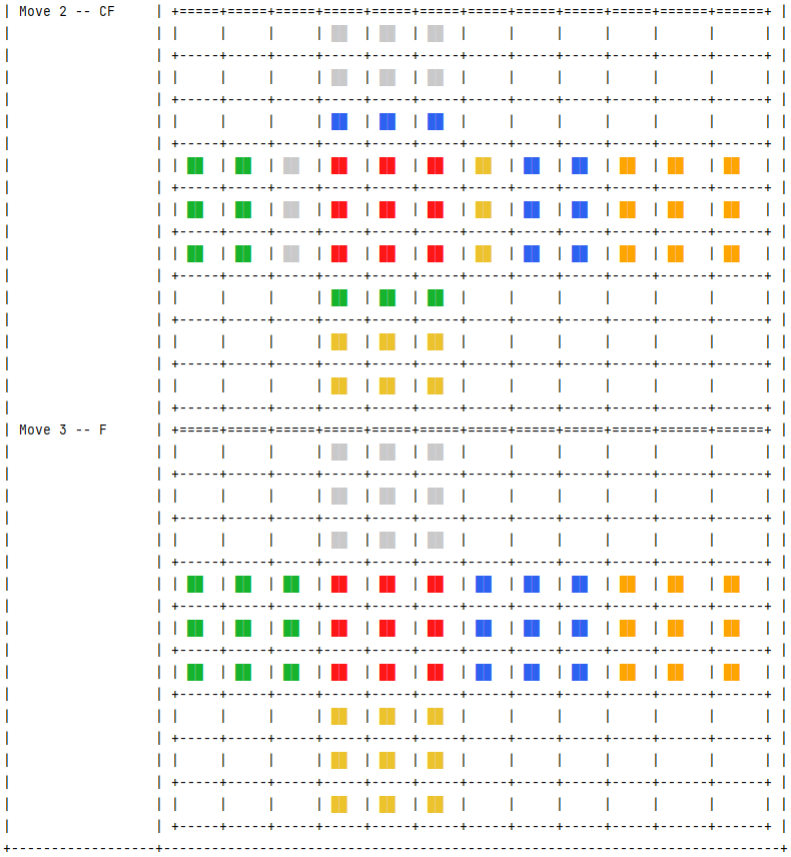


Figure 39: 3x3x3 **RC** – Fixed kociemba interface