Chess Assignment

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Abstract—This document is a model and instructions for LaTeX. This and the IEEEtran.cls file define the components of your paper [title, text, heads, etc.]. *CRITICAL: Do Not Use Symbols, Special Characters, Footnotes, or Math in Paper Title or Abstract. 1 sentence summary, 1 sentence method, and 1 sentence results, and 1 sentence conclusion.

Index Terms—reinforcement learning, chess

I. INTRODUCTION

A. - describe general setting

In this assignment, we explore three different reinforcement learning algorithms to learn how to play a simplified version of chess. These three algorithms are SARSA, Q-Learning and DQN¹.

B. - touch on methods

Throughout the report we indicate in footnotes which task a particular section is referring to in terms of answering the task. We do this as the solutions to certain tasks are spread throughout multiple sections, e.g. task 3 is answered in Section II and Section III. Even though this assignment was not solved in a group, we decided to also answer some of the "group only" and we stick to the numbering of the assignment in order to avoid confusion.

C. - touch on results and conclusion

seeds and nonseeded experiments foreshadow results from glearning

II. METHODS

A. Environment

This version of chess takes place on a 4 by 4 board and can be thought of as a late game where the agent has a king and a queen, and the opponent has only a king. Since this game can only end in a win for the agent or in a draw, it is the agent's goal to learn how to win the game and avoid draws. For all experiments considered, the agent will be given a reward of 1 for winning, 0 for drawing, and 0 for all intermediate steps.

For DQN no sequence is needed, because chess fulfills Markov property and gives rise to a Markov Decision Process (MDP). Also no preprocessing of sequence is needed anymore because state encoding is already given. [1] [2]

¹SARSA serves as answer to task 3 and DQN serves as answer to task 5.

Chess has/fulfills the Markov property, so applying reinforcement learning algorithms like Q-Learning and SARSA is theoretically justified.

(1) Describe the algorithms Q-learning and SARSA. Explain the differences and the possible advantages/disadvantages between the two methods. No coding is needed to reply to this question.

B. SARSA and Q-Learning²

1) Temporal-Difference Algorithms: maybe SARSA and Q-Learning are two very related model-free types of temporal-difference (TD) algorithms for learning expected rewards, also known as Q-values, when rewards are not immediate and possibly sparse. The learning takes place via interaction with an environment through trial and error. These Q-values are in general represented by an action-value function Q and, for finitely many state-action pairs (s, a), can be considered as a Q-table where each state-action pair, (s,a), maps to a single Q-value, thus providing an estimate of the quality of any given state-action pair (s, a). In this assignment however we use neural networks to approximate the action-value function, which outputs the Q-values for all possible actions for any given state. This helps to avoid computing large Q-tables. All algorithms explored in this assignment, including DQN, require the environment to fulfill the Markov property. why? else what?

2) differences/what they have in common: SARSA and Q-Learning address the temporal-credit-assignment problem [3], that is, trying to attribute future rewards to previous actions. These future rewards get discounted with the hyper-parameter γ (see Section III-C). Both algorithms repeatedly choose and take actions in the environment according to some policy π , e.g. an ϵ -greedy policy.

However, this is where they differ. SARSA is an on-policy algorithm, which means that consecutive actions are chosen according to the same policy π , even during the update step of the Q-values, which leads to the update rule:

$$Q_{\pi}(s, a) \leftarrow Q_{\pi}(s, a) + \eta(r + \gamma Q_{\pi}(s_{t+1}, a') - Q_{\pi}(s, a))$$

for some future action a' chosen according to policy π .

Q-learning, on the other hand, is an off-policy algorithm, which means that it takes its actions a according to its policy π , but during the update steps it assumes a greedy policy, i.e.

²Answer to task 1.

optimal play, for future actions $a^\prime.$ Q-Learning has the update rule:

$$Q_{\pi}(s, a) \leftarrow Q_{\pi}(s, a) + \eta(r + \gamma \max_{a'} Q_{\pi}(s_{t+1}, a') - Q_{\pi}(s, a)).$$

3) - advangages/disadvantages: This leads to one of Q-Learning's major advantages: Because of Bellman's optimality equation, Q-Learning is guaranteed to learn the values for the optimal policy, i.e. $Q_*(s,a) = \max_{\pi} Q_{\pi}(s,a)$, and in a greedy stetting will take the optimal actions, at least if it was trained sufficiently. However, this can in certain cases mean that the online performance of Q-Learning will be worse than the one from SARSA, as Sutton et al. [4] demonstrate with their "gridworld" example "Cliff Walking". Our chess game is a similar situation, because a win and a draw can be very close, thus during exploration Q-Learning can accidentally create a draw because it is going for the optimum when exploiting. Q-Learning is however relatively unstable and the parameters can even diverge when it is combined with non-linear function approximators [2], making the guarantee to learn the optimal policy irrelevant.

SARSA will learn to take a safer path, because it keeps its policy in mind when updating the Q-values, i.e. it keeps in mind that it will explore in future actions. This has the advantage that SARSA in general tends to explore more than Q-Learning.

C. Experience Replay³

replay memory of fixed size, queue (get code in appendix) (2) [Group Only] Describe the experience replay technique. Cite relevant papers.

Experience replay is a technique proposed by Lin [5] to speed up the training process for reinforcement learning algorithms by reusing past experiences for future training. This is analogous to the human ability to remember past experiences and learn from them even after the fact. The past experiences are stored in a replay memory of fixed size at each time step t as a tuple $e_t = (s_t, a_t, r_t, s_{t+1})$. This essentially allows us to transform the learning process from online learning to minibatch learning, where a batch of experiences e_j is randomly sampled for each update step. Experience replay can only be used in combination with off-policy algorithms, because otherwise the current parameters determine the next sample and create unwanted feedback loops [1], [2].

Experience replay provides many benefits over online Q-Learning, especially when neural networks are used to approximate the action-value function. First, it enables the agent to learn from past experiences more then once, leading to increased data efficiency and faster convergence [1], [5]. Second, since for each update step past experiences are sampled randomly, the correlations between the individual actions are reduced, which then reduces the variance of the updates [1]. This leads to the experience samples e_j being closer to i.i.d. and thus guaranteeing better convergence when using optimization algorithms such as stochastic gradient descent as most convergence proofs assume i.i.d. data.

D. Deep Q-Networks $(DQN)^4$

A first version of the DQN algorithm was proposed by Mnih et al. [1] and combined experience replay with Q-learning, where a neural network was used as a non-linear function approximator for the action-value function. Mnih et al. [2] later improved upon the method and presented the DQN algorithm, as it is known today, where they address the problem of the Q-values Q(s,a) being correlated to the target values $y=r+\gamma\max_{a'}Q(s',a')$ because they are generated using the same neural network. In the DQN algorithm they separated the Q-network from the target network and only update the target network every C steps, which helps to break this correlation and combat diverging network parameters.

E. Experiments

In order to address all tasks, we divided the tasks into several independent experiments. First, we conducted seeded runs⁵ for all three algorithms using seed 21 for reproducibility, which was chosen a-priori. These seeded runs serve as examples to compare the algorithm's online performance qualitatively. The seeds are used such that the weights of all neural networks are instantiated identically for all algorithms and they subsequently serve as seeds for any random number used during training. This makes sure that all agents start with the same initial conditions and that the results are reproducible (see Section V-1). All algorithms were run for 100000 episodes using identical model architecture and hyper-parameters (see Section II-F).

Since the seeded runs are heavily influenced by the choice of the seed, we could end up with anything between a very lucky and well performing seed, or with a very unlucky one. Also the interpretation of the seeded runs is more difficult as we just have one run for each algorithm. Therefore, we decided to perform a simulation study and complete 30 non-seeded runs for each algorithm in order to get a better idea of how the algorithms perform on average. For computational reasons we limited these runs to 40000 episodes as we realized with test runs that by then most of the training progress has already taken place.

To analyze the impact of the hyper-parameters β and γ^6 we trained 49 agents with different combinations for β and γ but keeping all other hyper-parameters and model architecture identical. We chose SARSA for this experiment as we found it to have very low variance between its unseeded runs, which makes it an ideal candidate for comparing individual runs (see Figures 4 and 5). These runs are seeded identically to the seeded runs mentioned above.

F. Implementation and Hyper-parameters

1) Implementation: We implemented all algorithms from scratch according to Sutton et al. [4] (SARSA and Q-

³Answer to "group only" task 2.

⁴Answer to task 5: Describing the used method.

⁵Answers to task 3 and 5.

⁶Answer to task 4.

Learning⁷) and Mnih et al. [2] (DQN⁸). For the implementation see file neural_net.py on GitHub or Listing 1. All algorithms use a neural network with 58 input neurons, 200 hidden neurons and 32 output neurons, not including the biases for the input and hidden layer. The neural network automatically adds a constant input for the bias and the hidden layer. The implementation treats the biases like any other weights and thus they are part of any matrix multiplication. We used a ReLU activation function for the hidden layer and no activation on the output layer. The weights were initialized using Glorot initialization [6], such that the weights are sampled from a normal distribution with mean 0 and variance $\frac{2}{n_{\rm in}+n_{\rm out}}$, where $n_{\rm in}$ and $n_{\rm out}$ denote to the number of input and output neurons of the respective layer. This helped preventing exploding gradients for the most part.check again with results

2) Hyper-Parameters: For all experiments we used the default hyperparameters provided in the Assignment.ipynb file unless otherwise noted. For DQN we updated the weights of the target network after every C=10 steps, as most games take fewer steps than that. We used a replay memory of size 100000 and a batch size of 32.

III. RESULTS

A. Seeded Runs9

(3) We provide you with a template code of the chess game. Fill the gaps in the program file chess implementing either Q Learning or SARSA; detailed instructions are available inside the file. We provide indicative parameter values. Produce two plots that show the reward per game and the number of moves per game vs training time. The plots will be noisy. Use an exponential moving average.

The rewards and number of moves for the seeded runs are depicted in Figures 1 and 2 respectively. Since the curves are very noisy, we smoothed them using an exponential moving average (EMA) with a weight on the most recent observation of $\alpha=0.001$.

As expected, the online performance of Q-Learning in terms of the rewards is generally lower than the rewards for SARSA but they converge slowly as ϵ decreases (Figure 1). Also in Figures 1 and 2 we can see that Q-Learning experiences instable learning behavior as both plots are a lot more noisy and at about 20000 and 90000 episodes the rewards decrease for some period. SARSA and DQN don't show this behavior.

Even though the number of steps is not punished, all agents still learn to reduce the number of steps over time, as they do not give rewards and their goal is to take actions that do. SARSA seems to do the best job at this, which perhaps is caused by its tendency to explore more and find better strategies. Q-Learning however seems to struggle to reduce the number of steps it takes.

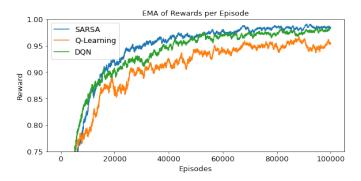


Fig. 1: Exponential moving average of the rewards achieved during training. All three algorithms, Q-Learning, SARSA and DQN were initialized with identical weights and trained with identical network architecture and hyper-parameters.

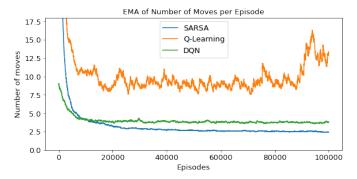


Fig. 2: caption

(5) Implement another Deep RL algorithm (it could be SARSA if you chose before Q Learning and vice versa). Compare the new results with your previous results.

As suggested by Mnih et al. [1], [2], DQN¹⁰ was able to overcome the downsides of Q-Learning which lead to an online performance which is comparable to that of SARSA in terms of reward and number of moves it achieved, and also in terms of the stability during training. It did however not learn to reduce the amounts of steps as much as SARSA.

B. Simulation Study (Non-seeded Runs)

We can confirm that the qualitative results from the seeded runs reasonably well represent the average case. The only notable exception being Q-Learning, for which most runs performed equally well to the seeded run, but some runs experienced huge increases in the number of steps, which influenced the average run dramatically, leading to an average of about 23 moves per episode after 40000 episodes. For the learning curves see Figures 4 and 5 in the Appendix.

We observed that DQN and SARSA show very comparable learning curves with DQN showing slightly faster convergence in the first 5000 episodes. SARSA showed the lowest variance in all runs and seems to be a very stable algorithm. Q-Learning on the other hand showed clear signs of divergence as for

⁷SARSA as answer to task 3 and Q-Learning as additional algorithm.

⁸Answer to task 5.

 $^{^9\}mbox{Answer}$ to task 3 (SARSA and Q-Learning as additional algorithm) and 5 (DQN).

¹⁰Answer to task 5 for comparing DQN to SARSA and Q-Learning.

some runs the rewards consistently dropped while the number of moves consistently increased. This shows that the measures taken by Mnih et al. [2] to combat the disadvantages of Q-Learning worked and increased the stability as well as the convergence speed.

We can conclude that the seeded runs in our initial experiment truthfully represent the average run and therefore some level of inference is justified.

We also found out that, unsurprisingly, the effective training time is mainly dependent on the number of steps an algorithm takes per episode. This leads to Q-Learning having by far the longest training time, especially when the parameters diverge and the number of steps increase. DQN and SARSA have relatively short training times, with SARSA being the fastest.

C. Hyper-parameters

- (4) Change the discount factor γ and the speed β of the decaying trend of ϵ (for a definition of β please see code). Analyse the results.
- 1) gamma: Figure 3(a) depicts the rewards and number of moves per episode as a function of β and γ . We can see that the reward increases monotonically as γ is increases, suggesting that a value of $\gamma \in [0.80, 1)$ should be chosen. This intuitively makes sense, as we have very sparse rewards and want the agent to "backpropagate" this reward through its sequence of actions.
- 2) beta: We can not see a clear relationship between β and the rewards, apart from $\beta=0$ being an inferior choice. In Figure 3(b) we can see that the that the number of steps taken by the agent decreases drastically when increasing γ from very low levels, but again there is no clear pattern visible for β . In summary, for reasonalby chosen values of γ the choice of β seems to not have much of an influence for training periods up to 40000 episodes.
- (6) [Group Only] Change the state representation or the administration of reward. Interpret your results.
- (7) [Group Only] The values of the weights could explode during learning. This issue is called exploding gradients. Explain one possible way to fix this issue and implement it. For example, search and study RMSprop). Show in a plot how your solution fixed this issue.

IV. CONCLUSION

We are aware that the performance of the individual algorithms could be improved by tuning the hyper-parameters, however, this was not explicitly asked for and the focus on this assignment lies on the comparison of these algorithms.

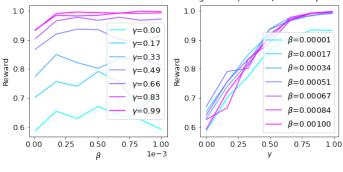
summarize results, takeaway

get correct bib format and complete entries

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[1] V. Mnih, K. Kavukcuoglu, D. Silver, A. Graves, I. Antonoglou3 D. Wierstra, and M. A. Riedmiller, "Playing atari with deept reinforcement learning," *CoRR*, vol. abs/1312.5602, 2013. [Online]5 Available: http://arxiv.org/abs/1312.5602

1A Reward for different values of beta and gamma (SARSA, 40000 episode



umber of Moves for different values of beta and gamma (SARSA, 40000 e

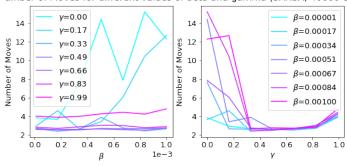


Fig. 3

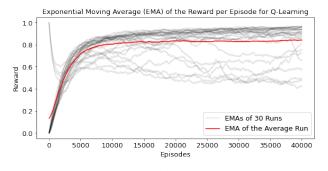
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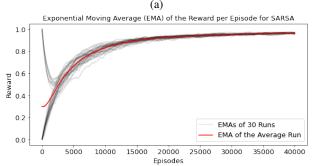
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V. APPENDIX

1) Reproducibility: put the appendix after the bibliography?

```
# import libraries
from types import MethodDescriptorType
import numpy as np
from tqdm.notebook import tqdm
import os
import json
```





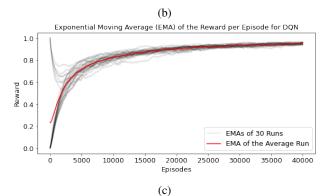
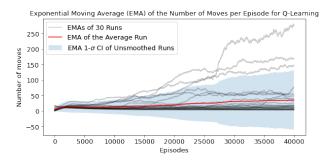
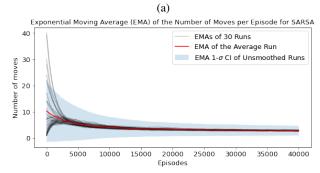


Fig. 4

```
import time
                                                           27
    import random
                                                           28
8
                                                           29
Q
    from collections import namedtuple, deque
                                                           30
11
                                                           31
   # import from files
12
    from Chess_env import *
                                                           32
13
                                                           33
14
                                                           34
15
                                                           35
   # ==== Epsilon-greedy Policy =====
16
                                                           36
17
18
    def EpsilonGreedy_Policy(Qvalues, allowed_a, epsilon
                                                           37
19
20
                                                           38
        returns: tuple
21
            an action in form of a one-hot encoded
                                                           39
                 vector with the same shapeensions as
                 Qvalues.
                                                           40
22
            an action as decimal integer (0-based)
                                                           41
23
24
        Assumes only a single state, i.e. online
                                                           42
            learning and NOT (mini-)batch learning.
25
                                                           43
26
        # get the Qvalues and the indices (relative of
                                                           44
            all Qvalues) for the allowed actions
                                                           45
```





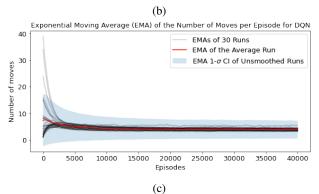


Fig. 5

```
allowed_a_ind = np.where(allowed_a==1)[0]
Qvalues_allowed = Qvalues[allowed_a_ind]
        ---- epsilon greedy -
# draw a random number and compare it to epsilon
rand_value = np.random.uniform(0, 1, 1)
if rand_value < epsilon: # if the random number
     is smaller than epsilon, draw a random
    action
    action_taken_ind_of_allwed_only = np.random.
       randint(0, len(allowed_a_ind))
else: # greedy action
    action_taken_ind_of_allwed_only = np.argmax(
        Qvalues_allowed)
# get index of the action that was chosen (
    relative to all actions, not only allowed)
ind_of_action_taken = allowed_a_ind[
    action_taken_ind_of_allwed_only]
          — create usable output —
```

```
115
                                                                           if len(self) < batch_size:</pre>
46
47
         # get the shapeensions of the Qvalues
                                                             116
                                                                                batch_size = len(self)
 48
         N_a, N_samples = np.shape(Qvalues) # N_samples17
                                                                           return random.sample(self.memory, batch_size
              must be 1
 49
 50
         # initialize all actions of binary mask to 0
                                                             119
                                                                       def __len__(self):
 51
         A_{binary_mask} = np. zeros((N_a, N_samples))
                                                             120
                                                                           return len(self.memory)
 52
         # set the action that was chosen to 1
                                                             121
 53
         A_binary_mask[ind_of_action_taken ,:] = 1
                                                             122
 54
                                                             123
 55
         return A_binary_mask, ind_of_action_taken
                                                             124
 56
                                                             125
                                                                  # ===== Neural Network ======
 57
                                                             126
                                                                  class NeuralNetwork(object):
 58
                                                             127
     # ==== activation functions and it's derivatives
                                                            128
                                                             129
                                                                       def __init__(self, N_in, N_h, N_a,
         ======
 60
                                                                            activation_function_1 = "relu",
 61
     # relu and its derivative
                                                                           activation_function_2=None, method="
     def relu(x):
                                                                           qlearning", seed=None, capacity=100_000, C
 62
 63
         return np.maximum(0,x)
                                                                           =100):
 64
                                                             130
                                                                           activation functions: "relu", "sigmoid", "
 65
     def heaviside(x):
                                                             131
                                                                           tanh", None methods: "qlearning", "sarsa", "dqn"
 66
         return np.heaviside(x,0)
                                                             132
 67
     # sigmoid and its derivative
                                                             133
     def sigmoid(x):
 69
                                                             134
                                                                           self.D = N_in # input dimension (without)
 70
         return 1 / (1 + np.exp(-x))
                                                                                bias)
 71
                                                             135
                                                                           self.K = N_h
                                                                                            # nr hidden neurons (without
 72
     def gradient_sigmoid(x):
                                                                                bias)
 73
         return sigmoid(x) * (1 - sigmoid(x))
                                                             136
                                                                           self.O = N_a
                                                                                            # nr output neurons (letter O
 74
                                                                                , not digit 0)
 75
     # tanh and its derivative
                                                             137
 76
     def tanh(x):
                                                             138
                                                                           # store method and seed
 77
                                                             139
                                                                           self.method = method
         return np.tanh(x)
 78
                                                             140
                                                                           self.seed = seed
 79
     def gradient_tanh(x):
                                                             141
 80
                                                                           if self.method == "dqn":
         return 1 - np.tanh(x)**2
                                                             142
                                                                                self.capacity = capacity
 81
                                                             143
 82.
     # identity and its derivative
                                                             144
                                                                                self.replay_memory = ReplayMemory(
     def identity(x):
 83
                                                                                    capacity)
         return x
                                                             145
                                                                                self.C = C
 84
 85
                                                             146
 86
     def const(x):
                                                             147
                                                                           # set activation function and gradient
 87
         return np.ones(x.shape)
                                                                                function
 88
                                                             148
                                                                           self.act_f_1_name = activation_function_1
                                                                           self.act_f_2_name = activation_function_2
 89
                                                             149
                                                                           self.act_f_1, self.grad_act_f_1 =
 90
     def act_f_and_gradient(activation_function="relu"):150
 91
         if activation_function == "relu":
                                                                                act\_f\_and\_gradient \, (\, activation\_function\_1 \,
 92
              return relu, heaviside
         elif activation_function == "sigmoid":
 93
                                                             151
                                                                           self.act_f_2, self.grad_act_f_2 =
 94
              return sigmoid, gradient_sigmoid
                                                                                act\_f\_and\_gradient \, (\, activation\_function\_2 \,
 95
         elif activation_function == "tanh":
         return tanh, gradient_tanh
else: # identity and constant 1
 96
                                                             152
 97
                                                             153
 98
              return identity, const
                                                             154
                                                                           # initialize the weights and biases and set
 99
                                                                                grobal seed
100
                                                             155
                                                                           np.random.seed(self.seed)
101
102
     # ===== Replay Memory for Experience Replay (with 157
                                                                           \# self.W1 = np.random.randn(self.K+1, self.D
         DQN) =====
                                                                                +1)/np.sqrt(self.D+1) # standard normal
103
                                                                                 distribution, shape: (K+1, D+1)
     Transition = namedtuple('Transition', ("state", "
    action", "reward", "next_state", "done"))
                                                             158
104
                                                                           # glorot/xavier normal initialization
                                                             159
                                                                           # self.W1 = np.random.randn(self.K+1, self.D
105
                                                                                +1)*np.sqrt(2/(self.D+1 + self.K+1)) #
106
     class ReplayMemory(object):
                                                                                 standard normal distribution, shape: (K
         def __init__(self, capacity):
    self.memory = deque(maxlen=capacity)
107
                                                                                +1, D+1)
108
                                                             160
                                                                           self.W1 = np.random.standard_normal((self.K
                                                                                +1, self.D+1))*np.sqrt(2/ (self.D+1 +
109
                                                                                self.K+1)) # standard normal
distribution , shape: (K+1, D+1)
110
         def push(self, *args):
111
              self.memory.append(Transition(*args))
112
                                                             161
                                                                           # self.W1 = np.random.randn(self.K+1, self.D
                                                                                +1) # standard normal distribution,
113
         def sample(self, batch_size):
114
              # if less data than batch size, return all
                                                                                shape: (K+1, D+1)
                  data
                                                             162
```

```
if future_reward: # future reward
             # self.W2 = np.random.randn(self.O, self.K214
                 +1)/np.sqrt(self.K+1) # standard norm215
                                                                            delta = R_rep + gamma*Q_prime - Qvalues
                  distribution, shape: (O, K+1)
                                                                                \# \rightarrow shape (O, 1)
             # glorot/xavier normal initialization
                                                                               # immediate reward
164
                                                                            delta = R_rep - Qvalues # -> shape (O,
165
             self.W2 = np.random.standard_normal((self.Q17
                  self.\overline{K+1})*np.sqrt(2/(self.K+1 + self.
                                                                                1)
                 O)) # standard normal distribution,
                 shape: (O, K+1)
                                                                        # update only action that was taken, i.e.
             # self.W2 = np.random.randn(self.O, self.K
                                                                            all rows apart from the one
166
                 +1) # standard normal distribution,
                                                                            corresponding to the action taken (
                 shape: (O, K+1)
                                                                            action index) are 0
167
                                                          220
                                                                        delta = delta * action_binary_mask
168
             if self.method == "dqn":
                                                          221
169
                 self.W1_target = np.copy(self.W1)
                                                          222
170
                 self. W2_target = np.copy(self.W2)
                                                          223
                                                                        self.compute_gradients(delta, a1, h1, a2, x)
171
                                                          224
                                                                        self.update\_parameters \, (\, self \, . \, eta \, )
172
                                                          225
173
         def forward(self, x, target=False):
                                                          226
                                                          227
174
                                                                   def backward_dqn(self, batch, gamma):
175
             x has shape: (D+1, 1) (constant bias 1 mus228
                 be added beforehand added)
                                                          229
                                                                        backward for method "dqn"
176
             target: if True, use the weights of the
                                                          230
                                                          231
                 target network
177
                                                          232
                                                                       # ===== compute targets y and feature matrix
178
179
                 last logits (i.e. Qvalues) of shape (O233
                                                          234
                                                                        # turn batch into individual tuples, numpy
                     1)
                                                                            arrays, or lists
180
181
                                                          235
                                                                        states = batch.state
182
             if target == True:
                                                          236
                                                                        rewards = np.array(list(batch.reward))
183
                                                                        actions = np.array(list(batch.action))
                 W1 = np.copy(self.W1_target)
                                                          237
                                                          238
184
                 W2 = np.copy(self.W2_target)
                                                                        next_states = list(batch.next_state)
185
             else:
                                                          239
                                                                       dones = np.array(list(batch.done))
                 W1 = np.copy(self.W1)
186
                                                          240
187
                 W2 = np.copy(self.W2)
                                                          241
                                                                       # compute targets y and feature matrix X
                                                                       y = np. zeros((self.O, len(dones)))
188
                                                          242
189
             # forward pass/propagation
                                                          243
                                                                        for j in np.arange(len(dones)):
                                                                            if dones[j]: # if done, set y_j = r_j
190
             a1 = W1 @ x
                                                          244
191
             h1 = self.act_f_1(a1)
                                                          245
                                                                                y[actions[j], j] = rewards[j]
192
             h1[0,:] = 1 # set first row (bias to secon 246
                                                                            else:
                  layer) to 1 (this ignores the weights 247
                                                                                # compute Q_prime
                  for the k+1th hidden neuron, because
                                                                                Q_target = self.forward(next_states[
                 this should not exist; this allows to
                                                                                    j], target=True)[-1]
                 only use matrix multiplication and
                                                                                y[actions[j], j] = rewards[j] +
                  simplify the gradients as we only need 2
                                                                                    gamma*np.max(Q_target)
                  instead of 4)
                                                          250
193
                                                          251
             a2 = W2 @ h1
                                                          252
                                                                        # convert states to feature matrix X
194
             h2 = self.act_f_2(a2)
195
                                                          253
             return a1, h1, a2, h2
                                                                       X = np.hstack((states))
196
                                                          254
197
198
         def backward (self, R, x, Qvalues, Q_prime, a1, 256
                                                                       # ===== compute TD error (aka delta) =====
             h1, a2, gamma, future_reward,
                                                          257
             action_binary_mask):
                                                          258
                                                                       a1, h1, a2, Qvalues = self.forward(X)
199
                                                          259
                                                                        delta = y - Qvalues # -> shape (O,
200
             backward for methods "qlearning" and "sarsa"
                                                                            batch_size)
201
                                                          260
             x has shape (D+1, 1) (constant bias 1 must 261
                                                                        self.compute_gradients(delta, a1, h1, a2, X)
                 be added beforehand)
                                                          262
                                                                        self.update_parameters(self.eta)
203
             set future_reward=True for future reward
                                                          263
                 with gamma>0, False for immediate rewa264
                                                                   def compute_gradients(self, delta, a1, h1, a2, x
                                                          265
204
             Q_prime must be chosen according to the
                 method on x_prime (on- or off-policy) 266
                                                                        # ==== compute gradient of the loss with
205
                                                                            respect to the weights =====
206
                                                          267
207
             # backward pass/backpropagation
                                                                        # common part of the gradient TODO: check
                                                          268
             # compute the gradient of the square loss
                                                                            dimensions
                                                          269
                                                                        self.dL_da2 = delta * self.grad_act_f_2(a2)
                 with respect to the parameters
209
                                                          270
210
             # ==== compute TD error (aka delta) ===== 271
                                                                        # gradient of loss wrt W2
211
                                                          272
                                                                        self.dL_dW2 = self.dL_da2 @ h1.T
212
             # make reward of shape (O, 1)
                                                          273
213
             R_{rep} = np.tile(R, (self.O, 1))
                                                          274
                                                                       # gradient of loss wrt W1
```

163

275		$self.dL_dW1 = ((self.W2.T @ self.dL_da2)$	*	
		self.grad_act_f_1(a1)) @ x.T		## SET DONE TO ZERO (BEGINNING
276		<u> </u>		OF THE EPISODE)
277			335	i = 1
278				
279	def	update_parameters(self, eta):		## COUNTER FOR NUMBER OF ACTIONS
280			336	
281		# gradient clipping	337	$S, X, allowed_a = env.$
282				Initialise_game() ##
283		# dL_dW1_norm = np.linalg.norm(self.dL_dW	1)	INITIALISE GAME
284		<pre># if dL_dW1_norm >= self.gradient_clip:</pre>	338	$X = np.expand_dims(X, axis=1)$
285		<pre># self.dL_dW1 = self.gradient_clip *</pre>		## MAKE X A
		self.dL_dW1 / dL_dW1_norm		TWO DIMENSIONAL ARRAY
286			339	X = np.copy(np.vstack((np.array)))
287		# dL_dW2_norm = np.linalg.norm(self.dL_dW	2)	([[1]]), X)) # add bias term
288		# if dL_dW2_norm >= self.gradient_clip:	340	([[-]]),//) " " " " " " " " " " " " " " " " " "
289		# self.dL_dW2 = self.gradient_clip *	341	if self.method == "sarsa":
20)		self.dL_dW2 / dL_dW2_norm	342	# compute Q values for the given
290		Serr. db_d w 2 / db_d w 2_norm	3.2	state
291		# update W1 and W2	343	a1, h1, a2, Qvalues = self.
292		$self.W2 = self.W2 + eta * self.dL_dW2$	545	forward (X) # -> shape $(O,$
293		$self.W2 = self.W2 + eta * self.dL_dW2$ $self.W1 = self.W1 + eta * self.dL_dW1$		1) $\pi = \sin \mu c (0, 1)$
		$SEII.WI = SEII.WI + Eta * SEII.UL_UWI$	344	1)
294				# -14: A:
295			345	# choose an action A using
296			246	epsilon-greedy policy
297			346	A_binary_mask, A_ind =
298	def	train (self, env, N_episodes, eta, epsilon_		EpsilonGreedy_Policy (Qvalues
		beta, gamma, alpha=0.001, gradient_clip=	1,	, allowed_a , epsilon_f) #
		batch_size=32, run_number=None):		-> shape (O, 1)
299		"""	347	
300		alpha is used as weight for the exponenti	a B48	
		moving average displayed during train:	in3 ⊈ 9	while Done==0:
				##
301		batch_size is only used for the DQN method	d.	START THE EPISODE
302		"""	350	
303			351	<pre>if (self.method == "qlearning")</pre>
304		# add training hyper parameters		or (self.method == "dqn"):
305		self. N_episodes = N_episodes	352	# compute Q values for the
306		self.eta = eta	332	given state
307		self.eta = eta self.epsilon_0 = epsilon_0	353	a1, h1, a2, Qvalues = self.
308		self.beta = beta	333	
308				forward (X) # -> shape (
		self.gamma = gamma	254	0, 1)
310		self.alpha = alpha	354	II 1
311		self.gradient_clip = gradient_clip	355	# choose an action A using
312		self.batch_size = batch_size	256	epsilon-greedy policy
313			356	A_{binary_mask} , $A_{ind} =$
314				EpsilonGreedy_Policy(
315		training_start = time.time()		Qvalues, allowed_a,
316				epsilon_f) # -> shape (
317		try:		0, 1)
318			357	
319		# initialize histories for important	358	
		metrics	359	# take action and observe reward
320		self.R_history = np.full([self.		R and state S_prime
		N_episodes, 1], np.nan)	360	S_prime, X_prime,
321		self. N_moves_history = np. full ([self.		allowed_a_prime, R, Done =
		N_episodes, 1], np.nan)		env. OneStep(A_ind)
322		self.dL_dW1_norm_history = np.full([s	e B 6 1	X_prime = np.expand_dims(X_prime
5 		. N_episodes, 1], np.nan)	0.001	, $axis=1$)
323		self.dL_dW2_norm_history = np.full([s	e B62	$X_{prime} = np.copy(np.vstack((np.$
323		. N_episodes, 1], np.nan)	C DD2	array ([[1]]), X_prime))) #
224		. N_episodes, 1j, np. nan)		array ([[1]]), X_prime))) #
324		# 1	262	add bras term
325		# progress bar	363	
326		episodes = tqdm(np.arange(self.	364	n_steps += 1
227		N_episodes), unit="episodes")	365	
327		ema_previous = 0	366	<pre>if self.method == "dqn":</pre>
328			367	
329		$n_steps = 0$	368	# store the transition in
330				memory
331		for n in episodes:	369	self.replay_memory.push(X,
332		•		A_ind, R, X_prime, Done)
333		$epsilon_f = self.epsilon_0 / (1 +$	370	_ , , _r , , ,
-		beta * n) ## DECAYING EPSILO		# sample a batch of
334		Done = 0		transitions
		-		

372	transactions = self. 409	
	replay_memory.sample(410	if self.method == "qlearning
	self.batch_size)	":
373	# turn list of transactions411	# chose next action off-
	into transaction of	policy
	lists 412	$Q_{prime} = np.max(self.$
374	batch = Transition(*zip(*	forward (X_prime)
57.	transactions))	[-1])
375	413	[-]/
376	# backward step and 414	<pre>elif self.method == "sarsa":</pre>
	parameter update 415	# chose next action on-
377	self.backward_dqn(batch,	policy
577	self.gamma) 416	policy
378	417	al_prime, hl_prime,
379	# update Q values indirectly by	a2_prime,
319		•
	updating the weights and	Qvalues_prime = self
200	biases directly	. forward (X_prime) #
380	of Dame 1. # THE EDICODE HAC 410	\rightarrow shape $(N_a, 1)$
381	if Done==1: # THE EPISODE HAS 418	
	ENDED, UPDATEBE CAREFUL419	# chose next action and
	THIS IS THE LAST STEP OF THE	save it
	EPISODE 420	A_binary_mask_prime ,
382		A_ind_prime =
383	if (self.method == "	EpsilonGreedy_Policy
	qlearning") or (self.	(Qvalues_prime,
	method == "sarsa"):	allowed_a_prime,
384	# compute gradients and	epsilon_f)
	update weights 421	· F · · · · · · · · · ·
385	self.backward(R, X, 422	# get Qvalue of next
303	Qvalues, None, a1,	action
		Q prime = Qvalues prime
	, , , , , , , , , , , , , , , , , , , ,	
	future_reward=False,	A_ind_prime]
	action_binary_mask 2 4	
	A_binary_mask) 425	
386	426	if (self.method == "
387	# store history	qlearning") or (self.
388	# todo: record max possible	method == "sarsa"):
	reward per episode 427	# backpropagation and
389	$self.R_history[n] = np.copy($	weight update
	R) # reward per episod 28	self.backward(R, X,
390	self.N_moves_history[n] = np	Qvalues, Q_prime, a1
570	copy(i) # nr moves per	, h1, a2, self.gamma
	episode	, future_reward=True
391	cpisode	· · · · · · · · · · · · · · · · · · ·
392	# store norm of anodients	, action_binary_mask
	# store norm of gradients	=A_binary_mask)
393	self.dL_dW1_norm_history[n]429	
	= np.linalg.norm(self.430	# NEXT CELEBRATE AND CO. DECOME
	$dL_{dW1}) 431$	# NEXT STATE AND CO. BECOME
394	self.dL_dW2_norm_history[n]	ACTUAL STATE
	= np.linalg.norm(self.432	<pre>if self.method == "sarsa":</pre>
	dL_dW2) 433	$A_{binary_mask} = np.copy($
395		A_binary_mask_prime)
396	# compute exponential movir#34	$A_{ind} = np.copy($
	average (EMA) to	A_ind_prime)
	display during training435	$a1 = np.copy(a1_prime)$
397	ema = $alpha*R + (1-alpha)*436$	$h1 = np.copy(h1_prime)$
	ema_previous 437	$a2 = np.copy(a2_prime)$
398		Qvalues = np.copy(
399	ema = R	Qvalues_prime)
400		$S = np.copy(S_prime)$
401	if run_number is not None: 440	$X = np.copy(X_prime)$
402	episodes.set_descriptio441	allowed_a = np.copy(
	$(f"Run = \{run_number\})$	allowed_a_prime)
	$\}$; EMA Reward = $\{er442$	
	:.2 f}") 443	i += 1 # UPDATE COUNTER FOR
403	else:	NUMBER OF ACTIONS
404	episodes.set_descriptio444	
	$(f''EMA Reward = {er445}$	if (self.method == "dqn") and (
	:.2f}")	n_{steps} % self.C == 0):
405	446	# update target network
406	break	•
407		every C steps
	447	self.W1_target = np.copy(
408	else: # IF THE EPISODE IS NOT	self.W1)
	OVER 448	self.W2_target = np.copy(

```
self.W2)
                                                                        name extension=None):
449
                                                              510
450
                                                              511
                                                                       # read values and store in neural network
451
                  training_end = time.time()
                                                                            instance
                                                                       name = f''\{method\}_{act_f_1}_{act_f_2}''
452
                  self.training_time_in_seconds =
                                                              512
                                                              513
                                                                        if name_extension is not None:
                       training_end - training_start
453
                                                              514
                                                                            name += f"_{name_extension}"
454
                  return None
                                                              515
                                                                       path = f"models/{name}"
455
                                                              516
                                                              517
                                                                        # print(f"loading from: {path}")
456
457
              except KeyboardInterrupt as e:
                                                             518
458
                  # return nothing
                                                              519
                                                                       # initialize neural network
459
                  training_end = time.time()
                                                              520
                                                                       nn = NeuralNetwork(0,0,0, activation_function_1 =
460
                  self.training_time_in_seconds =
                                                                            act_f_1, activation_function_2=act_f_2,
                       training_end - training_start
                                                                            method=method)
461
                                                              521
462
                  return None
                                                              522
                                                                       # network weights
                                                                       nn.W1 = np.load(f"{path}/W1.npy")
463
                                                              523
                                                                       nn.W2 = np.load(f"{path}/W2.npy")
464
                                                              524
465
          def save(self, name_extension=None):
                                                              525
466
              # create directory for the model
                                                              526
                                                                       # network training history
              name = f"{self.method}_{self.act_f_1_name}_527
self.act_f_2_name}"
467
                                                                       nn.R_history = np.load(f"{path}/
                                                                            training_history_R.npy")
468
                                                                        nn.N_moves_history = np.load(f"{path}/
              if name_extension is not None:
                                                              528
                                                                            training_history_N_moves.npy")
                  name += f"_{name_extension}"
469
470
                                                              529
                                                                       nn.dL_dW1\_norm\_history = np.load(f"{path}/
471
              path = f"models/{name}"
                                                                            training_history_dL_dW1_norm.npy
472
              if not os.path.isdir(path): os.mkdir(path) 530
                                                                       nn.dL_dW2_norm_history = np.load(f"{path}/
                                                                            training_history_dL_dW2_norm.npy")
473
              print(f"saving to: {path}")
474
                                                              531
                                                                       # network training parameters
475
              # save weights
                                                              532
              np.save(f"{path}/W1.npy", self.W1)
np.save(f"{path}/W2.npy", self.W2)
476
                                                              533
                                                                       with open(f"{path}/training_parameters.json", "r
477
                                                                             ") as f:
478
                                                              534
                                                                            params = json.load(f)
479
              # save training history
                                                              535
                                                                            # set parameters to the network instance
nn.method = params["method"]
480
              np.save(f"{path}/training_history_R.npy",
                                                             536
                   self.R_history)
                                                              537
                                                                            nn. N_episodes = int(params["N_episodes"])
481
              np.save(f"{path}/training_history_N_moves.
                                                             538
                  npy", self.N_moves_history)
                                                              539
                                                                            nn.eta = float(params["eta"])
                                                                            nn.epsilon_0 = float(params["epsilon_0"])
nn.beta = float(params["beta"])
              np. save (f"{path}/
                                                              540
482
                   training_history_dL_dW1_norm.npy", self41
                   dL_dW1_norm_history)
                                                              542
                                                                            nn.gamma = float (params ["gamma"])
483
              np.save(f"{path}/
                                                              543
                                                                            nn.alpha = float (params ["alpha"])
                   training_history_dL_dW2_norm.npy", se1544
                                                                            # nn.gradient_clip = float(params["
                   dL_dW2_norm_history)
                                                                                 gradient_clip"])
484
                                                              545
                                                                            try:
485
              # save training parameters and other gener 546
                                                                                nn.seed = int(params["seed"])
                   info
                                                              547
                                                                            except:
486
              params = {
                                                              548
                                                                                nn.seed = params["seed"]
                   "method": self.method,
487
                                                              549
                                                                            nn.D = int(params["D"])
                                                                            nn.K = int(params["K"])
                  "N_episodes": self.N_episodes,
488
                                                              550
                  "eta": self.eta,
489
                                                              551
                                                                            nn.O = int(params["O"])
490
                  "epsilon_0": self.epsilon_0,
                                                              552
                                                                            nn.training_time_in_seconds = float(params["
                  "beta": self.beta,
491
                                                                                 training_time_in_seconds"])
                  "gamma": self.gamma,
492
                                                              553
                  "alpha": self.alpha,
493
                                                              554
                                                                            if nn.method == "dqn":
494
                     gradient_clip": self.gradient_clip,555"
                                                                                nn.capacity = int(params["capacity"])
                  "seed": self.seed,
                                                                                nn.batch_size = int(params["batch_size"
495
                                                              556
                  "D": self.D,
496
497
                  "K": self.K,
                                                              557
                                                                                nn.C = int(params["C"])
498
                  "O": self.O,
                                                              558
                  "training_time_in_seconds": self.
                                                              559
499
                                                                        if nn.method == "dqn":
                       training_time_in_seconds
                                                              560
500
                                                              561
                                                                            nn.W1\_target = np.copy(nn.W1)
              if self.method == "dqn":
501
                                                              562
                                                                            nn.W2\_target = np.copy(nn.W2)
                  params["capacity"] = self.capacity 563
params["batch_size"] = self.batch_size 564
502
503
                                                                        return nn
                  params["C"] = self.C
504
              with \ open(\ \tilde{f}\ "\{path\ \}/\ training\_parameters\ .\ json"
505
                                                                                        Listing 1: caption
                     "w") as f:
                  json.dump(params, f)
506
507
508
```

509

def load_from(method, act_f_1, act_f_2,