Fast Polyhedra Analysis with deep Q-networks

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Abstract

We use deep Q-networks to increase the performance of numerical analysis whilst retaining a good precision. In this work, we reuse an existing framework using reinforcement learning to leverage the precision loss for performance gain inside of polyhedra analysis. We expand this framework with the use of nonlinear Q-function approximations. We then further optimise this method by testing new features, reward functions as well as other problem specific optimisations. We also try to increase the flexibility of the proposed algorithm. Finally, we train and test our resulting algorithm. Using its final version, we are able to achieve a considerable gain in both performance and precision.

Contents

Introduction

1

The number of domains controlled by computers has grown exponentially in the recent years. As the complexity of the structures surrounding us grows, the need for their automatisation grows with it. And so, more and more of the systems around us, become controlled by computers. From simple things such as automatic doors to vastly more complex and important systems such as self-driving cars, medical software or nuclear weapons software. In some of these applications, a program bug could only be a slight nuisance, but in others its existence could have major implications. A few infamous examples of these exist where buffer overflows, rounding errors or division by zeros have caused space craft crashes or lethal radiation overdoses. As such, the importance of some of these devices demands their invulnerability and its verifiability. Unfortunately, as the complexity of these programs increases their verification can no longer be simply done by hand and the need for complete and formal verification methods becomes critical.
Static analysis is a sub-branch of computer science. Its task is to analyse a program without its execution. It does this in the goal of discovering weaknesses inside of the code that could lead to vulnerabilities. As such, it should help with debugging and provide a better notion of safety about the code. Static analysis has seen a growing commercial use in the recent years mostly in safety-critical domains. Recent advances in this field use clever mathematical properties in order to increase the capabilities of such methods. Other techniques, leverage the domain of artificial intelligence to increase the fields capacities. For, until ai is capable of writing invulnerable software for us, we can at least use it to verify ours.

1.1 Problem Statement

The main focus of static analysis is observing the effects that program expressions and statements have on the variables inside of the program. In order for these methods to work, a numerical abstract domain is needed that can capture the relationships between the variables. An important attribute of a domain is its expressivity, that is to say, how complex are the constraints between variables that the domain can represent. The more expressive a domain is the more complicated relationships it can represent. The most expressive domain is the polyhedra domain that represents the constraints with different polyhedra. However, its expressivity comes at a cost. It is notoriously time and space complex, having worst case exponential complexities in both. Other domains also exits that do not suffer from these problems. Unfortunately, to achieve this, they loose their expressivity. Modifications to the polyhedra domain are also possible, some of these modifications try to leverage precision loss against performance gain.

However, finding the right balance between these two is not an easy task.

1.2 Goals

The goal of this thesis is to use some of the recent developments in new areas of reinforcement learning. To adapt and optimise these novel methods in order to to use them with polyhedra analysis. The goal is then to optimise these methods with some problem specific knowledge from polyhedra analysis, in order to render the analysis more efficient and learn an action selection policy that achieves the correct balance between precision and performance, hopefully outperforming preexisting methods.

1.3 Structure of this Document

Chapter 2 briefly introduces reinforcement learning, explaining the important concepts and its main goals. It will also describe some of the recent advances inside of the field and the achievements of these methods.

Chapter 3 addresses Polyhedra analysis. It will explain its usefulness inside of static analysers and how it works. It will also introduce some of the modifications made to the domain, in order to reduce some of its shortcomings.

Chapter 4 addresses the work done throughout this thesis. It will first address how the two previous chapters were combined and the basic algorithm was designed. It will also show the different methods tested to further optimise the results.

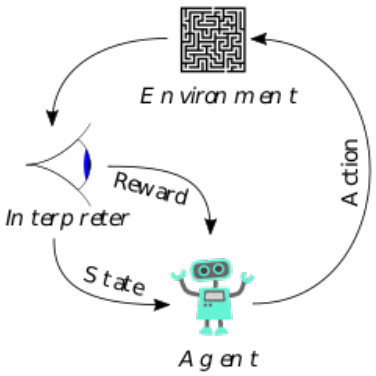
Chapter 5 discusses the different experiments that were run whilst finding the optimal combination of parts for the algorithm. It will also present the results of the execution of the finalised versions of our algorithms on different benchmarks.

Chapter 6 will be a final discussion on what was achieved during this thesis and the results we were able to obtain.

Reinforcement Learning

2

Reinforcement Learning[Kaelbling et al. 1996] is a very general problem of machine learning studied in a multitude of different fields, such as game theory, information theory or statistics. It is a very broad concept and the foundations are the following. An agent interacts with a given environment, at its disposal, it has a set of various different actions. When an action is performed it receives a reward. The goal of the agent is to devise an action selection strategy that should maximise the cumulative reward of the actions.



2.1 Concepts

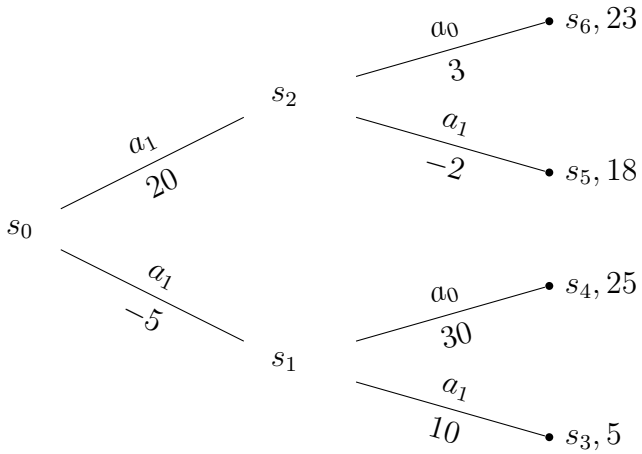
In order to be able to solve a problem with reinforcement learning, it first has to be mapped to the following RL concepts:

- A set of agent states S, with the initial state $s_0 \in S$
- A set of actions A
- A function giving the reward of performing an action from s_t to s_{t+1}, $r(s_t, a_t, s_{t+1}) \in \mathbb{R}$

During the execution of the program, the agent will first start in the initial state s_0. Then, at each timestep $t = 0, 1, ...$, the agent will pick an action $a_t \in A$, this action will then be executed, the agent will move from s_t to s_{t+1} and receive the reward $r(s_t, a_t, s_{t+1})$. This process will be repeated until a final state is reached. In RL, state transitions typically satisfy the Markov property. This property states that the next state s_{t+1} only depends on the current state s_t and on the action taken at this state a_t. We call the sequence of actions and states from the initial to

the final state an episode. The goal of the agent is to devise an action picking strategy so as to maximise the cumulative reward. I will demonstrate the idea of the cumulative reward with the following example.

Example 2.1
Let's assume we have an episode with two time-steps and an action set with only two possible actions. In the following tree, we can see the different actions we can take at each state and their respective reward.



The cumulative reward, is the summed reward of all the actions taken during an episode. This is shown at the end of the leaf nodes in the example above. Therefore, an ideal decision policy would choose the actions $\{a_1, a_0\}$ in that order for the above episode.

2.2 Q-function

We call Q-function or quality function, a mapping $Q : S \times A \to \mathbb{R}$ that specifies the cumulative reward of picking an action a_t in state s_t. If this function was known the reinforcement learning problem would become quite trivial, as it would simply suffice to pick, at every time step, the action with the highest Q-value.
Unfortunately, as in most real world cases the state space is very large or even infinite. Computing the Q-function exactly is, in most practical cases, infeasible.

2.3 Q-function approximation

The goal of reinforcement learning is to obtain the best possible Q-function approximation. To achieve this, the agent is allowed to interact freely inside of the environment, picking actions randomly or with the till now learned policy. It observes the different results it obtains and updates its policy accordingly.
We shall now briefly introduce a few concepts used during training.

Exploration-exploitation

As mentioned above, during training we either pick the best action with the till-now learned policy or we just pick a random action. The trick is in finding a correct balance between the both of these as each has its own particular advantage. This is called the exploration-exploitation dilemma[Yogeswaran and Ponnambalam 2012]. If we always pick the best action we will converge quickly but the risk of getting stuck in a local minima is fairly high. On the other hand, if we only pick random actions, the convergence will be very slow and we might simply diverge and not be able to find a strategy at all. Most training algorithms start with a high probability of exploration and then as training progresses increase the exploitation probability as to solidify the learned policy.

Learning rate

The learning rate is also part of the exploration-exploitation dilemma. With this ratio we can modify the importance that we give to newly acquired information. The lower it is the harder it will be to overwrite a already learned policy. With a high learning rate we will adapt easier to new problems, but the risk of overfitting will also be higher.

Discount factor

In reinforcement learning, we mostly approximate the Q-function with the following equation:

$$Q'(s,a) = \max_{\pi} \mathbb{E}[r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} | s_t = a, a_t = a, \pi] \tag{2.1}$$

where π is the learned policy.
We call γ the discount factor. It represents the importance that we give to the feature reward. If $\gamma = 0$ then only the immediate reward will be considered and if $\gamma \approx 1$ then we will look for a policy that will give the same importance to the future rewards as to the immediate reward. The same as before one has to choose between a faster convergence and a higher risk of getting stuck in local minima and not learning a global policy.

2.3.1 Q-learning

Q-learning[Watkins and Dayan 1992] is one of the main algorithms used in reinforcement learning for the Q-function approximation. It models the Q-function as a set of basis function where each basis function assigns a value to a (state,action) pair and each feature has its own basis function. Q-learning offers several advantages, it is efficient and converges relatively quickly and the learned policy can be quite easily interpreted. By definition, Q-learning uses a linear function approximation. In most cases this should not cause much of a problem. But, in the case where the ideal decision policy is non-linear, Q-learning will never achieve optimal results.

2.3.2 Deep Q-networks

Deep Q-networks[Mnih et al. 2013] are a novel method used for reinforcement learning that has gained a lot of attention in the recent years. The reason why it has gained so much notice

lately, is due to the ability of a single algorithm being able to achieve very good results on a broad array of tasks without the need of any specialised knowledge about the task beforehand, leading some to call it as the first major steps towards general artificial intelligence.
What separates deep Q-networks from other reinforcement learning methods, is that they use neural networks in order to approximate the Q-function. Neural networks are nonlinear functions. Reinforcement learning has been known to diverge when non-linear function approximators have been used. Various techniques have been developped to combat the divergence of the methods, such as neural fitted Q-iteration [Riedmiller 2005] or experience replay memory [Mnih et al. 2015]. These methods have allowed neural networks to become a viable tool for reinforcement learning and to achieve some very remarkable results. Most notably, [Mnih et al. 2015] were able to design an algorithm that, without the need of any prior knowledge about the task, achieved human level performance on a large number of different games.

Polyhedra Analysis

3

Polyhedra analysis is one of the main tools of static analysis[Cousot and Cousot 1977]. During the execution of a program variables can become bounded, either by numbers or by other variables. Polyhedrons are the most expressive ways of modelling all the different relations that can appear between a set of variables. Different alternatives exist for constraint representation instead of polyhedra, but none are as expressive. Unfortunately, it has worst case exponential space and time complexity meaning that using it on most real-world sized applications would very often cause it to either timeout or to run out of memory making it very impractical. Therefore, other domains have been more widely used such as octagon [Miné 2006], zone [Miné 2001] or pentagon [Logozzo and Fähndrich 2010] , but all of these are less expressive and therefore less precise by design. In the recent years several techniques have been developed that have managed to speed up polyhedra analysis without the loss of precision[Gange et al. 2016, Jourdan 2017, Maréchal and Périn 2017]. We shall now briefly present some of these methods that are useful for this work.

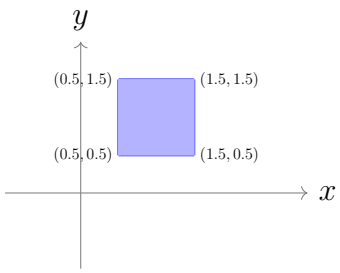
3.1 Polyhedra representation

One of the technique used to increase the performance of static analysis involves the way in which we represent our domain[Singh et al. 2015]. Polyhedra, for example, can be represented with both their constraint representation and their generator representation[Motzkin 1953] . To illustrate these different representations I will proceed with the following example. Lets assume we have the following set of commands:

Example 3.1

$$
\begin{aligned}
&if\ x \geq 0.5 \wedge x \leq 1.5 \wedge y \geq 0.5 \wedge y \leq 1.5 : \\
&\qquad\qquad ... \\
&end
\end{aligned}
$$

Inside of the if statement, the polyhedron would have the following shape:



We can represent this information in two different possible ways.

3.1.1 Constraint representation

In constraint representation we model the polyhedron as the intersection of a finite number of closed half spaces and a finite number of subspace. The resulting polyhedron can be written as:

$$P = \{x \in Q^n | Ax \leq b \wedge Dx = e\} \tag{3.1}$$

where A,D are matrices and b,e are vectors of natural numbers. Therefore, the constraint representation of the above example would be:

$$C = \{-x \leq -0.5, x \leq 1.5, -y \leq -0.5, y \leq 1.5\} \tag{3.2}$$

3.1.2 Generator representation

In order to encode a Polyhedron with the generator representation, we have to model it as the convex hull of three items:

- A finite set $V \in Q^n$ of vertices $v_i \in V$.
- A finite set $R \subseteq Q^n$ of rays. $r_i \in R$ are direction vectors of infinite edges of the polyhedron with one end bounded. The rays start from $v \in V$.
- A finite set $Z \subseteq Q^n$ of lines. $z_i \in Z$ are direction vectors of infinite edges of the polyhedron with both ends unbounded. The lines pass through $v \in V$.

The result of generator representation on the previous example would have the following form:

$$G = \{V = \{(0.5, 0.5), (1.5, 0.5), (1.5, 1.5), (0.5, 1.5)\}, R = \emptyset, Z = \emptyset\} \tag{3.3}$$

3.1.3 Polyhedra domain

Now that we can represent our Polyhedra we can do some interesting calculations with them. The polyhedra abstract domain consists of the polyhedral lattice: $(P, \sqsubseteq, \sqcup, \sqcap, \bot, \top)$, and a set of operators that we can apply on them. The different operators are the following:

- Inclusion test: $P \sqsubseteq Q$
- Equality test: $P = Q$
- Join: $P \sqcup Q$
- Meet: $P \sqcap Q$
- Widening, this operator is applied to accelerate convergence since the polyhedral lattice has infinite height:

$$C_{P \nabla Q} = \begin{cases} C_Q \text{ if } P = \bot; \\ C'_P \bigcup C'_Q, \text{ otherwise;} \end{cases}$$

  where $C'_p = \{c \in C_P | C_Q \vdash c\}$, and
  $C'_Q = \{c \in C_Q | \exists c' \in C_P, C_P \vdash c$ and $((C_P\text{'}) \bigcup \{c\}) \vdash c'\}$ where $C \vdash c$, test wether c can be entailed from constraints in C
- Conditional: let $\otimes \in \{\leq, =\}, 1 \leq 1 \leq n, \alpha \in Q$ then $\alpha x_i \otimes \delta$ adds the constraint $(\alpha - a_i)x_i \otimes \delta - a_i x_i$ to the constraint set C
- Assignement: $x_i = \delta$, first adds x_i to P then augments C with $x_i - \delta = 0$

In the following table we can see the respective complexities of the different operators according to the representation

Operator	Constraint	Generator	Both
Inclusion ($\sqsubseteq$)	$O(mLP(m,n))$	$O(gLP(g,n))$	$O(ngm)$
Join ($\bigsqcup$)	$O(nm^{2^{n+1}})$	$O(ng)$	$O(ng)$
Meet ($\sqcap$)	$O(nm)$	$O(ng^{2^{n+1}})$	$O(nm)$
Widening ($\bigtriangledown$)	$O(mLP(m,n))$	$O(gLP(g,n))$	$O(ngm)$
Conditional	$O(n)$	$O(ng^{2^{n+1}})$	$O(n)$
Assignment	$O(nm^2)$	$O(ng)$	$O(ng)$

$m = |C|, g = |G|, LP(m,n)$ is the complexity of solving a linear program with m constraints and n variables
As we can see no representation is faster than the other, as some of the operators are quicker in one but others in the other. But, as we can see in the last table, when both representations are available all the operators are polynomial.

Chernikova's Algorithm

The first optimisation that one can do is to keep both representations of the the polyhedron and

for each operator pick the representation that minimises the time complexity. A conversion between the two representations is possible thanks to Chernikova's algorithm[Chernikova 1968].

3.2 Polyhedra Decomposition

Another technique used to increase the efficiency of polyhedra analysis, is that of online decomposition [Singh et al. 2017]. It is based on the observation that during the execution of a program, not all it's variables are dependent on one another. Using this observation, we can separate the set of all variables into smaller, independent sets. Therefore, instead of having to represent the whole set of variables with one large polyhedron we can instead represent it with various smaller ones.
Let's assume we have a set of variables χ in a Polyhedron P. The set χ can be partitioned as $\pi_P = \{\chi_1, \chi_2, .., \chi_r\}$, $\chi_i \subseteq \chi$. We call the partitioning of the set permissible iff $\chi_i \cap \chi_j = \emptyset$, $\forall i \neq j$. Once the decomposition has been done in this way, during the execution of an operator, it only has to be executed on the subset of blocks that contain it. This allows for a very large performance gain, giving us the following time complexity for the various operators.

Table 2 Asymptotic time complexity of Polyhedra domain operators with decomposition

Operator	Decomposed
Inclusion ($\sqsubseteq$)	$O(\sum_{i=1}^{r} n_i g_i m_i)$
Join ($\bigsqcup$)	$O(\sum_{i=1}^{r} n_i g_i m_i + n_{max} g_{max})$
Meet ($\sqcap$)	$O(\sum_{i=1}^{r} n_i m_i)$
Widening ($\bigtriangledown$)	$O(\sum_{i=1}^{r} n_i g_i m_i)$
Conditional	$O(n_{max})$
Assignment	$O(n_{max} g_{max})$

Example 3.2
Let's consider the with variables $X = \{x_1, x_2, x_3, x_4\}$ and $C = \{x_1 + 2 \cdot x_3 \leq 10, x_2 = 1\}$. This polyhedron can be partitioned into three blocks $\pi_P = \{\{x_1, x_3\}, \{x_2\}, \{x_4\}\}$ and its corresponding factors are equal to:

$$C_{P_1}\{x_1 + 2 \cdot x_3 \leq 10\}, C_{P_2}\{x_2 = 10\}$$

3.2.1 Decomposition operators

As we change the model of our domains we must equally update the operators inside of these domains. For sake of brevity I will not go into detail about each of them, but I will only talk

about the join operator as it plays an important role for this paper.
During the join of P and Q, most of the time their factors will not be equal($\pi_P \neq \pi_Q$). Therefore, we have to remake their partitions in order for their factors to be equal $\pi = \pi_P \sqcup \pi_Q$. During most joins of a normal execution this will not cause much problem, but during some cases the join can merge all blocks producing the $\top$ partition. In order to rebuild the $\top$ partition from all its blocks we use the following formula:

$$P = P_1 \bowtie P_2 \bowtie ... \bowtie P_r = (C_{P_1} \cup C_{P_2} \cup ... \cup C_{P_1}, G_{P_1} \times G_{P_2} \times ... \times G_{P_r}) \tag{3.4}$$

Due to the cartesian product, building the $\top$ partition can blow up the number of generators and therefore seriously slow down online decomposition.

3.3 Reinforcement Learning for polyhedra analysis

Both of the techniques presented in chapters 3.2 and 3.3, manage to achieve considerable performance gain without having to sacrifice any precision. Unfortunately, at some point compromises have to be made. Analysers that tune the precision and cost based on the program they are analysing are called parametric program analysers. Several such approaches already exist. [Oh et al. 2015, Liang et al. 2011, Heo et al. 2016]
As explained in 3.3.1. one bad constraint can significantly decrease the performance of the whole program. The trick is being able to identify this variable at the correct time. One of the explored solutions to this problem that we shall explore, is training a reinforcement learning algorithm in order to decide when to apply abstractions [Singh et al. 2018].
Intuitively, using reinforcement learning for polyhedra analysis seems quite straight. Let's imagine that for all the operators we have presented above, we have two versions of these O_{pr} and O_{pe}. One of these is a slower and more precise operator and the other, using some sort of abstraction, is faster but not as precise. The goal of the reinforcement learning method would then simply be to select the correct operator at the right time, so that we get the most precise result in as little time as possible. Before this can be done, it is first necessary to initiate polyhedra analysis for reinforcement learning.

3.3.1 Adapting polyhedra analysis for Reinforcement Learning

As explained in 2.1., reinforcement learning uses a defined set of concepts. In some way, these concepts have to be translated into the domain of polyhedra analysis. A possible mapping can be done in the following way.

RL concept	Polyhedra analysis concept
Agent	Static analyzer
State $s \in S$	some features describing the polyhedron
Action $a \in A$	Abstract transformer
Reward function r	some function representing the runtime and precision of a polyhedron

A more in-depth explanation of these concepts will come in the following chapter.

3.3.2 Linear function approximation methods

Existing methods already exploit this idea [Singh et al. 2018]. Using techniques such as Q-learning in order to learn their decision making policies. Q-learning is a common linear Q-function approximation technique and has shown some very good results when applied to the polyhedra domain.
However, recently, new reinforcement learning methods seem to be more focused on the use of nonlinear Q-function approximators, as they seem to give very good results on some complex tasks. When the Q-function of the particular problem is nonlinear, Q-learning will never be able to learn the ideal policy. In these cases, deep Q-networks have a very real opportunity of exceeding the performance of the Q-learning based methods.
The use of nonlinear approximators has not yet been tested on the domain of static analysis. In the following chapters we shall explore the idea of using such methods in order to construct a new decision policy based on neural networks.

Fast polyhedra analysis with deep Q-networks

4

The goal of this work was to build upon the existing solutions used to make polyhedra analysis more efficient and use deep Q-networks to further improve the performance. Specifically, the goal was to extend the Elina Framework [ELINA], the version of it that uses reinforcement learning for polyhedra analysis, in order to replace the Q-learning method with deep Q-networks for the Q-function estimation. Our work can be separated into three major subtasks. First of all, it was necessary to figure out a way of calling a deep neural network from Elina, so that it could be used for the Q-function estimation. Secondly, In order to test out the validity of deep Q-networks on polyhedra analysis and to have a baseline for further optimisation. We decided to implement the basic deep Q-network training algorithm. Finally, we attempted to further optimise this problem with some task specific knowledge.

4.1 Incorporating Neural Networks inside Elina

The first part, whilst definitely being the least interesting was probably the most laborious and a very key part of the whole work. The problem was that for the Q-value estimation we wanted to use neural network regression from the Keras framework in Python. We decided to use this framework as it is very widely used for this type of problem, is relatively easy and intuitive to use whilst remaining very powerful. However, Elina being written in C, the link between the python and C code had to be made. This was finally achieved by using the Python/C API and embedding the python code into the Elina framework. Initialising all the python code as well as importing all the necessary libraries such as Keras, is done in the $op\_pk\_manager\_alloc()$ function so that it does not have to be done every time the join function is called. Inside the join function we simply have to call the learning or prediction algorithms.
One advantage of such a modification to the framework, is that we can now learn online. In comparison to [Singh et al. 2018] where the training was done offline. Online training allows the algorithm to pick the best action according to the current decision policy. This is a very important feature for deep Q-networks, as it allows us to set an exploration rate and to reinforce the already learned policy, this is vital to prevent divergence.

4.2 Basic algorithm

In order to get the basic training algorithm working, first the domain of polyhedra analysis has to be made compatible with the domain of reinforcement learning. Therefore the following list of items have to be initialised inside of the polyhedra domain:

- A set of features describing the polyhedra to use as states S
- A set of actions A
- A reward function r

Luckily, since a reinforcement learning method [Singh et al. 2018] has already been used for polyhedra analysis we can simply reuse what has already been developed for our baseline algorithm.

4.2.1 Features

The reinforcement learning method uses a set of nine different features.

- The number of blocks.
- The minimal, maximal and average size of a block.
- The minimal, maximal and average size of the generator set off the union of input factors corresponding to a block.
- The number of variables with finite upper and lower bound.
- The number of variables with one finite and one infinite bound.

We will start off by reusing the same features. However we will modify their bucketing, since, due to the nature of the Q-learning method, it is very restrictive. The new bucketing will be discussed in section 4.3.2.

4.2.2 Actions

As we discussed in 3.3.1., the bottleneck of the decomposed analysis is the join. Therefore, the set of actions will be composed of various joins of different precision and performance.
First of all, the cost of the joins depends on the size of the block. Therefore, bounding the the size of the block with a threshold would increase the performance. These four different thresholds are used $threshold \in [5, 9], [10, 14], [15, 19], [20, \infty)$
Once we have decided on the size of a threshold we have to equally decide on what to do if the block has a greater size than the threshold. Their are different possibilities of how to split a large block into smaller ones, but basically, one has to pick a subset of constraints to remove from the block so as to make some of the variables no longer dependant and then it can be further partitioned. The following three constraint removals are used:

Stoer-Wagner min-cut

This algorithm is based on the simple idea of removing the minimal amount of constraints in order to be able to split the block into two separate permissible partitions [Stoer and Wagner 1997].

Weighted constraint removal

The second and third constraint removal techniques are based on the same principal. They associate a certain weight to each constraint and then remove the constraint with the highest weight. Two different weight distribution techniques are considered.
In the first one, we first compute for each variable $x_i \in X$ the number of constraints it appears in, we can call this n_i. Then for each constraint c_i we set its weight to the sum of n_i of all the variables that are in the constraint.
The second method, we first compute for each pair of variables $x_i, x_j \in X$, n_{ij} the number of constraints containing both x_i and x_j. The weight of the constraint is then the sum of all the n_{ij} of all the pairs of variables x_i, x_j contained in the constraint.
The idea behind removing the constraint with maximal weight, is that, most likely the variables with a large weight also occur in other constraints and therefore will not become unbounded once the constraint is removed. In this way we retain precision.

Merging blocks

The next three actions are various block merging strategies. The idea is to select different blocks and merge them together as long as the resulting blocks remain below the threshold in order to increase the precision of the subsequent join. The following three block merging strategies are used:

- No merge, no blocks are merged
- Merge smallest first, we first merge the smallest two blocks together. We then remove the smallest block and continue as long as the resulting merge remains below the threshold.
- Merge small with large, similar to the previous strategy but this time me merge the smallest block with the largest.

In total we have four different thresholds, three different constraint removal algorithms and three different block merging strategies. We can mix and match these together as we please, which means that in total we have $4 \cdot 3 \cdot 3 = 36$ different actions we can pick.

4.2.3 Reward

As a reminder, the objective of the reward is to guide our learning policy, rewarding it when it takes actions towards our global goal and penalising it when it does otherwise. Therefore, the reward developed by the Q-learning method was the following:

$$r(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} - \log_{10}(cyc) \tag{4.1}$$

Where n_s is the number of exactly defined variables of the resulting polyhedron after the join. n_b is the number of bounded variables and n_{hb} the number of semi-bounded variables of the resulting polyhedron. cyc is the number of cycles required to perform the join.

4.2.4 Back to deep Q-networks

As we have finally initialised polyhedra analysis for the use with reinforcement learning. We can finally proceed to the more interesting part of designing the training algorithm. Under its most basic form, the training algorithm could simply be the following. Pick a random reward or maximal action, observe the reward and then retrain the network with the observed reward plus the discounted future reward on the given action. This very basic algorithm however does not work very well as it runs into two major complications.

Divergence of decision policy

The first of which is the divergence of the action selection strategy. Meaning that the neural networks were not able of creating a consistent strategy but would be picking different actions almost randomly all the time.

Divergence of the action value prediction

The second problem was that the predictions of the estimators would diverge towards infinity. This is also known as the exploding gradient problem.

These problems are not new and are a fundamental problem of trying to use non-linear functions for the Q-function approximation. Several techniques exist to combat these problems. Many of which reduce the complexity of the network and/or the problem in general. However, some new methods have been developed recently that would allow the training of the estimators whilst retaining the problems original complexity. We decided the use the following two concepts inside of the algorithm.

4.2.5 Experience replay memory

Experience replay memory [Mnih et al. 2015] is a biologically inspired mechanism. That gives the estimator a very basic concept of a memory and instead of directly learning from the current events happening. The agent learns from a random subset of its memory. More formally, during training, an array of a certain size filled with the past memory objects is kept. Each memory item contains the following items: $mem(s_t, a_t, r_t, s_{t+1})$. The current state, the action taken at this state, the observed reward and the next state. For training we then simply pick a random subsample from the memory array and train from these examples.
The objective of the memory is to homogenise the training data. It comes from the observation that during the execution of a program, often a particular strategy would be optimal for a certain period of time and afterwards another one would be the new optimal. This causes two major problems. First of all, it is not very time efficient as we do not gain much information by learning from the same data. Secondly, as there is low diversity in the training data and the decision strategy would frequently abruptly change. This either leads to the neural network getting stuck in local minima or simply to diverge and not obtain a policy.
Picking a random subsample from memory helps increase the variance amongst the training data allowing the network to learn a more global policy.

4.2.6 Separating target from max Q estimators

The other method used to reduce the divergence of the predicted Q-values towards infinity, was to reduce the correlation between the training and the prediction data [Mnih et al. 2015]. This was done because, since the networks are being fitted partly on the maximum Q-value estimation, diverging towards infinity reduces their error and therefore is a valid strategy that the networks can exploit. In order to reduce this correlation, the networks predicting the maximum Q-value and the ones predicting the Q-value can be separated. The weights of the maximum Q-value estimators are then updated every n steps in order for them to remain up to date.

Further modifications were also made on the neural network level in order to reduce these problems. We will get into these in part 4.4.
Once these modifications have been made the basic training algorithm has the following form.

Pseudo code of basic learning algorithm

Algorithm 1: DQN Training algorithm

function learn $(S, A, r, \gamma, \alpha, \phi, N, l\_freq, b\_size, update\_nn\_freq, \varepsilon)$;

Input :

$S \leftarrow states, A \leftarrow Actions, r \leftarrow reward,$
$\gamma \leftarrow discount\ factor, \alpha \leftarrow learning\ rate,$
$\phi \leftarrow$ set of feature functions over S and A
N $\leftarrow$ size of memory, l_freq$\leftarrow$ learning frequency,
b_size $\leftarrow$ batch size, $\varepsilon \leftarrow$ random action probability,
update_nn_freq $\leftarrow$ frequency of updating max Q estimators

Output:

$\theta \leftarrow$ trained weights of the estimator

$\theta =$ initialise random weights and learning rate α
$\theta_{max} =$ initialise random weights and learning rate α
$M =$ initialise an empty memory with size N
for *each episode* **do**
  start from initial state $s_0 \in S$
  for $t = 0, 1, 2, ...$ **do**
    Initialise new memory item m_t
    With probability ε take random or maximal action a_t
    observe next state s_{t+1} and $r_t(s_t, a_t, s_{t+1})$
    Set $m_t.a = a_t, m_t.s_1 = s_t, m_t.s_2 = s_{t+1}, m_t.r = r_t$
    if $M_{size} \geq N$ **then**
      del M_0
      $M_N = m_t$
    else
      push m_t on M
    if $t \mod l\_freq = 0$ **then**
      select a random batch of size b_size from m
      compute $Q(:, s_t)$ estimation with θ
      compute $Q(:, s_{t+1})$ estimation with θ_{max}
      set $Q(a, s_t) = Q(a, s_t) + \gamma * max(Q(:, s_{t+1}))$
      Fit weights θ with new training data
    if $t \mod update\_nn\_freq = 0$ **then**
      set $\theta_{max} = \theta$
  end
end
return θ

4.3 Further optimisations

Once the basic version of the deep Q-network algorithm was designed we were able to train it, test it and obtain our first set of results. The discussion of these will be done in chapter 5. These results can from now on be used as a baseline and we will attempt to further improve our results.
In the search of a more efficient algorithm, we decided to incorporate some problem specific knowledge to the deep Q-network algorithm. As well as further optimisations to the feature vector and reward functions. The modifications made will be discussed in the rest of this section.

4.3.1 Separating the problem into two

The first problem specific modification was subdividing the problem into two independent subproblems. The objective of Polyhedra Analysis is to obtain the most precise result in the quickest way possible. These are two independent objectives. The goal was therefore to separate these two tasks and create two independent subsystems, one focusing on making the results as precise as possible, and the other on the time complexity of getting there.
Such a division of the problem, offers two main advantages. Firstly, a greater flexibility during training. The parameters of each system can be tuned for its specific needs. So for example, the characteristics of the neural network or the discount factor. Furthermore, the optimal features used for precision and performance estimation, are most likely different. The separation therefore allows us to use only the necessary features for each subsystem making the learning and prediction less complex and therefore more precise and converge faster. The reward as well can be fine tuned for the needs of the specific subsystem.
Secondly, two separate subsystems also allow for a more flexible algorithm post training. Since during training, we will have two different Q-function estimators, during prediction we will have a greater possibility of optimising our results by changing the importance we give to each subsystem at different points in time according to the specific needs. We will get into more detail about this in the section 4.3.4.
The pseudo code for the training algorithm with separated estimators has the following form:

Pseudo code of the separated training algorithm

Algorithm 2: DQN Training algorithm

function learn $(S, A, r, \gamma, \alpha, \phi, len, l\_freq, b\_size, update\_nn\_freq)$;

Input :

$S \leftarrow states, A \leftarrow Actions, r \leftarrow reward,$
$\gamma \leftarrow discount\ factor, \alpha \leftarrow learning\ rate,$
$\phi \leftarrow$ set of feature functions over S and A
len $\leftarrow$ size of memory, l_freq$\leftarrow$ learning frequency,
b_size $\leftarrow$ batch size,
update_nn_freq $\leftarrow$ frequency of updating max Q estimators

Output:

$\theta_1 \leftarrow$ trained weights of neural network for performance
$\theta_2 \leftarrow$ trained weights of neural network for precision

$\theta_1 =$ initialise random weights
$\theta_2 =$ initialise random weights
$\theta_{1\_max} =$ initialise random weights
$\theta_{2\_max} =$ initialise random weights
$m =$ initialise an empty memory
for *each episode* **do**
  start with initial states $s_{pr\_0} \in S, s_{pe\_0} \in S$
  for $t = 0, 1, 2, ...$ **do**
    Initialise new memory item m_t
    Take action a_t according to the action selection algorithm
    observe next state s_{pr_t+1}, s_{pe_t+1} and $r_{pe}(s_{pe\_t}, a_t, s_{pe\_t+1}), r_{pr}(s_{pr\_t}, a_t, s_{pr\_t+1})$
    Set $m_t.a = a_t, m_t.s_{pr\_1} = s_{pr\_t}, m_t.s_{pe\_1} = s_{pe\_t}, m_t.s_{pr\_2} = s_{pr\_t+1}, m_t.s_{pe\_2} = s_{pe\_t+1}, m_t.r_{pr} = r_{pr}, m_t.r_{pe} = r_{pe}$
    if $m_{size} \geq len$ **then**
      del m_0
      $m_{len} = m_t$
    else
      push m_t on m
    if $t \mod l\_freq = 0$ **then**
      select a random batch of size b_size from m
      compute $Q(:, s_t)$ estimation with θ_1, θ_2
      compute $Q(:, s_{t+1})$ estimation with $\theta_{1\_max}, \theta_{2\_max}$
      set $Q(a, s_t) = Q(a, s_t) + \gamma * max(Q(:, s_{t+1}))$
      Fit weights θ_1, θ_2 with new computations from this batch
    if $t \mod update\_nn\_freq = 0$ **then**
      set $\theta_{1\_max} = \theta_1, \theta_{2\_max} = \theta_2$
  end
end
return θ_1, θ_2

4.3.2 Feature selection

Before we get into the specific features that were used for the estimators, lets go a bit more in-depth about the theory of features and states. In the case of polyhedra analysis states would be the concrete Polyhedra. However, during our analysis we do not use the concrete polyhedra as this would be too complicated, but rather some information that we extract from them, we collect this information inside of the feature vector. As explained in section 2.1., for reinforcement learning, states should respect the Markov property, which states that state s_{t+1} only depends on s_t and on a_t. Whilst this is the case for the polyhedra, our feature vectors do not necessarily obey this property as they do not represent the polyhedra themselves but only some information about them. The more precisely we manage to describe our polyhedron the closer we will be to respecting the Markov property and the better will be the results of reinforcement learning.

With regards to the old set of features. One big inconvenience of using Q-learning, is that, since we want to represent our Q-function with basis functions, the size and dimensions of our feature vector is very limited. This constraint no longer holds when using more advanced methods such as deep Q-networks. This allowed us to make two major changes about the feature vector.

Adding new features

The first change we made, was adding some new features.First of all, we reused the nine features from the Q-learning algorithm. As a reminder these features are the following: the first seven features are used to characterise the complexity of the join. They are the number of blocks, minimal, maximal and average size of the blocks and the minimal, maximal and average size of the generator set. The last two features are used to characterise the precision of the inputs and they are the number of variables with a finite upper and lower bound, as well as the number of variables with a finite upper or lower bound, in both Polyhedra.
We further extended this set with four new features, in order to further increase the description accuracy of the feature vector. The selection of these features was done by trial and error, with an experimental observation of an increase, or lack thereof, of accuracy. It is also possible to check whether a particular feature is useful once training is finished by analysing the neural network and observing the impact a particular feature has on the end result. However, since at the end our network has a total of four layers, this made its analysis somewhat complicated.
At the end, we decided to add a total of four new features, three of which are used for modelling the precision and one for the complexity. For the complexity, we added the number of variables. As for the precision, we added the number of unconstrained variables, the number of exactly constrained variables and finally, the sum of the values the bounded variables can have (i.e. an approximation of the circumference of the polyhedra). We also attempted using some features that would have perhaps modelled the precision more accurately, such as most notably approximating the volume of the polyhedra. Unfortunately, one must also consider the complexity of computing the features. The computation of the volume approximation was far too time complex, which greatly increased the learning time making the feature not viable.

Bucketing

Due to the limitations of Q-learning the old algorithm uses a very restrictive bucketing policy.

Deep reinforcement learning does not suffer from such restrictions. It was therefore possible for us to remove the bucketing from the feature selection. We still decided to implement a version of bucketing inside of the algorithm for three main reasons.
Firstly, for features with very big values an exact precision is not needed. For example, for the feature that approximates the circumference of the polyhedra, its total value can be very big and and if it is a million and one or just a million doesn't impact the resulting precision much, therefore bucketing does not impact it either.
The second reason, for the use of bucketing is that it greatly decreases the learning time and helps convergence.
Finally, the last reason is, so that the decision policy does not give more importance to some features simply because they are larger in value than others. In total we have thirteen different features and they can all have very different values. For example, the number of blocks varies mainly between one and ten and the circumference of the polyhedra can go up to 10^9. This does not mean that the circumference has a greater impact on the overall description of the polyhedron. Bucketing assures that all features have a similar impact on the decision policy.
In order to decide the values of the bucketing that would be used, the algorithm was run on a big number of benchmarks computing the maximal, minimal and average values the different features could have. Finally, they were scaled in such a way, so that they would all approximately remain between the bounds of zero and ten. The resulting bucketing has the following form:

Feature	Extraction complexity	Approximate range	Scaling
$\lvert\beta\rvert$	$O(1)$	1-10	$x/1.$
$min(\lvert\chi_k\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-50	$round((x/5), 0.5)$
$max(\lvert\chi_k\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-50	$round((x/5), 0.5)$
$avg(\lvert\chi_k\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-50	$round((x/5), 0.5)$
$min(\lvert\bigcup G_{P_m}(\chi_k)\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-10000	$round((x/1000), 0.1)$
$max(\lvert\bigcup G_{P_m}(\chi_k)\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-10000	$round((x/1000), 0.1)$
$avg(\lvert\bigcup G_{P_m}(\chi_k)\rvert : \chi_k \in \beta)$	$O(\lvert\beta\rvert)$	1-10000	$round((x/1000), 0.1)$
$\{\lvert x_i \in X : x_i \in (-\infty, \infty)$ in $P_m\rvert\}$	$O(ng)$	1-100	$round((x/10), 0.5)$
$\{\lvert x_i \in X : x_i \in [l_m, \infty)$ in $P_m\rvert\}+$ $\{\lvert x_i \in X : x_i \in (-\infty, u_m]$ in $P_m\rvert\}$	$O(ng)$	1-50	$round((x/5), 0.5)$
$\{\lvert x_i \in X : x_i \in [l_m, u_m]$ in $P_m\rvert\}$	$O(ng)$	1-50	$round((x/5), 0.5)$
$\{\lvert x_i \in X : x_i \in [u_m, u_m]$ in $P_m\rvert\}$	$O(1)$	1-200	$round((x/20), 0.2)$
$\lvert X\rvert$	$O(ng)$	1-50	$round((x/5), 0.5)$
$\sum(u_m - l_m) : u_m, l_m \in \{[l_m, u_m]$ in $P_m\}$	$O(ng)$	$2 * 10^9$	$round((x/2 * 10^8), 0.01)$

One thing to note is, that opposed to the reinforcement learning algorithm, these features do not have a maximal possible value. We believe that this increases the precision of the Q-function

estimation, especially for the approximation of the complexity. Certain features can have very large values and we believe that when this arrives, it has a major impact on the complexity of the join. However, these very large values were ignored by the bucketing of the Q-learning algorithm.

4.3.3 Reward Function modelling

Due to the nature of the new algorithm, the modelling of the reward function was separated into two separate subproblems.

Performance reward

Firstly, the reward for the precision estimator and then the reward for the performance estimator. Modelling the complexity is fairly simple and very straight forward, as simply counting the number of cycles needed for the computer to execute the join perfectly models the joins complexity and is exactly what we want to optimise. One thing to note is that we want this reward to be as small as possible, two simple solutions for this are either to invert it or to negate it. After some experimentation with both of these we decided that negating it produces better results. This is probably due to the fact, that inverting the reward makes it have a nonlinear curve and its derivative looses importance the higher the CPU cycles are, which is not something we want to model. Another thing to note is that modelling the complexity reward in this way give us another advantage over the reinforcement learning version of the algorithm. The Q-learning algorithm took the $\log_{10}$ off the CPU Cycles in order for the complexity and the precision reward to have similar values. We believe that this produces a similar problem as inverting the reward. The reward is no longer linear and its differences loose importance the higher it gets. Once again, this is not something that we want to model. The final rewards has the following form:

$$r_{pe}(s_t, a_t, s_{t+1}) = -1 \cdot cyc \tag{4.2}$$

Where cyc is the number of CPU cycles needed to perform the join.

Precision reward

As to the second reward, modelling the precision of the resulting join. This is considerably more difficult than modelling the complexity as there is no trivial element giving us the precision of our polyhedron. In order to choose the reward, we proceeded by intuitively picking a small set of options and verifying them experimentally at the end. At the end, we tested out three different reward.

We took the first one from the reinforcement learning algorithm, that is, its objective is to maximise the amount of exactly bounded, bounded and half bounded variables. The second is a further extension by penalising the amount of values a bounded variable can have in the resulting Polyhedra. The final, reward function is slightly different. In this one, we penalise the loss of an exactly bounded, bounded or half bounded variable. Reward the loss of a unbounded variable and penalise the amount of values a bounded variable can have. We also tried basing a reward function on an approximation of the volume of the resulting Polyhedra, unfortunately, the complexity of this computation was too high which made it too impractical to use. The final

rewards have the following form:

$$r_{pr_1}(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} \tag{4.3}$$

$$r_{pr_2}(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} - \log_{10}(|n_b|) \tag{4.4}$$

$$r_{pr_3}(s_t, a_t, s_{t+1}) = 3 \cdot (n_{s_f} - n_{s_i}) + 2 \cdot (n_{b_f} - n_{b_i}) + (n_{hb_f} - n_{hb_i}) - \log_{10}(|n_b|) \tag{4.5}$$

Where n_s is the number of exactly defined variables of the resulting polyhedron after the join. n_b is the number of bounded variables and n_{hb} the number of semi-bounded variables of the resulting polyhedron. n_{x_f} is the number of variables after the join and n_{x_i} before the join.

4.3.4 Action selection algorithms

As discussed before, the Q-function estimation was separated into two independent subproblems. As we have already mentioned earlier, this allows a certain amount of benefits that would not be possible otherwise. However, it also imposes one major complication. These two subproblems are not totally separable, as once we have predicted the two Q-function estimations, we have to somehow merge the information contained in both of these estimations and pick an ideal action accordingly. We tried out a few different action selection algorithms in order to find the one that maximises precision and performance the most. One thing to note is that it is at least partially possible to test out these algorithms post training. That is to say that we do not have to train using these in order to measure their performance afterwards. This only works if we train purely randomly however. As if, if we were to train using one selection algorithm and then test with another, this would surely deteriorate the results for the other algorithm. The fact that we are able to test the selection algorithms after random training is still very helpful as the training time is relatively high and having to train for each algorithm would be very time intensive.

Algorithm 1

The first selection algorithm we used is perhaps the most intuitive one. First scaling both predictions. The performance one between [-1,0] and the precision one between [0,1]. Adding the values together and picking the action with the maximal value. Whilst seeming very fair this type of selection has a couple of fundamental flaws. First of all, reinforcement learning estimates the best action to take in order to maximise the long-term objective, it however has less of a guarantee about the second to best and third to best action. This means that if the network is well trained, the chances that the action with the maximal Q-value prediction is also the best action to take at this point in time should be quite high. However, the guarantee that the action with the second highest Q-value prediction is the second-best action to take is much smaller. Using this selection algorithm tends to quite often not choose the best action but the second best or the third etc... making the probability that they are also good actions also a lot smaller. The second problem with this type of selection algorithm is that scaling the reward function causes a loss of information that could be very important. Lets demonstrate this with an example, let's say we have four joins j1,j2,j3,j4. J1 takes one second, j2 ten seconds, j3 one hour and j4 ten hours. Let's also say that j1 and more precise than j2 and j3 is more precise than

j4. This algorithm is going to treat the difference between j1 and j2 the same as the one between j3 and j4, even though the gain in precision might be worth to loss in performance for the case of j1 and j2, whilst this would probably not be case for j3 and j4.

Pseudo code of algorithm 1

Algorithm 3: Action selection algorithm 1

function select1 (Q_{pr}, Q_{pe});
  Input :
    Q_{pr} ←array of Q-function estimations for precision,
    Q_{pr} ←array of Q-function estimations for performance
  Output:
    a ← action to take
  $Q_{pr} = Q_{pr}/max(Q_{pr})$
  $Q_{pe} = Q_{pe}/min(Q_{pe})$
  $a = max_{arg}(Q_{pr} + Q_{pe})$
  return a

Algorithm 2

The second algorithm used, that was designed to confront both problems of the previous algorithm, proceeds as follows. We set some sort of threshold for the performance. We then look at the action that has the maximal Q-value for precision. If this actions Q-value for performance is above the threshold we take it otherwise we take the second-best action and continue until we find an action that is above the threshold. Again, this algorithm seems quite good at first glance and maybe if it was executed perfectly it would be the best option, but like the one before it has some fundamental problems. First of all, picking a threshold is not a very simple task. The predictions are done with regression neural networks, the activation function of there last layers are linear, this means that the output values are unbounded and they do not have a direct correlation with Realtime CPU cycles. In order to pick a threshold, we had to experimentally try different possible values and observe the resulting precision and adjust accordingly, however this threshold would vary according to the benchmark and therefore choosing an optimal one was a very difficult task on its own. Another problem of this algorithm is that if no action has a Q-performance estimation above the threshold the algorithm will choose the action with the worst precision, and this one does not even have to have the best performance estimation.

Pseudo code of algorithm 2

Algorithm 4: Action selection algorithm 2

```
1 function select2 (Q_pr, Q_pe, PE_thresh);
      Input  :
               Q_pr ←array of Q-function estimations for precision,
               Q_pr ←array of Q-function estimations for performance,
               PE_thresh ←performance threshold
      Output:
               a ← action to take
2     while max(Q_pr) ≠ 0 do
3         a = max_arg(Q_pr)
4         if Q_pe(a) ≥ PE_thresh then
5             break;
6         Q_pr(a) = 0
7     end
8     return a
```

Algorithm 3

Another possibility is to slightly modify the previous algorithm in order to minimise some of its short comings. This time we set both some sort of a threshold for the performance and a certain number x. if the action that has the highest precision estimation is under the threshold for performance, we take the x best actions according to their precision and take the one that has the highest performance estimation. The problem of picking an appropriate threshold remains the same and this time we have the further problem of picking a correct value for x. However, the case that all actions are under the threshold is no longer a problem. It is worth noting that this algorithm also has a greater time complexity, however this is still greatly outweighed if the correct action is taken.

Pseudo code algorithm 3

Algorithm 5: Action selection algorithm 3

```
1  function select3 (Q_pr, Q_pe, PE_thresh, N_act);
       Input  :
                Q_pr ←array of Q-function estimations for precision,
                Q_pr ←array of Q-function estimations for performance,
                PE_thresh ←performance threshold,
                N_act ←number of actions to consider if below threshold
       Output:
                a ← action to take
2      a = max_arg(Q_pr)
3      if Q_pe(a) ≤ PE_thresh then
4          a_max = a
5          val_max = Q_pr(a)
6          Q_pr(a) = 0
7          for i ∈ N_act do
8              a = max_arg(Q_pr)
9              if Q_pe(a) ≥ val_max then
10                 a_max = a
11                 val_max = Q_pe(a)
12             Q_pr(a) = 0
13         end
14     return a_max
```

Algorithm 4

Finally, the last selection algorithm that we will present here is based upon the previous one, but modified in such a way as to reduce the importance of correct parameter choosing. This time we begin by scaling the performance prediction to [-1,0]. We set a threshold between [0,1]. We pick the action that has the highest Q-precision estimation. If the absolute value of this action's performance estimation minus the maximal performance estimation is below the threshold, then we pick this action otherwise we pick the second-best precision action until we find one that is below the threshold. This time, since we compare to the best performance action we are guaranteed to be below the threshold at some point, therefore, in the worst case we will pick the action with the best performance. The threshold is also a lot easier to set since it is bounded. Unfortunately, once again we have the problem caused by the scaling of the performance estimation. However, after some experimental observation, we observed that when the join is fast all the Q-performance estimations tend to be quite close together, so hopefully this should not be all too much of a problem.

Pseudo code algorithm 4

Algorithm 6: Action selection algorithm 4

function select4 $(Q_{pr}, Q_{pe}, PE_{thresh})$;
Input :
Q_{pr} ←array of Q-function estimations for precision,
Q_{pr} ←array of Q-function estimations for performance,
PE_{thresh} ←performance threshold
Output:
$a \leftarrow$ action to take
$Q_{pr} = Q_{pr}/max(Q_{pr})$
$Q_{pe} = Q_{pe}/min(Q_{pe})$
while $True$ **do**
  $a = max_{arg}(Q_{pr})$
  if $Q_{pe}(a) + PE_{thresh} \geq max(Q_{pe})$ **then**
    break;
  $Q_{pr}(a) = 0$
end
return a

4.4 Neural network characteristics

As for the characteristics of the neural network that is used. We started with a relatively small neural network and then grew it progressively as the number and size of the features was expanded. In the final version we use a fully connected neural network with four hidden layers of two hundred nodes each. They have each thirteen inputs, one for each feature and thirty-six outputs, one for each action. The first three layers use the Relu activation function and the last one uses a linear activation, since the rewards can be either negative or positive. We use stochastic gradient descent for updating the weights of the nodes and clip its norm to 1. We do this in order to avoid the exploding gradients problem and prevent the predicted values to diverge towards infinity. To calculate the loss, the mean squared error is used. The characteristics of the neural networks are based on related work as these types of networks seem to be the most widely used ones for deep reinforcement learning. It is worth noting that we decided not to do much parameter optimisation on the neural networks as the training time for the algorithm is quite long which would make parameter optimisation a very tedious task. It is also worth noting that we used the same network models for both performance and precision prediction.

4.5 Training

The training of the algorithm was done in multiple stages. During the first stage, only random actions were picked. This was done in order for the algorithm not to get stuck in local maxima but have the most global policy possible. We also did not have too large time constraints about the length of training so we could afford to proceed in this way in order to get the best possible results. Throughout the next stages, the training was separated into two. One concentrating on

the precision and the other on the performance. All the actions were no longer chosen randomly, but now the action with the highest predicted value was chosen. The probability with which we chose a random action was progressively decreased throughout training. This was done in order to reinforce the choice of the best action and increase convergence speed. Once these stages finished, we would have two separate systems each optimised for their own task. In the final stage, we would then combine both of the systems and do a final training phase with the chosen action selecting algorithm as described above. We did this in order to further optimise the decision policy for the particular action selection algorithm.
There were two major complications that came up during training, that had to be dealt with. The first of these was that, especially during random training the likelihood of getting stuck on some join and not finishing the analysis of a benchmark was quite high. To confront this we set a timeout of thirty minutes on each benchmark. The goal of this is to find a compromise between having enough time to get to interesting joins and not wasting too much time in case the analysis gets stuck on a certain join. The other problem was that the analysis is very sensitive. That is to say, that one bad action can have severe consequences on the end precision of the analysis. This means that training with a low probability of picking random actions was essential for the estimators and had to be given enough time, but not too much so that we would avoid overfitting. This method of training is quite time intensive. We decided to proceed in this way since time was not a big factor but the end results were more important. A more efficient training strategy can surely be found if this is needed.

Experimental Results

5

As described in the previous chapter, different strategies were elaborated for the reward function and the action selection algorithm. Training all possible combinations and then observing the end precision would be a viable way of finding the optimal combination of these. However, due to the training and testing complexities of the algorithms, this would be very time intensive. Instead, we designed a set of experiments that should be able to indicate which methods are more optimal.

Precision measuring

In order to measure the precision of the result, we observe the fraction of program points at which the Polyhedra invariants generated by our various algorithms is semantically the same as the one generated by ELINA without any abstraction.

Training/Testing set

The algorithms were trained on 328 different benchmarks following the steps mentioned in 4.8. The testing set consist of 81 different benchmarks that were chosen part randomly and part due to their complexity. To avoid overfitting, the testing and training sets do not overlap.

5.1 Reward function selection

As a reminder, if we view the problem as a decision tree, and the role of reinforcement learning to pick the best path at each node. The reward function can be viewed as the compass of the reinforcement learning algorithm that should lead it to the end in such a way as to maximise the global goal.

We decided to measure the effectiveness of each reward function by observing if the direction it steered the algorithm to, was indeed correctly maximising this global goal. To achieve this, we would first train an algorithm with each of the different reward functions. Once this was done, we modified the Q-learning version of the algorithm so that during testing it would measure each of the different reward functions. As a reminder, the Q-learning algorithm was trained with the following reward function:

$$r(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} - \log_{10}(cyc) \tag{5.1}$$

We then ran the Q-learning algorithm with each of the reward functions, measuring their reward during the execution. The decision of wether or not the reward function was correct was then

made with the following rule:
If the reward of the deep Q-network algorithm was higher than the one of the Q-learning algorithm, but its overall precision was not higher. This would imply that the deep Q-network was correctly learning to maximise the reward, but that this reward was not maximising the overall performance of the algorithm and therefore that it was not a good reward.
As a reminder, the rewards tested are the following:

$$r_{pr_1}(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} \tag{5.2}$$

$$r_{pr_2}(s_t, a_t, s_{t+1}) = 3 \cdot n_s + 2 \cdot n_b + n_{hb} - \log_{10}(|n_b|) \tag{5.3}$$

$$r_{pr_3}(s_t, a_t, s_{t+1}) = 3 \cdot (n_{s_f} - n_{s_i}) + 2 \cdot (n_{b_f} - n_{b_i}) + (n_{hb_f} - n_{hb_i}) - \log_{10}(|n_b|) \tag{5.4}$$

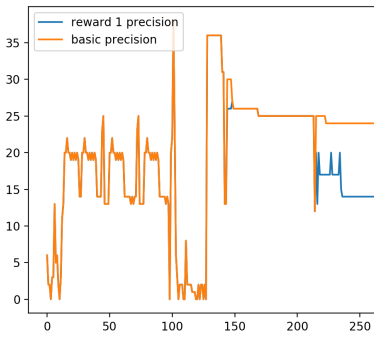


Figure 5.1: *Reward one*

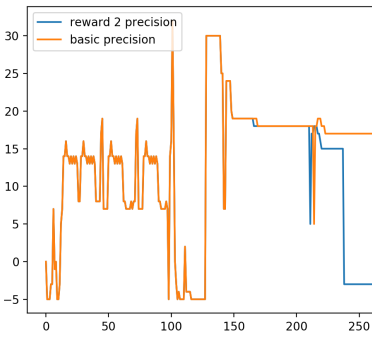


Figure 5.2: *Reward two*

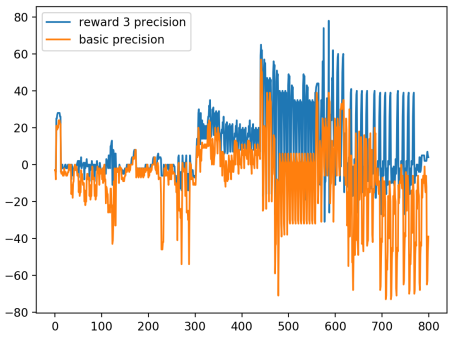


Figure 5.3: *Reward three*

These are the graphs of the evolution of the precision reward according to the number of joins. The orange line represents the measured reward whilst running the Q-learning algorithm and the blue line the measured reward of the deep Q-network algorithm trained with this reward as well. The overall precision of the end polyhedra are the following: For Figure 5.1. 99% for Q-learning and 96% for DQN. For figure 5.2. 99% for Q-learning and 94% for DQN. For figure 5.3. 97% for Q-learning and 90% for DQN. Whilst these graphs behave as expected in the first two scenarios, that is that the reward is lower for the algorithm with lower end precision as well. In the last graph we can see something unexpected. Whilst the DQN algorithm has a higher reward throughout most of the execution of the program having an average of 9 versus -8 for the Q-learning algorithm. This tells us that whilst the DQN has learned a correct strategy for maximising the reward, this reward does not guide us to the overall goal of maximising the end precision and therefore reward three is not an optimal reward function. These experiments do not give us much information on the differences between reward one and two as they both behave as normally. This is to be expected as reward one and two are similar.
It is worth noting that whilst these experiments do give us some interesting information about the optimality of the different reward function, the results are heavily dependant of the benchmark we run them on and therefore the results cannot be fully trusted. However, with the information gathered by these experiments as well as some overall testing I decided to use the second reward function in further experiments.

5.2 Action selection algorithm

The second problem was selection the best action selection algorithm. In section 4.8., four different action selection algorithm were described. In order to select the best one of these four, I proceeded by training an algorithm using each of these four selection algorithms and then comparing the overall precision. Not all the training had to be done separately for the four different action selections. Firstly, we could train estimators from only random actions and then simply specialise each of them with their own action selection algorithm. I then compared the results on a set of seven different benchmarks.

Benchmark	Q-learning	Algorithm 1	Algorithm 2	Algorithm 3	Algorithm 4
driver-media	99.0	98.6	97.6	93.2	98.0
linux-kernel-locking-spinlock	99.9	94.4	63.6	79.9	95.0
linux-usb-dev	58.2	51.8	60.3	56.5	59.3
linux-kernel-locking-mutex	77.1	73.2	95.5	95.6	76.1
complex-emg-drivers-net	57.1	97.3	94.6	96.0	96.9
complex-emg-drivers-media	57	50.1	58.9	55.4	54.9
complex-emg-linux-alloc-spinlock	44.9	72.2	69.9	91.8	72.0

As to the choice of benchmarks for this experiment. I had several criteria. First, I picked benchmarks where achieving a high level of accuracy was not too easy in order to have more informative results. Second, I picked benchmarks that were fast to compute so that the testing time would be fast. I also picked fast benchmarks because my goal was to find an algorithm that maximised the precision as each of these algorithms can be then optimised with its own parameters in order to ameliorate performance and in this way I only had to concentrate on precision.
As to the results of these experiments. Unfortunately there is not overall best algorithm. As discussed in section 4.8., each of these algorithms has its advantages and shortcomings. However, the main objective I was looking for from these experiments was finding an algorithm that would be stable. We can see that algorithms two and three can obtain very good on some benchmarks. Unfortunately, they also perform very bad on others. This is due to the fact that both of these are threshold based and picking an optimal threshold that would work well for all benchmarks is very difficult, making both of these algorithms not practical. Afterwards, between the first and fourth algorithm, the last one outperforms the first on average and therefore is the one I will use from here on. Whilst the last algorithm does not have the best precision on some benchmarks its stability over all benchmarks made it the preferred candidate.

5.3 Final algorithm

Once both of these decisions had been made. The architecture of the final separated algorithm was fully decided and could be further trained and optimised.
For the testing of the different algorithm, we decided to run them on a large set of benchmarks. In this way, we could see if we managed to learn a global policy or simply find a local minima. In the end we settled on a set of 81 different benchmarks of varying sizes on complexities. Due to the relatively large amount of benchmarks, we set the timeout to be quite short to thirty minutes. This was done so that the experiments could be run in a reasonable amount of time. For each benchmark, we saved the resulting invariants of the analysis and the runtime.

We test on the benchmarks with four different analyses:

- Using the decomposed Polyhedra domain.
- Rl trained with Q-learning
- Basic deep Q-network algorithm
- Deep Q-network with separated estimators

The following table shows the results of the experiments. It shows the average of the precision percentages as compared to the decomposed analysis. The total runtime on all benchmarks, the number of benchmarks that the analysis timed out on. Finally, for the reinforcement learning algorithms, the number of benchmarks where they outperform the other RL algorithms with regards to precision.

Results	Elina	Q-learning	DQN	Separated DQN
Avg. prec. (%)	100	87.1	94.9	91.6
Runtime (hr.)	18:28	14:05	15:35	11:21
n° timeouts	33	23	23	17
n° bench. most precise		1	36	2

Result discussion

We can see that we are able of outperforming the Q-learning method with both the deep Q-network and the separated deep Q-network algorithms. What is interesting to note, is that the regular DQN outperforms the separated one in terms of precision. This is most likely due to the action selection algorithm. Even though, in 5.2., we attempted to pick an algorithm that would be as stable as possible and be able to maintain good results over all benchmarks. If we observe the concrete results, on a few benchmarks the separated DQN performs very poorly which makes it drop its overall precision. However, it is worth noting that the separated DQN outperforms all the other algorithms in terms of speed, as it manages to finish the analysis of all the benchmarks quite a lot faster than the others, most notably, it is faster than the Q-learning algorithm whilst remaining more precise as well. The separated DQN also has the least timeouts out of all the analysis. In terms of precision however, the normal DQN algorithm is the most

precise on average on all the benchmarks. It is also more precise on 36 of the 81 benchmarks and is only beaten by the other algorithms on one benchmark by Q-learning and on two by the separated DQN, the precision is the same for the rest.

Conclusion

In conclusion, in this work we managed to build a framework for the training and testing of various deep reinforcement learning algorithms inside of polyhedra analysis. We were then able of designing a series of such algorithms. These algorithms ranged from very global reinforcement learning methods, too ones more optimised with problem specific knowledge as well as having a greater flexibility towards the various subproblems. We then tested out the different subparts of our algorithms that we had come up with, in the goal of finding an optimal combination.
Once our algorithms were designed, we were than able of testing them on a broad array of different benchmarks. They managed to outperform the other preexisting reinforcement learning methods on both accuracy and performance.
It is also worth noting that we managed to highlight the overall effectiveness of the global deep Q-network algorithm, as after all it was able to craft the decision policy that was the most accurate. When designing new training algorithms that used more domain specific knowledge, we were only able to increase the performance at the loss of some accuracy.

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