Describing the role of Artificial Neural Networks in Reinforcement Learning

Thilo Stegemann
University of Applied Sciences
Applied Computer Science
12459 Berlin, Wilhelminenhofstraße 75A
Email: t.stegemann@gmx.de

***Abstract*—TODO : Write an awesome abstract at the end!**

I. Introduction

Artificial Intelligence (AI) is a huge, rewarding, rising and complex research field. More and more people are interested in AI every day. Students, researchers, economics, engineers, CEO's and investors are highly encouraged to use, understand and/or improve AI technologies. At some point in time an AI newcomer will get to the problems of Reinforcement Learning (RL) and therefore to Artificial Neural Networks (ANN's). Andrew Ng. describes AI as the new upcomming electricity: AI will change many different industries and it will have a huge general impact in everyday life.

In this paper we will concentrate on the use of ANN's in Reinforcement Learning. To understand the relationship between those two big concepts we explain key parts of both. For RL key parts are the problem definition, especially sequential stochastic decision processes (Markov Decision Process), discounted sums of delayed rewards, policy and value functions and approximation approaches of those functions. Additionally it is needed to define what the RL algorithms have to achieve in form of a loss function (also called objective or cost function) and how this function can be optimized with gradient methods. This mechanism of defining a loss function and optimize it with gradient methods is also widely used in other machine learning sub domains like supervised learning. RL is one of three main machine learning sub domains: Supervised Learning (SL) where a "teacher" defines whether something is good or bad, Reinforcement Learning (RL) where no "teacher" is given and the algorithm only learns from trial and error experience and delayed reward signals and Unsupervised Learning (UL) where no "teacher" or reward signal is given and the algorithm learns considering the special clustering or structure of the input data. Inside the paper we will strongly concentrate on reinforcement learning, but sometimes we refer to supervised learning for a better understanding of certain concepts.

Policy and value functions represent the behaviour and learning result of an RL algorithm. One generalization approach (as we will see later) is approximating policy and value functions using ANN's. For ANN's key parts are convolutional neural networks (CNN'S), recurrent neural networks (RNN's) and backpropagation. CNN's and RNN's are special kinds of ANN's. CNN's are often used for image classification and RNN's are often used in sequential settings when we have input over time. Combination of both special types are also possible and practically used. Another approach for approximating policy and value functions is using a linear combination of features, but this will not be part of this paper. After we explained both concepts RL and ANN's we switch to practical case studies done by scientific researchers, which all used ANN's in RL successfully. We will have a closer look onto the results and how they realized their experiments. Last part of the paper is a discussion and conclusion part about how well ANN's are used in RL and which opportunities for ANN's in RL are in the future.

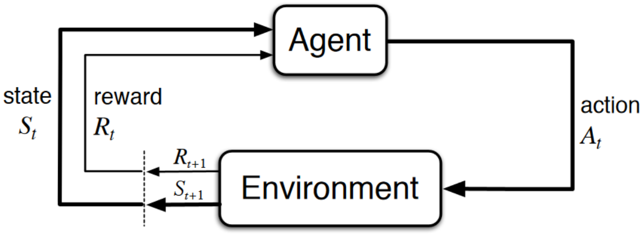


Fig. 1. Agent-environment interaction [1].

II. Reinforcement Learning (RL)

Reinforcement learning (RL) problems consider an agent-environment interaction framework. Basics of reinforcement learning are mentioned in [2]–[6]. As an in depth guide for reinforcement learning see [1]. The following part is about summarizing those background RL introductions. The agent (implementation of the learning algorithm) will interact with the environment (a Markov Decision Process). The interaction is continuous in time t, so the start state at time $t = 0$ is s_0 and a trajectory (decision sequence) looks like $(s_0, r_0) \rightarrow a_0 = (s_1, r_1) \rightarrow a_1 ... a_{t-1} = (s_t, r_t) \rightarrow a_t$. The agent environment interaction is graphically displayed in Fig. 1. The agent will get a reward R_t and a state S_t from the environment and the environment will get an action A_t from the agent. This action A_t is a calculated decision based on the received reward R_t and state S_t. After the environment received action A_t it will return a state S_{t+1} and a reward signal R_{t+1}. The agent tries to learn optimal behaviour through trial and error attempts. The agent wants to know which actions in which states get the most long-term reward and fit this knowledge into a policy representation. A few main problems of this RL framework are:

- The agent only gets a numerical reward from the environment at the end of a decision-sequence.
  ∼ *Delayed Reward*
- How should the reward be assigned to the different steps of a decision-sequence?
  ∼ *Credit Assignment Problem*
- How to handle vast action- and state-spaces?
  ∼ *Generalization Problem*

This paper focuses heavily on the last mentioned problem. How to handle vast action- and state-spaces? In my bachelor thesis I also had the problem of high dimensional action- and state-spaces. I implemented a variant of table lookup Q-learning with a SQLite database for storing the agent experience. The agent should try to learn TicTacToe and Reversi (two board strategy games). Although the algorithm did OK for the TicTacToe (3x3 board) problem it completely failed for bigger game fields of TicTacToe or Reversi. The reason for failure was the exponential time increase proportional to the increasing dimensionality of action and state spaces. Q-functions cannot be represented in a table lookup, because the dimensions of most RL problems will lead to databases with more entries then particles in the universe (compare chess board positions and actions [7] S. 114 ff). One big and promising solution for this problem is function approximation in general and artificial neural networks in concrete.

A major goal of RL is to find a global optimal policy. A policy is a function which maps states to actions. This policy will additionally get a vector of parameters. The parameter-vector changes the policy output. This parametrisation of the policy function is called “function approximation” and Artificial Neural Networks are an approach for approximating a policy function. Combining ANN’s with reinforcement learning algorithms have so far shown spectacular results e.g.: The Google DeepMind Team programmed an AI which plays Go (a very complex strategy board game) at human grandmaster level [5]. With this approximation the problem of vast action- and state-spaces can be solved. To optimise the parameter vector, methods like Policy Gradient or Temporal Difference (e.g. Q-Learning) approaches are used. Applications like TD-Gammon by Gerald Tesauro proved that learning complex strategy games with Artificial Neural Networks is possible and promising.

A. *Q-learning*

Q-Learning (Watkins [8], 1989) is a reinforcement learning algorithm for agents to learn how to act optimally in controlled Markov decision processes. Watkins showed in his paper that Q-Learning converges to the optimum action-value with probability 1 so long as all actions are repeatedly sampled in all states and the action-value are represented discretely. We will describe the Q-Value update in detail now, because in a later chapter Q-Learning is a fundamental part of the implementation. The update rule of one-step Q-Learning is [1]:

$$\begin{aligned} Q(S_t, A_t) \leftarrow & Q(S_t, A_t) + \alpha[R_{t+1} + \\ & \gamma \max_a Q(S_{t+1}, a) - Q(S_t, A_t)]. \end{aligned} \tag{1}$$

This equation defines how to update a Q-value in one time step. Step size (or learning rate) α should be $0 \leq \alpha < 1$ but often closer to 0. This hyper parameter defines how much the agent can trust its experience. So if α is close to 0 that means the agent should update its Q-values just a little bit in the direction of the temporal difference (TD), because the complete Q-Function is initialized randomly and the agent can’t trust those values completely until a certain amount of updates is done. The temporal difference is the mathematical difference between two timely successive Q-Values: $\max_a Q(S_{t+1}, a) - Q(S_t, A_t)$. TD represents the error between the two Q-Values, if TD is 0, then there is no difference between the states. Another hyper parameter is γ which is a discounter. γ defines how relevant future experience is for the agent. If γ is close to 1 or is 1, then there is no discounting and every experience is equal important. If γ is close to 0, then future experience gets more irrelevant proportional to the time distance. When γ is 0, then no future experience is considered at all. $\max_a$ is a function which should return the highest Q-value for every possible action a in state S_{t+1} (also denoted as S').

B. *Loss Function*

A loss function $J(f)$ (or objective function) always defines how good or bad a function f is. The result of a loss function is a scalar. Sometimes the loss function is also called a cost function, because if the resulting scalar is a high value, then its like the cost of function f is high. There are several different loss functions for different tasks. In supervised learning tasks for example linear regression a mean squared error (MSE) loss is used. Mathematically MSE loss looks like this:

$$J_D(\Theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\Theta(x^{(i)}) - y^{(i)})^2).$$

D is the data or the training set which includes all training values x and all target values y (labels). m is the amount of training examples inside D. Θ is a parameter vector containing several different Parameters $(\theta_0, \theta_1, ..., \theta_n)$. Parameter vector Θ affects the output of the linear hypotheses h_Θ. Using the MSE loss function $J_D(\Theta)$ and a gradient descent method it is possible to fit the linear hypothesis to the given data. Fig. 2. displays the start point and the result of a linear regression as described above. The blue data points are not measured data, these points are calculated with a Gaussian normal distribution. So to all y values a Gaussian noise is added. The

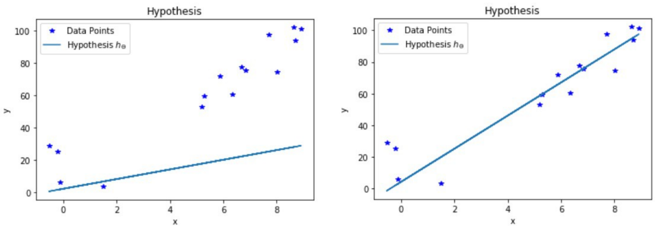


Fig. 2. Fitting a linear hypothesis with linear regression.

left graph is the not fitted random initialized hypothesis h_Θ and the right graph is the fitted hypothesis after 400 iterations using MSE loss and gradient descent. For completeness the parameter vector Θ is optimized and so the hypothesis will fit the data, because the hypothesis h_Θ is dependent on Θ.

In reinforcement learning tasks loss functions look and behave similar as in supervised learning. Later we will examine a successful Q-Learning implementation with a neural network as function approximation using a loss function $L_i(\theta_i)$ and to understand this loss function it is helpful to understand the example loss function given above.

C. *Batch vs. Stochastic Gradient Decent*

In the privious chapter we already talked about gradient descent metodes, but we did not defined how gradient descent works. Now we will explain two different gradient descent methodes in detail. The following differentiation of batch and stochastic gradient descent is based on [9] and [10]: In general gradient methods are used to optimize a function respective to its partial derivatives. A parameter update with batch gradient descent will consider the whole training set for its calculation. So in large scale machine learning problems there are training sets with several millions or billions of examples. For every update step the batch gradient descent calculates the sum of the partial derivatives in respective to all examples. To find the minimum of a function multiple update steps are needed. Batch gradient descent will have an exponential computational cost for larger machine learning problems.

A Solution for this problem is the stochastic gradient descent. Instead of computing the gradient of the function exactly, each iteration (update step) estimates the gradient on the basis of a single randomly picked example. The trade-off between batch and stochastic gradient descent is that batch gradient descent achieves linear convergence, when the initial estimate is close enough to the optimum and when the gain of the discounting factor is sufficiently small. The stochastic gradient descent will not converge to a minimum like batch gradient descent does, rather the parameters which are updated will oscillate around the minimum but will may never converge to the minimum. But often the stochastic gradient descent gets the parameters close to the minimum much faster than batch gradient descent.

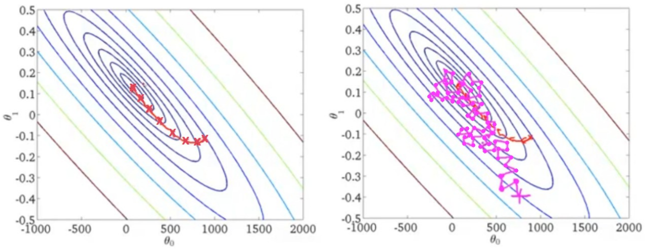


Fig. 3. Contour plots of cost function $J(\theta)$ with marked batch (left) and stochastic gradient descent (right) [11].

Algorithm 1 Stochastic gradient descent [11]

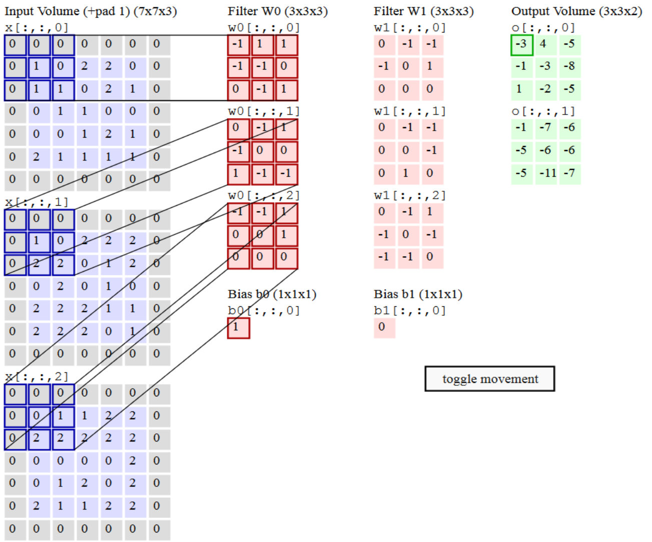
```
Randomly shuffle (reorder) training examples
repeat
  for  $i := 1, ..., m$ do
    for $j := 0, ..., n$ do
      $\theta_j := \theta_j - \alpha(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$
    end for
  end for
until 1-10 times
```

Figure 3 illustrates how batch and stochastic gradient descent converge to a minimum. The coloured ovals define the contour of a cost function $J(\theta)$. The cost function is minimal in the middle of the smallest oval and gets higher in the outer ovals. The parameters θ_0 and θ_1 are two parameters of a parameter vector θ. Those parameter values will change the cost of function $J(\theta)$. In the left part of figure 3 parameters θ updated by batch gradient descent converges "relatively straight" to a minimum after several iterations. Whereas in the right part of figure 3 parameters θ updated by stochastic gradient descent are in general moved in the direction of the minimum but not always and in the end the parameters are wondering around close to the minimum.

Algorithm 1 is a pseudocode example of stochastic gradient descent from Andrew Ng [11]. The term m denotes the amount of training examples, n is the amount of parameters θ, hyper parameter α is the step size or learning rate which we already mentioned in chapter Q-learning and $h_\theta(x^{(i)}) - y^{(i)}$ is a part of the error term mentioned in chapter loss function. For a concrete example with $m = 300.000.000, 00$ training examples the algorithm 1 will update all parameters θ_n for every training example. So in one single stochastic gradient descent step the parameter vector $\Theta = \theta_0, ..., \theta_n$ is updated m times. Batch gradient descent will in contrast calculate an update of all parameters θ_n considering all training examples at once and then just performing one single batch gradient descent update of the parameter vector Θ.

III. Artificial Neural Networks (ANN's)

In neural networks in general between the output and the input layers are hidden layers. If there is more then one hidden



Input Volume (+pad 1) (7x7x3)

x[:,:,0]

0	0	0	0	0	0	0
0	1	0	2	2	0	0
0	1	1	0	2	1	0
0	0	1	1	0	0	0
0	0	0	1	2	1	0
0	2	1	1	1	1	0
0	0	0	0	0	0	0

x[:,:,1]

0	0	0	0	0	0	0
0	1	0	2	2	2	0
0	2	2	0	1	2	0
0	0	2	0	1	0	0
0	2	2	2	1	1	0
0	2	2	2	0	1	0
0	0	0	0	0	0	0

x[:,:,2]

0	0	0	0	0	0	0
0	0	1	1	2	2	0
0	2	2	2	2	2	0
0	0	0	0	0	2	0
0	0	1	2	0	2	0
0	2	1	1	2	2	0
0	0	0	0	0	0	0

Filter W0 (3x3x3)

w0[:,:,0]

-1	1	1
-1	-1	0
0	-1	1

w0[:,:,1]

0	-1	1
-1	0	0
1	-1	-1

w0[:,:,2]

-1	-1	1
0	0	1
0	0	0

Bias b0 (1x1x1)

b0[:,:,0]

1

Filter W1 (3x3x3)

w1[:,:,0]

0	-1	-1
-1	0	1
0	0	0

w1[:,:,1]

0	-1	-1
0	0	-1
0	1	0

w1[:,:,2]

0	-1	1
-1	0	-1
-1	-1	0

Bias b1 (1x1x1)

b1[:,:,0]

0

Output Volume (3x3x2)

o[:,:,0]

-3	4	-5
-1	-3	-8
1	-2	-5

o[:,:,1]

-1	-7	-6
-5	-6	-6
-5	-11	-7

Fig. 4. Computation inside a convolution layer [12].

layer between input and output layer, then the neural network is called a deep neural network.

A. Convolutional Neural Network (CNN/ConvNet)

To better understand the later experiment [6] (Deep Q-network) it is helpful to get into CNN's first. Knowledge base of this chapter is a Stanford class CS231n about "Convolutional Neural Networks for Visual Recognition" [12]. A convolutional neural network is a specific ANN which assumes that every input is an image. This assumption allows to reduce the amount of parameters and so improve the performance for image processing with CNN's in contrast to more general ANN's. More general because ANN's don't assume a specific input. A CNN consists of layers. There are different kinds of layers: input layer (INPUT), convolutional layer (CONV), rectified linear unit layer (RELU), pooling layer (POOL), fully connected layer (FC) and an output layer. Some of these layers can appear multiple times. A simple ConvNet architecture for classification could be INPUT → CONV → RELU → POOL → FC. In the following every different layer will be explained in detail.

a) The Input layer: can be high dimensional sensory data. Considering the Atari 2600 arcade gaming environment [2]–[4] the input is a video stream of pixels at different time steps. At time step t a video signal reduces to just an image of pixels and the complete sequence of images at all time steps equals the video signal. There is still more then the raw pixels from the video stream like the score value at each time step [4]. In terms of reinforcement learning the score signal is a reward signal and the video stream at each time step describes the state in which the agent is in. Another example is the CIFAR-10 dataset which contains images of shape 32x32x3 (32 wide, 32 high, 3 color channels).

b) The convolution layer: is the most computationally expensive layer, because much matrix multiplications are performed on raw data (not reduced data expect preprocessing). In general this layer applies filters on input images. A filter is a window with fixed size for the CIFAR-10 example the filters could have a size of 5x5x3. These filters are shifted around the width and height of the input images and for every position a matrix multiplication between the input image and the filter is performed. The matrix multiplication results in scalar values stored in a result matrix (feature map). Every filter produces an own feature map. Filters represent the weights of CNN's. For every filter there is an additional bias weight which need to be considered inside the computation. The output of this layer is controlled by three hyperparameters: depth, stride and zero-padding.

- Depth
- Stride
- Zero-padding

A filter can be a representation for edges, lines or other shapes. A combination of those low level filters results in more complex filters like an eye or an ear. Those low and high level filters are like extracted features from the CNN. The computation inside a convolution layer is represented in Fig. 4. Three input matrices of shape 7x7 are independently drawn, because each matrix represents the red, green or blue color channel so the input layer has a shape of 7x7x3 (7 wide, 7 high, 3 color channels). The outer lines (matrix borders) are all zero

c) The rectified linear unit layer: will apply an elementwise activation function, such as the $max(0, x)$ thresholding at zero. If $max(0, x)$ gets values below zero then it will return just zero and if the values are greater then zero max will return the value itself. The blue circles in Fig. 5 with a white line after CONV and FC layers represent the RELU activation function. The $max(0, x)$ rectifier is used for deep learning rather then e.g. the logistic sigmoid, because of better practical efficiency.

d) The pooling layer:

e) The output layer: Aim of the CNN is to predict which of 10 different CIFAR classes an image belongs to.

B. Recurrent Neural Networks (RNN's)

IV. Successful case studies using ANN's for RL

The following part is about summarising successful case studies which used ANN's for RL.

A. Asynchronous Methods for Deep Reinforcement Learning

The scientists from Google DeepMind and Montreal Institute for Learning Algorithms introduced asynchronous deep learning algorithms [2]. These asynchronous algorithms are based on four standard reinforcement learning algorithms: One-step Q-learning, one-step Sarsa, n-step Q-learning and advantage actor-critic. The paper explains the background of reinforcement learning and how the asynchronous reinforcement learning methods works. The study was approved by an experiment in an Atari 2600 evaluation environment . All four asynchronous algorithms where tested within the

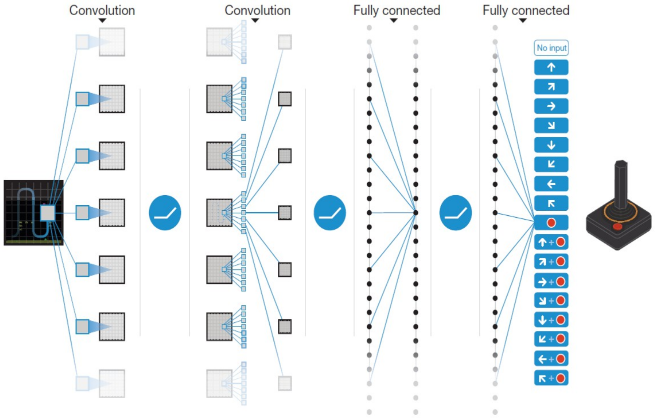


Fig. 5. Schematic illustration of the convolutional neural network [4].

test environment . The Atari 2600 environment tests where used to compare the performance of the four algorithms. The main finding of this study is that all four asynchronous deep reinforcement learning algorithms are able to train neural network controllers on a variety of domains in a stable manner. In addition their results show that stable train ing of neural networks through reinforcement learning is possible with both value-based and policy-based methods, off-policy as well as on-policy methods, and in discrete as well as continuous domains.

B. *Deep Reinforcement Learning with Double Q-Learning*

Aim of this paper is to determine if the recent DQN (Deep Q Network) algorithm, which combines Q-learning with a deep neural network, suffers from substantial overestimations in some games in the Atari 2600 domain [3]. Furthermore the Google DeepMind contributors point out how the Double Q-learning algorithm can be generalized to work with large-scale function approximation to successfully reduce the DQN overoptimism, resulting in more stable and reliable learning. Finally they propose a specific adaptation to the DQN algorithm and show that the resulting algorithm (Double DQN) not only reduces the observed overestimation, as they hypothesized, but that this also leads to much better performance on several Atari 2600 games.

C. *Human-level controll through deep reinforcement learning*

The paper is about how to reach human-level control through a deep Q-network, that can learn successful policies directly from high-dimensional sensory inputs using end-to-end reinforcement learning [4]. The deep Q-network agent (in reinforcement learning an agent is the executing learning algorithm) is tested on the challenging classic Atari 2600 game environment. The result of this test demonstrated that the deep Q-network agent, receiving only the pixels and the game score as inputs, was able to surpass the performance of all previous algorithms and achieve a level comparable to that of a professional human games tester across a set of 49 games, using the same algorithm, network architecture and hyperparameters.

D. *Mastering the game of Go with deep neural networks and tree search*

The paper from Google concerns two different algorithm approaches for deep reinforcement learning [5]. The first approach uses 'value networks' to evaluate board positions and 'policy networks' to select moves. These deep neural networks are trained by a novel combination of supervised learning from human expert games and reinforcement learning from games of self-play. They proof through experiments that this deep RL algorithm approach is capable of playing Go at the level of state-of-the-art Monte Carlo tree search. The second deep RL approach is a new seach algorithm that combines Monte Carlo simulation with value and policy networks. They used this search algorithm inside the application AlphaGo and the application achieved a 99.8% winning rate against other Go programs and it defeated the human European Go champion by 5 games to 0.

E. *Playing Atari with Deep Reinforcement Learning*

The paper from DeepMind Technologies is about a deep learning model to successfully learn control policies directly from high-dimensional sensory input using reinforcement learning [6]. They defined the model as a convolutional neural network (CNN). This CNN is trained with a variant of Q-learning. Input of the CNN is row pixels and output is a value function estimating future rewards. They apply this deep learning model to seven Atari 2600 games from the Arcade Learning Environment, with no adjustment of the architecture or learning algorithm. Result of this experiment is that it outperforms all previous approaches on sex ot the games and surpasses a human expert on three of them.

V. Deep Reinforcement Learning

In depth explaining of the experiment done in paper "Playing Atari with Deep Reinforcement Learning".

A. *Deep Q-network*

A deep Q network (DQN) is a combination of a convolutional neural network and the reinforcement learning algorithm Q-learning.

"A deep Q network (DQN) is a multi-layerd neural network that for a given state s outputs a vector of action values $Q(a, ; \theta)$, where θ are the parameters of the network. For an n-dimensional state space and an action space containing m actions, the neural network is a function from $\mathbb{R}^n$ to $\mathbb{R}^m$. Two important ingredients of the DQN algorithm as proposed by Mnih et al. (2015) are the use of a target network and the use of experience replay. The target network, with parameters θ^-, is the same as the online network except that its parameters are copied every t steps from the online network, so that then $\theta_t^- = \theta_t$, and kept fixed on all other steps. The target used by DQN is then

$$Y_t^{DQN} \equiv R_{t+1} + \gamma \max_a Q(S_{t+1}, a; \theta_t^-).$$

For the experience replay (Lin, 1992), observed transitions are stored for some time and sampled uniformly from this memory bank to update the network. Both the target network and the experience replay dramatically improve the performance of the algorithm (Mnih et al. 2015)."

VI. Discussion & Conclusion

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