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1 Summary of Notation

Symbol	Description	Reference
s	state	
a	action	
r	reward	
t	timestep	
T	terminal timestep	
0	partially observable environment frame	
γ	discount	
x	hidden state	
G^N	N-step return	
δ	TD-error or value diff	5.3.14
V	value function	
Q	state-action value function	
\mathcal{A}^e	environment action space	5.3.3
\mathcal{A}^a	agent action space	5.3.3
\mathcal{S}	state space	
0	observation space	
\mathcal{T}_t	step sample	5.3.7
\mathcal{T}	trajectory sample	
\mathcal{L}	loss function	
h	representation function	
g	dynamics function	
f	prediction function	
ϱ	projection function	
X	hidden state	
v^i	value prediction	
B	batch size	
H	height	5.3.1
W	width	5.3.1
C_e	environment channels	5.3.1
C_h	history channels	5.3.4
C_x	hidden space channels	
K	number of unrolled steps	5.3.7
L	history length	5.3.7
N	bootstrap length for N-step return	5.3.7
A	dimension of action	
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2 Introduction

Deep Learning (DL) is a branch of **Artificial Intelligence (AI)** that emphasizes the use of neural networks to fit the inputs and outputs of a dataset. The training of a neural network is done by computing the gradients of the loss function with respect to the weights and biases of the network. A better trained neural network can better approximate the function that maps the inputs to the outputs of the dataset.

Reinforcement Learning (RL) is a branch of AI that emphasizes on solving problems through trials and errors with delayed rewards. RL had most success in the domain of game playing, including boardgames and Atari games. An extension to game playing is General Game Playing (GGP), whose goal is to design a single algorithm that can play many different games without having much prior knowledge of the games.

Deep Reinforcement Learning (DRL) is a rising branch that combines DL and RL techniques to solve problems. In a DRL system, RL techniques lay out the structure of the algorithm such as the use the **agent-environment interface**

reference

, a value function, a reward signal, e.t.c., while DL techniques are used approximate specific functions such as the value function.

Planning refers to any computational process that analyzes generated actions and their consequences in an environment. In the RL terms, planning specifically means the use of a model to improve a policy. RL algorithms that use planning had great success in playing boardgames, with the most significant achievement of beating human experts in Computer Go.

A distributed system is a computer system that uses multiple processes with various purposes to complete tasks. DRL systems for solving large problems are both data and compute intensive. Utilizing concurrency to increase efficiency and throughput for these DRL systems are sometimes necessary. Building a distributed system to achieve such concurrency is a common practice in the industry but requires significant engineering effort.

2.1 Contribution

In this thesis we present the project **MooZi**, a general game playing system that play games by planning with a learned model. The systems

- a collection of environment bridges that connect the system to various environments using a unified interface
- a neural network model that learns representation and could be used for planning
- a MCTS based planner that uses the learned model to perform planning.
- a distributed training system that efficiently trains the agent.
- a thesis with empirical studies and analysis

3 Literature Review

3.1 Planning and Search

Many AI problems can be reduced to a search problem [56, p.39]. Such search problems can be solved by determining the best plan, path, model, function, and so on, based on some metrics of interest. Therefore, search has played a vital role in AI research since its dawn. The terms **planning** and **search** are widely used across different domains. Here we adopt the definition by Sutton and Barto [53].

Planning refers to any process by which the agent updates the action selection policy $\pi(a \mid s)$ or the value function $V_{\pi}(s)$. We will focus on the case of improving the policy in our discussion. We view the planning process as an operator \mathcal{I} that takes the policy as input and outputs an improved policy $\mathcal{I}\pi$.

Planning methods can be categorized based on the target state s they aim to improve. If the method improves the policy for arbitrary states, we call it **background planning**. That is, for any timestep t and a set of states $S' \subset S$:

$$\pi(a \mid s) \leftarrow \mathcal{I}\pi(a \mid s), \ \forall s \in \mathcal{S}'$$

Typical background planning methods include **dynamic programming** and **Dyna-Q** [53]. In the case of dynamic programming, a full sweep of the state space is performed and all states are updated. In the case of Dyna, a subset of the state space is selected for update.

An other type of planning focuses on improving the policy of the current state s_t . We call this **decision-time planning**. That is, for any timestep t:

$$\pi(a \mid s) \leftarrow \mathcal{I}\pi(a \mid s), s = s_t$$

Algorithms such as AlphaGo use both types of planning when they use self-play for training. For decision-time planing, a tree search is performed at the root node and updates the policy of the current state. For background planning, a neural network uses past experience to train and updates policy for all states.

An early example of the use of search as a planning method is the **A*** algorithm. In 1968, Hart, Nilsson, and Raphael designed the A* algorithm for finding a shortest path from a start vertex to a target vertex [19]. Although A* works quite well for many problems, especially in early game AI, it falls short in cases where the assumptions of A* do not hold. For example, A* requires a heuristic, and an optimal solution under stochastic environments. It is computationally infeasible on large problems. To address this problem, Korf framed the problem of **Real-Time Heuristic Search**, where the agent has to make a decision in each timestep with bounded computation, and developed the **Real-Time-A*** algorithm as a modified version of A* with bounded computation per step [32]. Tree-based search algorithms such as **MiniMax** and **Alpha-Beta Pruning** were developed to play and solve two-player games [29]. Monte Carlo techniques are designed to handle complex environments.

3.2 Monte Carlo Methods

In 1873, Joseph Jagger observed the bias in roulette wheels at the Monte Carlo Casino. He studied the bias by recording the results of roulette wheels and won over 2 million francs over several days by betting on the most favorably biased wheel [40]. Therefore, **Monte Carlo (MC)** methods gained their name as a class of algorithms based on random samplings.

MC methods are used in many domains but in this thesis we will primarily focus on its usage in search. In a game where terminal states are usually unreachable by the limited search depth, evaluation has to be performed on the leaf nodes that represent intermediate game states. One way of obtaining an evaluation on a state is by applying a heuristic function. Heuristic functions used this way are usually hand-crafted by human based on expert knowledge, and hence are prone to human error. The other way of evaluating the state is to perform a rollout from that state to a terminal state by selecting actions randomly. This evaluation process is called **random rollout** or **Monte Carlo rollout**.

3.3 Monte Carlo Tree Search (MCTS)

Kocsis and Szepesvári developed the Upper Confidence Bounds applied to Trees (UCT) method as an extension of the Upper Confidence Bound (UCB) algorithm employed in multi-armed bandit problems [31]. Rémi Coulom developed the general idea of Monte Carlo Tree Search that combines Monte Carlo rollouts with tree search [8] for his Go program CrazyStone. Shortly afterwards, Gelly et al. implemented another Go program MoGo, that uses the UCT selection formula [17]. MCTS was generalized by Chaslot et al. as a framework for game AI [7]. This framework requires less domain knowledge than classic approaches to game AI while giving better results. The core idea of this framework is to gradually build the search tree by iteratively applying four steps: selection, expansion, evaluation, and backpropagation. The search tree built in this way emphasizes more promising moves and game states based on collected statistics in rollouts. More promising states are visited more often, have more children, have deeper subtrees, and rollout results are aggregated to yield more accurate values. Here we detail the four steps in the MCTS framework by Chaslot et al. (see Figure 1).

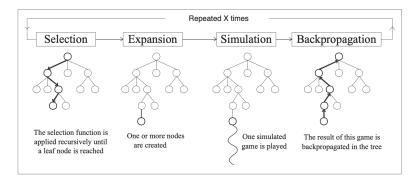


Figure 1: The Monte Carlo Tree Search Framework. Source: [7]

3.3.1 Selection

The selection process starts at the root node and repeats until a leaf node in the current tree is reached. At each level of the tree, a child node is selected based on a selection formula such as UCT or PUCT. A selection formula usually has two parts: the exploitation part based on the evaluation function E, and the exploration bonus function B. For actions $(s, a), a \in \mathcal{A}$ of a parent state s, the selection I(s) is defined as

$$I(s) = \operatorname*{argmax}_{a \in \mathcal{A}} \left[E(s, a) + B(s, a) \right]$$

The evaluation function E can be based on the value of the child, the accumulated reward of the child, or the prior selection probability based on the policy $\pi(a \mid s)$. The exploration bonus function B is usually based on the visit count of the child and the parent. The more visits a child has, the smaller the exploration bonus becomes. For example, the UCT algorithm uses

$$E(s, a) = \frac{V(s)}{N(s, a)}$$
$$B(s, a) = \sqrt{\frac{2 * \log(\sum_{b \in \mathcal{A}} N(s, b))}{N(s, a)}}$$

where V(s) is the value of the node, and N(s,a) is the visit count of the edge. This Gelly et al. used this selection rule in their implementation of MoGo, the first computer Go program that uses UCT [17]. Rosin developed the PUCB and the PUCT algorithm that utilize a predictor P(s,a) that estimates the prior probability of the action a being selected from state s and later being used in AlphaGo (3.5, [45]).

3.3.2 Expansion

The selected leaf node is expanded by adding one or more children. Each child represents a successor game state reached by playing the associated legal move.

3.3.3 Evaluation

The expanded node is evaluated, either by playing a game with a rollout policy, or by using an evaluation function, or by using a blend of both approaches. Many MCTS algorithms use a randomized policy as the rollout policy and the game result as the evaluation. Early work on evaluation functions focused on hand-crafted or machine learned heuristic functions based on expert knowledge. Recently, evaluation functions use deep neural networks specifically trained for the problems (3.4).

3.3.4 Backpropagation

After the expanded nodes are evaluated, the nodes on the path from the expanded nodes back to the root are updated. The statistics updated usually include visit count, estimated value and accumulated reward of the nodes.

3.3.5 MCTS Iteration and Move Selection

The four MCTS steps are repeated until the budget runs out. The budget is usually a limited number of simulations or a period of time. After the search, the agent acts by selecting the action associated with the most promising child of the root node. This could be the most visited child, the child with the greatest value, or the child with the greatest lower confidence bound value [46, 55].

3.4 AlphaGo

In 2017, Silver et al. developed **AlphaGo**, the first Go program that beat a human Go champion on even terms [51]. AlphaGo was trained with a machine learning pipeline with multiple stages. For the first stage of training, a supervised learning policy (or SL policy) is trained to predict expert moves using a neural network. This SL policy p is parametrized by weights σ , denoted p_{σ} . The input of the policy network is a representation of the board state, denoted s. The network outputs a probability distribution over all legal moves s through the last softmax layer. During the training of the network, randomly sampled expert moves are used as training targets. The weights s are then updated through gradient ascent to maximize the probability of matching human expert move:

$$\Delta\sigma \propto \frac{\partial \log p_{\sigma}(a \mid s)}{\partial \sigma}$$

For the second stage of training, the supervised policy p_{σ} is used as the starting point for training with reinforcement learning. This reinforcement learning trained policy (or RL policy) is parametrized by weights ρ and is initialized $p_{\rho} = p_{\sigma}$. Training data is generated in form of self-play games using p_{ρ} as the rollout policy. For each game, the game outcome $z_t = \pm r(s_T)$, where s_T is the terminal state, $z_T = +1$ for winning, $z_T = -1$ for losing from the perspective of the current player. Weights ρ are updated

using gradient ascent to maximize the expected outcome using the update formula:

$$\Delta \rho \propto \frac{\partial \log p_{\rho} \left(a_t \mid s_t \right)}{\partial \rho} z_t$$

Finally, a value function is trained to evaluate board positions. This value function is modeled with a neural network with weights θ , denoted V_{θ} . Given a state s, $V_{\theta}(s)$ predicts the outcome of the game if both players act according to the policy p_{ρ} . This neural network is trained with stochastic gradient descent to minimize the mean squared error (MSE) between the predicted value $V_{\theta}(s)$ and the outcome z.

$$\Delta\theta \propto \frac{\partial V_{\theta}(s)}{\partial \theta} \left(z - V_{\theta}(s)\right)$$

AlphaGo combines the policy network p_{ρ} and the value network V_{θ} with MCTS for acting. AlphaGo uses a MCTS variant called PUCT similar to that described in 3.3. In the search tree, each edge (s, a) stores an action value Q(s, a), a visit count N(s, a), and a prior probability P(s, a). At each time step, the search starts at the root node and simulates until the budget runs out. In the select phase of each simulation, an action is selected for each traversed node using the same base formula (??). In AlphaGo, the exploitation score of the selection formula is the estimated average value of the next state after taking the actions, namely Q(s, a). In AlphaGo's PUCT formula, The exploration bonus of edge (s, a) is based on the prior probability P and decays as its visit count N grows. As before, the action taken at time t maximizes the sum of the exploitation score and the exploration bonus

$$I(s) = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \left[E(s, a) + B(s, a) \right]$$

$$E(s, a) = Q(s, a)$$

$$B(s, a) \propto \frac{P(s, a)}{1 + N(s, a)}$$

AlphaGo evaluates a leaf node state s_L by blending both the value network estimation $V_{\theta}(s_L)$ and the game result z_L obtained by the rollout policy p_{π} The mixing parameter $\lambda \in [0, 1]$ is used to balance these two types of evaluations into the final evaluation $V(s_L)$

$$V(s_L) = (1 - \lambda)V_{\theta}(s_L) + \lambda z_L$$

3.5 AlphaGo Zero

AlphaGo Zero is a successor of AlphaGo that beat AlphaGo by 100-0 in 100 games [51]. In contrast, AlphaGo Zero learns to play Go from *tabula rasa*. This means it learns solely by reinforcement learning from self-play, starting from random play, without supervision from human expert data.

Central to AlphaGo Zero is a deep neural network f_{θ} with parameters θ . Given a state s as an input, the network outputs both move probabilities \boldsymbol{p} and value estimation v

$$(\mathbf{p}, v) = f_{\theta}(s)$$

To generate self-play games $s_1, ..., s_T$, MCTS is performed at each state s using the latest neural network f_{θ} . To select a move for a parent node p in the search tree, a variant of the PUCT algorithm is used:

$$I(s) = \operatorname{argmax}_{a \in \mathcal{A}} (E(s, a) + B(s, a))$$

$$E(s, a) = Q(s, a)$$

$$B(s, a) \propto P(s, a) \frac{\sqrt{\sum_{b \in \mathcal{A}} N(s, b)}}{1 + N(s, a)}$$

Self-play games are processed into training targets to update the network parameters θ through gradient descent on the loss function l

$$\mathcal{L}(\theta) = (z - v)^2 - \boldsymbol{\pi}^{\mathrm{T}} \log \boldsymbol{p} + c \|\theta\|^2$$

Here $(z-v)^2$ is the mean squared error of the prediction value, $-\boldsymbol{\pi}^{\mathrm{T}} \log \boldsymbol{p}$ is the cross-entropy loss of the move probabilities, and $c\|\theta\|^2$ is a L_2 weight regularization. Many other components of this system are similar to those in AlphaGo.

3.6 AlphaZero

AlphaZero reduces game specific knowledge of AlphaGo Zero even further so that the same algorithm can be also applied to Shogi and chess [50]. One generalization is that in AlphaZero the game result is no longer either winning or losing $(z \in \{-1, +1\})$, but can also be a draw $(z \in \{-1, 0, +1\})$.

3.7 MuZero

In 2020, Schrittwieser et al. developed **MuZero**, an even more algorithm that learns to play Atari, Go, chess and Shogi at superhuman level. Compared to the AlphaGo and AlphaZero, MuZero has no access to a perfect model of the game. MuZero plans with a neural network that learns the game dynamics through experience. Therefore, MuZero can be applied to games where either the perfect model is not known or is infeasible to compute with.

MuZero defines three main functions. The **representation function** h encodes a history of observations o_1, o_2, \ldots, o_t and actions $a_1, a_2, \ldots, a_{t-1}$ into a hidden state \mathbf{x}_t^0 . This hidden state is learned, and is the main conceptual change from AlphaZero. The **dynamics function** g implements action execution in the representation. Given a hidden state \mathbf{x}^k and action a^k , produces an immediate reward r^k and the next hidden

state \mathbf{x}^{k+1} . The **prediction function** f corresponds to the one network in AlphaZero. Given a hidden state \mathbf{x}^k , it produces a probability distribution p^k of actions and a value v^k associated to that hidden state. Three functions f, g, h are approximated jointly in a neural network with weights θ

$$\mathbf{x}_{t}^{0} = h_{\theta}(o_{1}, \dots, o_{t}, a_{1}, \dots, a_{t-1}) \tag{1}$$

$$\mathbf{x}_{t}^{0} = h_{\theta}(o_{1}, \dots, o_{t}, a_{1}, \dots, a_{t-1})$$

$$(\mathbf{x}^{k+1}, \hat{r}^{k+1}) = g_{\theta}(\mathbf{x}^{k}, a^{k})$$
(1)
(2)

$$(v^k, \mathbf{p}^k) = f_{\theta}(\mathbf{x}^k) \tag{3}$$

The superscripts of \mathbf{x} , a, v denote the depth of such values in the search tree, and depth 0 is at the search tree's root. Equivalently, the superscripts also mean the number of recurrent inferences (through the dynamics function q) the algorithm performs to obtain that value.

MuZero plans with a search method based on the MCTS framework (discussed in 3.3). Due to the lack of access to a perfect model, MuZero's MCTS differs from a standard one in numerous ways. The nodes are no longer perfect representations of the board states. Instead, each node is associated with a hidden state \mathbf{x} as a learned representation of the board state. The transition is no longer made by the perfect model but by the dynamics function q. Moreover, since the dynamics function also predicts a reward, edges created through inferencing with the dynamics function also contribute to the Q value estimation.

To act in the environment, MuZero plans following the MCTS framework described in section 3.3. At each timestep t, \mathbf{x}_t^0 is created using (1). A variant of PUCT is used to select an action during the search

$$I(s) = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \left(E(s, a) + B(s, a) \right)$$

$$E(s, a) = Q(s, a)$$

$$B(s, a) \propto P(s, a) \frac{\sqrt{\sum_{b \in \mathcal{A}} N(s, b)}}{1 + N(s, a)} \left[c_1 + \log \left(\frac{\sum_{b \in \mathcal{A}} N(s, b) + c_2 + 1}{c_2} \right) \right] .$$

Where c_1 and c_2 are two constants that adjust the exploration bonus. The selected edge (\mathbf{x}^k, a^k) at depth k is expanded using (2) and evaluated using (3). At the end of the simulation, the statistics of the nodes along the search path are updated. We denote the updated prior action probabilities \mathbf{p}^* , and the updated value estimation v^* . Notice since the transitions of the nodes are approximated by the neural network, the search is performed over hypothetical trajectories without using a perfect model. Finally, the action a^0 of the most visited edge (\mathbf{x}^0, a^0) of the root node is selected as the action to take in the environment.

Experience generated is stored in a replay buffer and processed into training targets.

The three functions of the model are trained jointly using the loss function

$$\mathcal{L}_{t}(\theta) = \underbrace{\sum_{k=0}^{K} \mathcal{L}^{p} \left(p_{t+k}^{*}, p_{t}^{k} \right)}_{(1)} + \underbrace{\sum_{k=0}^{K} \mathcal{L}^{v} \left(z_{t+k}, v_{t}^{*} \right)}_{(2)} + \underbrace{\sum_{k=1}^{K} \mathcal{L}^{r} \left(r_{t+k}, \hat{r}^{k} \right)}_{(3)} + \underbrace{c \|\theta\|^{2}}_{(4)}$$

$$(4)$$

where K is the rollout depth, (1) is the loss of the predicted prior move probabilities and move probabilities improved by the search, (2) is the loss of the predicted value and experienced N-step return, (3) is the loss of the predicted reward and the experienced reward, and finally (4) is the L_2 regularization.

3.7.1 MuZero Reanalyze

Schrittwieser et al. also developed **MuZero Reanalyze**, a sample efficient variant of MuZero [48]. This method generates training targets in addition to those generated through game play through re-executing search on old games using the latest parameters. **MuZero Unplugged** and **Efficient Zero** also use similar mechanisms to generate new data by updating search statistics of old data [49, 57]. In Efficient Zero, experiments are ran with a reanalyze ratio of 0.99, which means only 1% of the training data are generated through interacting with the environment, and the other 99% are generated by re-running search on old trajectories. In our project, we also implement a reanalyze worker to perform this task (see section 5.3.10, 5.3.13).

3.8 Atari Games Playing

3.8.1 Atari Learning Environment

The Atari 2600 gaming console was developed by Atari, Inc. and was released in 1977. Over 30 million copies of the console sold over its 15 years on the market [2]. The most popular game, PacMan, was sold over 8 million copies and was the all-time best-selling video game back then. Stella is a multi-platform Atari 2600 emulator released under the GNU General Public License (GPL) [52]. Stella was ported to popular operating systems such as Linux, MacOS, and Windows, providing Atari 2600 experiences to users without physical copies of the equipment. In 2013, Bellemare et al. introduced the Arcade Learning Environment (ALE) and the library has been publicly available since [3]. ALE provides interfaces of over a hundred of Atari game environments using Stella as the backend. Each ALE environment has specifications on its visual representation, action space, and reward signals. ALE environments are suitable for controlled machine learning research, because data are well-represented and evaluation metrics are clearly defined. Moreover, ALE environments are diverse in their characteristics: while some environments require more mechanical mastery of the agent, others require more longterm planning. This makes solving multiple ALE environments using the same algorithm a good general game playing problem (2).

3.8.2 Deep Q-Networks

Mnih et al. pioneered the study of using deep neural networks to learn in ALE environments [38]. They developed the algorithm **Deep Q-Networks (DQN)** that learned to play seven of the Atari games and reached human-level performance. The DQN agent has a neural network that approximates the Q function, parametrized by weights θ , denoted Q_{θ} . Experiences are generated through interacting with the environment by taking the action that maximizes the immediate Q value

$$\pi(a_t \mid (o_{t-L+1}, \dots, o_t)) = \operatorname*{argmax}_a Q_{\theta}(o_{t-L+1}, \dots, o_t, a)$$

where L is the length of history, and o_t is the "frame", a partial observation of the game state at timestep t (also see 5.3.4). Generated experience is stored in an experience replay buffer implemented as a FIFO queue. For each training step, a batch of uniformly sampled experience is drawn from the experience replay, and the loss is computed using

$$\mathcal{L}(\theta) \propto \mathbb{E}_{\pi} \left[r + \gamma \max_{a'} Q_{\theta'}(s', a') - Q_{\theta}(s, a) \right]$$

The network parameters θ' are updated less frequently than θ .

3.8.3 Double Q Learning

Hasselt analyzed the overestimation problem of Q values in Q-learning and developed **double Q learning**, where a double Q update replaces the traditional Q update [20]. Double Q learning reduces the overestimation problem by introducing an additional Q estimator's and updating two estimator using each other

$$Q^{A}(s, a) \leftarrow Q^{A}(s, a) + \alpha \left(r + \gamma Q^{B} \left(s', \operatorname*{argmax}_{a'} Q^{A}(s', a') \right) - Q^{A}(s, a) \right)$$
$$Q^{B}(s, a) \leftarrow Q^{B}(s, a) + \alpha \left(r + \gamma Q^{A} \left(s', \operatorname*{argmax}_{a'} Q^{B}(s', a') \right) - Q^{B}(s, a) \right)$$

where Q^A and Q^B are two different Q estimators updated alternately. Hasselt, Guez, and Silver applied the double Q learning in DQN [21]. Similar to the double Q update above, a double Q update for neural networks is formulated as

$$\mathcal{L}(\theta^{A}) \propto \mathbb{E}_{\pi} \left[r + \gamma Q_{\theta^{B}} \left(s', \operatorname*{argmax}_{a'} Q_{\theta^{A}}(s', a') \right) - Q_{\theta^{A}}(s, a) \right]$$

$$\mathcal{L}(\theta^{B}) \propto \mathbb{E}_{\pi} \left[r + \gamma Q_{\theta^{A}} \left(s', \operatorname*{argmax}_{a'} Q_{\theta^{B}}(s', a') \right) - Q_{\theta^{B}}(s, a) \right]$$

Here Q_{θ^A} and Q_{θ^B} are two sets of parameters of the same neural network architecture. This paragraph looks redundant. Should I trim this into two sentences instead?

3.8.4 Experience Replay

Schaul et al. studied the role of a experience replay in DQN and developed the **prioritized experience replay** method [47]. In the original work of DQN, all samples were drawn from the experience replay uniformly. In prioritized experience replay, however, samples are drawn according to a distribution based on their calculated priority

$$P(i) = \frac{p_i^{\alpha}}{\sum_k p_k^{\alpha}}$$

where P(i) is the probability of the *i*-th sample being drawn, α is a constant, and p_i is the priority of the sample. Schaul et al. developed two approaches to compute priorities of samples. In **proportional sampling**, the priority p of sample i is calculated by

$$p_i = |\delta_i| + \epsilon$$

where δ_i is the temporal-difference error of the sample, and ϵ is a small constant to give all samples a non-zero probability to be drawn. In **rank-based sampling**, the same temporal differences are calculated, but the final priority is computed based on the rank of the error,

$$score(i) = |\delta_i| + \epsilon$$

$$p_i = \frac{1}{rank(score(i))}$$

This formula looks redundant. Should I cut it?

Horgan et al. followed up by implementing a distributed version of prioritized experience replay [25]. Kapturowski et al. investigated the challenges of using experience replays for RNN-based agents and developed **Recurrent Replay Distributed DQN** [27].

3.8.5 Network Architectures

Wang et al. studied an alternative neural network architecture for ALE learning [54]. **Dueling Q-network** retains the input and output specifications of the Q-network used in DQN and structurally represented the learning of the advantage function A(s,a) defined as

$$A(s,a) = Q(s,a) - V(s)$$

The Q-network has three parts: θ , the shared trunk of the network; Λ , the advantage head; and Υ , the value head. The network approximates the value function internally through the shared trunk and the value head, denoted $V_{\theta,\Upsilon}$, and the advantage function,

denoted $A_{\theta,\Lambda}$. The values computed by the two heads are combined to form the Q-value as follows

$$Q_{\theta,\Upsilon,\Lambda}(s,a) = V_{\theta,\Upsilon}(s) + \left(A_{\theta,\Lambda}(s,a) - \frac{1}{|\mathcal{A}|} \sum_{a'} A_{\theta,\Lambda}(s,a')\right)$$

Similar to DQN, the dueling Q-network is trained through fitting to empirical data generated by interacting with the environment. Experiments show that this architecture encourages the network to learn to differentiate between the values of states and the values of state-action pairs, and leads to better performance of the agent.

3.8.6 Scalar Transformation

Pohlen et al. introduced enhancements to achieve more stable training in Atari games [43]. We focus on discussing the **transformed Bellman Operator** since both MuZero and MooZi use it. For different Atari games, reward signals can vary drastically both in density and scale. This leads to high variance in training targets during training of the algorithms, causing algorithms to have difficulty converging. In DQN, rewards are clipped the reward signal to a range of [-1,1] to reduce such variance [38]. However, this clipping discards the scale of rewards and consequently changes the set of optimal policies. The transformed Bellman Operator was developed to address this problem. The Q update of the new operator is as follows

$$Q(s, a) \leftarrow Q(s, a) + \alpha \phi \left(r + \gamma \max_{a' \in \mathcal{A}} \phi^{-1} \left(Q\left(s', a'\right) \right) \right)$$

where ϕ is an invertible transformation that contracts. One example of such a transformation is

$$\phi(x) = \operatorname{sign}(x) \left(\sqrt{|x| + 1} - 1 \right) + \varepsilon x$$

$$\phi^{-1}(x) = \operatorname{sign}(x) \left(\left(\frac{\sqrt{1 + 4\varepsilon(|x| + 1 + \varepsilon)} - 1}{2\varepsilon} \right)^2 - 1 \right)$$

Both MuZero and MooZi use this specific ϕ definition for both value transformations and reward transformations (5.3.6).

3.8.7 MinAtar

MinAtar, developed by Young and Tian, is an open-source project that offers RL environments inspired by ALE [58]. MinAtar offers five environments that pose similar challenges to ALE environments: learning representation from raw pixels, and learning behaviors that associate actions and delayed rewards. MinAtar environments are implemented in pure Python, have simpler environment dynamics, and are visually less rich than ALE environments. This makes MinAtar perfect test environment for university research.

3.8.8 Consistency Loss

One interesting characteristic of Atari-like games is that the environment frames are usually temporally consistent. For example, given the position of the player avatar for the last few frames, it is not difficult for a human to guess the position of the avatar in the next frame. To take advantage of this property, one common approach is to enforce temporal consistency in the loss function. De Vries et al. visualized the latent space of a learned model of MuZero in a 3D space, in which a hidden state is a point in the space [10]. As MuZero applies recurrent inferences to a hidden state, the transitions can be traced as a 1-D path in the 3D space. The consistency loss they developed creates a smoother path in the 3D space and improves performance. Ye et al. developed a project-then-predict structure similar to a Siamese network to enforce consistency [57, 30].

3.9 Deep Reinforcement Learning Systems

Deep reinforcement learning systems involve irregular computation patterns and complicated hardware interactions between CPUs and AI accelerators. Designing such systems efficiently a great challenge. Decisions the designer has to make include but are not limited to (1) Where and how to generate experience? (2) Where and how to store generated experience? (3) Where to store the model and copies of it? (4) Where is the gradient computation carried out? (4) How to orchestrate processes for stable training? Here we briefly review popular deep reinforcement learning system designs that utilize parallelization to achieve faster and more efficient training.

3.9.1 Mnih et al.'s Asynchronous Methods Framework

Mnih et al. developed asynchronous variants for four popular RL algorithms with a parallelization structure uses actor-learner processes [37]. Each actor-learner process holds a local copy of the model, generates experience locally using the model, and accumulates gradients locally. Once in a while, all local gradients are aggregated to update the global model. Delaying and aggregating updates to neural network parameters reduces gradient variance among processes and achieves a more stable learning. Among the asynchronous algorithm variants, **Asynchronous Advantage Actor Critic (A3C)** had the best performance and achieved the state-of-the-art at the time using only half the training time.

3.9.2 The IMPALA Architecture

Espeholt et al. developed **IMPALA**, a scalable distributed deep reinforcement learning agent [13]. IMPALA deploys two types of computation workers: *actor* and *learner*. A actor holds a copy of the neural network parameters and the environment. It performs model inferences locally to interact with its environments and generates experiences. Generated experiences are saved in a local storage and subsequently pushed into the learner's local storage. The learner holds the master copy of the neural

network parameters. Once the learner receives enough experiences from the actors, it samples experiences from its local queue and performs batched forward pass and back-propagation steps using its model. Figure 2 shows two variants of this structure.

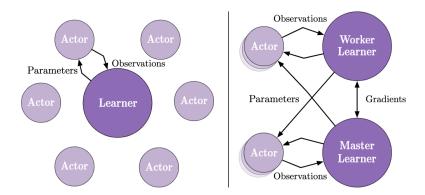


Figure 2: IMPALA Architecture, from [13]. Left: a single learner computes all gradients; Right: multiple worker learners compute gradients and one master learner collects and aggregates gradients.

3.9.3 The SEED Architecture

Espeholt et al. developed the Scalable, Efficient Deep-RL (SEED) architecture to effectively utilize accelerators using a centralized inference server [14]. Similar to IMPALA, SEED also uses two main types of workers: actors and learners. However, in SEED, actors do not hold copies of the model. Instead, SEED actors interact with their environments through querying the learner. The learner not only computes gradients and stores trajectories as in IMPALA, but also has a batching layer that batches actor queries and efficiently performs batched inference with the model. Since actors no longer need to pull neural network parameters from the learner, the IO overhead from serializing and messaging parameters is eliminated. Moreover, since the learner batches queries from all actors, the IO overhead from moving inputs and outputs to accelerators (GPUs or TPUs) is also reduced, increasing the overall inferencing throughput. One downside of the SEED architecture is that actors have to wait for a response from the learner to take an action, and thus have a higher latency for taking a step. Figure 3 illustrates a distributed SEED agent.

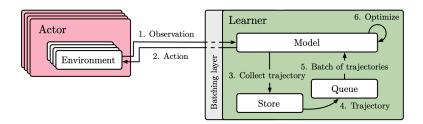


Figure 3: The SEED Architecture, from [14]. All inferences are computed on the learner and actors act through querying the learner.

3.9.4 The Acme Framework

Hoffman et al. developed the **Acme** research framework [24]. Acme similar to IMPALA: processes that interact with the environment are actors, and processes that collect experience and update gradients are learners. Additionally, Acme has a *dataset* component, which is synonymous to the replay buffer used in DQN. This component uses **Reverb**, a high-performance library developed by Cassirer et al. for storing and sampling collected experiences [6]. Figure 4 illustrates a distributed asynchronous agent in Acme.

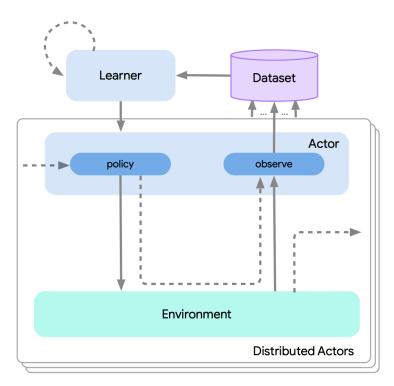


Figure 4: Example of a distributed asynchronous agent with Acme, from [24].

3.9.5 Ray and RLlib

Moritz et al. designed and implemented Ray, a framework for scalable distributed computing [41]. Ray enables both task-level and actor-level parallelization through a unified interface. Ray Core was designed with AI applications in mind and has powerful primitives for building distributed AI systems. For example, Ray uses shared memory to store inputs and outputs of tasks, allowing zero-copy data sharing among tasks. This is useful for DRL systems in which generated experiences are stored and sampled in a separate process. Liang et al. developed RLlib, an industrial-grade deep reinforcement learning library. RLlib is built on top of Ray Core and provides abstractions for a broad range of DRL systems could make use of. Figure 5 illustrates RLlib's abstraction layers. As of the writing of this thesis, RLlib implemented 24 popular DRL algorithms using its abstractions. One major difference between RLlib agents and other DRL agents is that RLlib deploys a hierarchical control over the worker processes. Our project uses Ray Core to implement its worker processes and deploys a hierarchical control paradigm similar to RLlib (see 5).

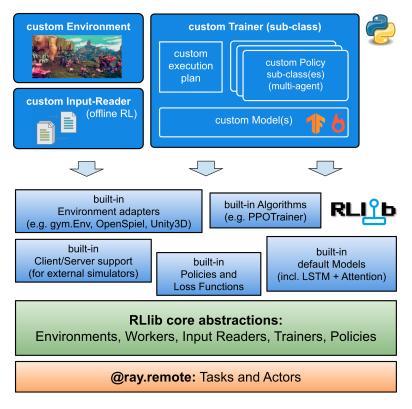
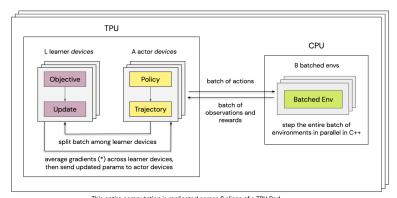


Figure 5: RLlib Abstraction Layers, from [34].

3.9.6 JAX and Podracer Architecture

Frostig, Johnson, and Leary designed JAX, a just-in-time (JIT) compiler that compiles computations expressed in Python code into high-performance accelerators code [15]. JAX is compatible with **Autograd**, so computation procedures expressed and compiled with JAX can be automatically differentiated. JAX also supports control flow, allowing more sophisticated logic to be expressed while taking advantage of accelerators. Our project uses JAX for both neural networks and search. As a result, we are able to compile the entire policy in rollout workers, including history stacking, planning, and neural networks inferencing, into a single optimized program that can be hardware-accelerated (??). Hessel et al. designed two paradigms to efficiently use JAX for DRL systems [23]. In the **Anakin** architecture, the environment is implemented with JAX and the entire agent-environment loop is compiled using JAX and computed with accelerators. Gymnax, developed by Robert Tjarko Lange, provides environment implementations in native JAX, and is compatible with the Anakin architecture [44]. However, pure JAX implemented environments are not always feasible, especially when environments involve external services, such as Stella or Unity in their backend. Alternatively, in the Sebulba architecture, environments run on CPUs, but policies could be compiled and computed on accelerators. Generated experiences in both architectures can be used to compute gradients directly on accelerators. Figure 6 illustrates the Sebulba architecture.



This entire computation is replicated across S slices of a TPU Pod, in which case gradients in (*) are averaged across all learner devices of all slices

Figure 6: Sebulba architecture, from [23]. The environments runs on CPUs. Inferences and gradient computations are compiled, optimized and executed on TPUs.

4 Problem Definition

4.1 Markov Decision Process and Agent-Environment Interface

A RL problem is usually represented as a Markov Decision Process (MDP). MDP is four-tuple (S, A, R, P): S is a set of states that forms the state space A, is a set of actions that forms the action space; $P(s, a, s') = Pr[S_{t+1} = s' \mid S_t = s, A_t = a]$ is the transition probability function; R(s, a, s') is the reward function. We use the agent-environment interface to solve a problem formulated as an MDP. Figure 7 illustrates the agent-environment interface. The MDP is represented as the environment. The decision maker that interacts with the environment is called the agent. At each time step t, the agent starts at state $S_t \in S$, takes an action $A_t \in A$, transitions to state $S_{t+1} \in S$ based on the transition probability function $P(S_{t+1} \mid S_t, A_t)$, and receives a reward $R(S_t, A_t, S_{t+1})$. These interactions yield a sequence of actions, states, and rewards $S_0, A_0, R_1, S_1, A_1, R_2, \ldots$ We call this sequence a trajectory. When a trajectory ends at a terminal state S_T at time t = T, this sequence is completed and we called it an episode.

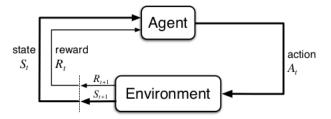


Figure 7: Agent-Environment Interface

my notation is messed up but I will fix them later for sure.

At each state s, then agent takes an action based on its **policy** $\pi(a \mid s)$. This policy represents the conditional probability of the agent taking an action given a state so that $\pi(a \mid s) = Pr[A_t = a \mid S_t = s]$. One way to specify the goal of the agent is to obtain a policy that maximizes the sum of expected reward from any state s

$$E_{\pi} \left[\sum_{k=0}^{T} R_{t+k+1} \mid S_t = s \right]$$
 (5)

where E_{π} denotes the expectation of the agent following policy π . Another way is to also use a discount factor γ so to favor short-term rewards

$$E_{\pi} \left[\sum_{k=0}^{T} \gamma^t R_{t+k+1} \mid S_t = s \right] \tag{6}$$

Notice that (5) is a special case of (6) where $\gamma = 1$.

Maybe I should use one formula here to unify both.

4.2 Our Approach

(5 pages)

5 Method

(20 - 25 pages)

5.1 Design Philosophy

5.1.1 Use of Pure Functions

One of the most notable differences of the MooZi implementation compared to other implementations is the use of pure functions. In MooZi, we separate the storage of data and the handling of data whenever possible, especially for the parts with heavy computations. We use **JAX** and **Haiku** to implement neural network related modules (3.9.6, [18, 26]). These libraries separate the **specification** and the **parameters** of a neural network. The **specification** of a neural network is a pure function that is internally represented by a fixed computation graph. The **parameters** of a neural network includes all learned variables that could be used with the specification to perform a forward pass. For example, say we have a simple neural network with a single dense layer that does the following

$$y = \tanh(Ax + b)$$

where \mathbf{x} is the input vector of shape (n,1), \mathbf{y} is the output vector of shape (m,1), \mathbf{A} is the learned weights of shape (m,n), and b is the learned bias of shape (m,1). We demonstrate how to build this simple network using JAX and Haiku in Algorithm 1. We visualize the computation graph of it in Figure 8.

```
import haiku as hk
import jax
import jax.numpy as jnp
m = 3
n = 2
# specify the computations to be performed
class Model(hk.Module):
  def __call__(self, x):
    A = hk.get_parameter('A', shape=(m, n), init=jnp.zeros)
b = hk.get_parameter('b', shape=(m, 1), init=jnp.zeros)
    return jax.nn.tanh(A @ x + b)
# haiku transforms the object-oriented model into a functional one
model = hk.without_apply_rng(hk.transform(lambda x: Model()(x)))
# construct a concrete input
x = jnp.ones((n, 1))
# initialize the parameters
params = model.init(jax.random.PRNGKey(0), x)
\# perform the forward pass
out = model.apply(params, x)
```

Algorithm 1: A simple dense layer implemented in JAX and Haiku. The model in the code is the specification of the neural network. The params in the code is the parameters of the neural network. Only params contains concrete data.

apply_fn args[0]: model/A f32[3,2] model dot_general f32[3,1] add f32[3,1] output tanh f32[3,1]

Figure 8: Computation graph of the simple dense layer in Algorithm 1. This computation graph show no concrete data, but the data types, shapes, and operators of the layer (f32 stands for *single-precision float*). To complete a forward pass, we need both concrete neural network parameters (\mathbf{A}, \mathbf{b}) and concrete input value (\mathbf{x}) .

Using these pure functions separates the *algorithm* of the agent and the *state* of the agent both conceptually and in implementations. The *algorithm* part of the agent could be abstracted into a computation graph that could be compiled and optimized using a specialized compiler, such as XLA, for hardware acceleration 3.9.6. The *state* part of the agent could be efficiently handled by tools specialized in data manipulations and transferring such as Ray (3.9.5). This way, our system efficiently performs inferences on accelerators and transfers data on CPUs.

5.1.2 Training Efficiency

In section 3.9 we reviewed common DRL systems in which developers gave training efficiency the highest priority in their system designs. We also designed our system so that it's efficient and scalable. Here we describe key features our system has to improve its efficiency. The first one is system parallelization. The computation throughput of a single process is simply not enough for DRL systems. In the published results of MuZero by [48], the agent generated over 20 billion environment frames for training. Let's do a quick back-of-envelope-calculation for what this means for a non parallelized system. Consider Gymnax's efficient MinAtar implementation where each environment step takes about 1 millisecond [44]. With a single process, it would take more than 200 days just to step the environment. As a result, we have to build a distributed system to increase total throughput through parallelism. The second one is the environment transition speed. In Atari games, especially Atari games in ALE (3.8.1), taking one environment step invokes a full-fledged Atari emulator in the backend and is much more time consuming than neural network inferences. Board games, especially those are implemented in performance focus languages, are much faster. We use MinAtar (3.8.7) for simpler variants of Atari games, and OpenSpiel for efficient implementations of board games to reduce the time cost on environment transitions. The third one is neural network inferences used in acting. DRL systems like IMPALA assume that the policy output can be computed by a single forward pass of a neural network. However, MuZero's policy not only requires dozens inferences per action taken, but also requires a planner that prepares inputs for the inferences and initiates inferences. Our system, utilizing JAX and MCTX, handles planning with multiple inferences per action efficiently.

5.1.3 Understanding is Important

Machine learning algorithms, especially those involve neural networks, have interpretability issues and sometimes could only be used as "black boxes" [35]. We believe that having a system that we can understand is much more useful for future research than having a system that "just works". Therefore, our project studies the behavior of the system through extensive logging and visualization utilities.

5.2 Architecture Overview

In MooZi, we use the **Ray** library designed by Moritz et al. for orchestrating distributed processes [41]. We also adopt the terminology used by Ray. In a distributed system with **centralized control**, a single **driver** process is responsible for operating all other processes. Other processes are either **tasks** or **actors**. **Tasks** are stateless functions that take inputs and return outputs. **Actors** are stateful objects that can perform multiple tasks. In the RL literature, **actor** is also a commonly used term for describing the process that holds a copy of the network weights and interacts with an environment [14, 13]. Even though MooZi does not adopt this concept of a RL actor, we will use the

terms **Ray task** and **Ray actor** to avoid confusion. In contrast to distributed systems with **distributed control**, ray tasks and actors are reactive and do not have busy loops. The driver controls when a ray task or actor is activated, what data is used as inputs, and where the outputs goes. The driver orchestrates the data and control flow of the entire system. Ray tasks and actors merely responded to instructions, process input and return output on command. We illustrate MooZi's architecture in Figure (9).

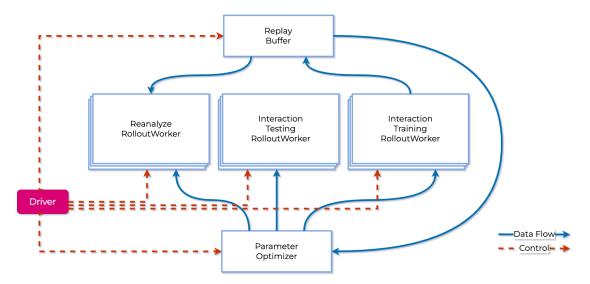


Figure 9: MooZi Architecture. The *driver* is the entrance point of the program and is responsible for setting up configurations, The *parameter server* stores the latest copy of the network weights and performs batched updates to them (5.3.15). The *replay buffer* stores generated trajectories and processes these trajectories into training targets (5.3.14). A *training worker* is a ray actor responsible for generating experiences by interacting with the environment (5.3.11). A *testing rollout worker* is a ray actor responsible for evaluating the system by interacting with the environment (5.3.12). A *reanalyze rollout worker* is a ray actor that updates search statistics for history trajectories (5.3.13).

5.3 Components

5.3.1 Environment Bridges

bridges wrap these environments again to produce a flat dictionary used by MooZi. The final environments share the same signature as follows:

• Inputs

 b_t^{last} : A boolean indicating the episode end.

 a_t : An integer encoding of the action taken.

• Outputs

 o_t : An N-dimensional array representing the observation of the current timestep as an image in the shape (H, W, C_e) . H is the height, W is the width, and C_e is the number of channels.

 b_t^{first} : A boolean indicating the episode start.

 b_t^{last} : A boolean indicating the episode end.

 r_t : A float indicating the reward of taking the given action.

 $m_t^{A^a}$: A bit mask indicating legal action indices. Valid action indices are 1 and invalid actions indices are 0 (see 5.3.3).

All environments are generalized to continuous tasks by passing an addition input b_t^{last} to the environment stepping argument. For an episodic task, the environment is reset internally when b_t^{last} is True. The policy still executes for the last environment step, but the resulting action is discarded. For a continuous task, the environment always step with the latest action and the b_t^{last} input is ignored. Algorithm 2 demonstrates the unified main loop interface.

```
# interact with the environment with a policy indefinitely
def main_loop(env, policy):
    action = 0
    while True:
        result = step(env, action, result.is_last)
        action = policy(result.observation)

def step(env, action, is_last):
    if env.type == "episodic":
        if is_last:
            return env.reset()
        else:
            return env.step(action)
    elif env.type == "continuous":
        return env.step(action)
```

Algorithm 2: Environment Adapter Interface. Both *episodic* environments and *continuous* environments are handled with the same main loop.

We also implement a mock environment using the same interface [39]. A mock environment is initialized with a **trajectory sample** \mathcal{T} , and simulates the

environment by outputting step samples one at a time. An agent can interact with this mock environment as if it were a real environment. However, the actions taken by the agent do not affect state transitions since they are predetermined by the given trajectory from initialization. This mock environment is used by the reanalyze rollout workers in section 5.3.13.

5.3.2 Vectorized Environment

We also implement a vectorized environment supervisor that stack multiple individual environments to form a single vectorized environment. The resulting vectorized environment takes inputs and produces outputs similar to an individual environment but with an additional batch dimension. For example, an individual environment produces a single frame of shape (H, W, C), while the vectorized environment produces a batched frame of shape (B, H, W, C). Previously scalar outputs such as reward are also stacked into vectors of size B. Since environment bridges generalize episodic tasks as continuous tasks, we do not need special handling for the first and the last timesteps in the vectorized environment and its main loop looks exactly like that in Algorithm 2. Using vectorized environments increases the communication bandwidth between the environment and agent and facilitates designing an vectorized agent that processes batched inputs and returns batched actions in one call.

The mock environment described in section 5.3.1 is less trivial to vectorize. Each mock environment has to be initialized with a trajectory sample. To vectorize B mock environments, at least B trajectories have to be tracked at the same time. These B trajectories usually have different length and therefore terminate at different timesteps. Once one of the mocked trajectories reaches its termination, another trajectory has to fill the slot. We create a trajectory buffer to address this problem. When a new trajectory is needed by one of the mocked environments, the buffer replenish it, so the vectorized mocked environment can process batched interactions like a regular vectorized environment until the trajectory buffer runs out of trajectories. An external process has to refill the buffer once in a while. The driver pulls the latest trajectories from the replay buffer and supplies the mock environment's trajectory buffer

reference training

.

5.3.3 Action Space Augmentation

We augment the action space by adding a dummy action a^{dummy} indexed at 0. This dummy action is used to construct history observations when the horizon extends beyond the current timestep. For example, if the history horizon is 3, we need the last three frames and actions to construct the input observation to the policy. However, if the current timestep is 0, the agent hasn't taken any actions yet. We use zeroed frames with the same shape as history frames, and the augmented dummy action as history actions. Moreover, MooZi's planner (5.3.5) does not have access to a perfect model, and

it does not know when a node represents a terminal state. Node expansions do not stop at terminal states and the tree search could simulate multiple steps beyond the end. Search performed in these invalid subtrees not only wastes precious search budget, but also back-propagates value and reward estimates that are not learned from generated experience. We address this issue by letting the model learn a policy that always takes the dummy action beyond a terminal state. This learned dummy action acts as a switch that, once taken, treats all nodes in its subtree as absorbing states and edges that have zero values and rewards respectively. This discourages the planner to search in invalid regions and improves search performance for near-end game states. To formally differentiate these two types of action spaces, we denote the original environment action space \mathcal{A}^e and the augmented action space \mathcal{A}^a , and

$$\mathcal{A}^a = \mathcal{A}^e \cup a^{\text{dummy}}$$
 $a_i = a^{\text{dummy}} \quad \forall i < 0$ (before the first timestep)
 $a_i = a^{\text{dummy}} \quad \forall i \geq T$ (after the last timestep)

Notice that the environment terminates at timestep T so the last effective action taken by the agent is a_{T-1} .

5.3.4 History Stacking

In fully observable environments, the state s_t at timestep t observed by the agent entails sufficient information about the future state distribution. However, for partially observable environments, this does not hold. The optimal policy might not be representable by a policy $\pi(a \mid o_t)$ that only takes into account the most recent partial observation o_t . Most Atari games are such partially observable environments. In DQN, Mnih et al. alleviated this problem by augmenting the inputs of the policy network from a single frame observation to a stacked history of four frames so that the policy network had a signature of $\pi(a \mid o_{t-3}, o_{t-2}, o_{t-1}, o_t)$ (3.8.2, [38]). AlphaZero and MuZero use not only a stacked history of environment frames, but also a history of past actions. MooZi uses the last L environment frames and taken actions, so the signature of the learned model through the policy head of the prediction function is $\mathbf{p} = f(a \mid o_{t-L+1}, \dots, o_t, a_{t-L}, \dots, a_{t-1})$. The greater L is, the better the stacked observation represents a full state. In a deterministic environment with a fixed starting state, the stacked history represents a full environment state when $L=\infty$. On the other hand, L=1 is sufficient for fully-observable perfect information environments.

The exact process of creating the model input by stacking history frames and actions is as follows:

- 1. Prepare L saved environment frames of shape (L, H, W, C_e) .
- 2. Stack the L dimension with the environment channels dimension C_e , resulting in shape $(H, W, L * C_e)$

- 3. Prepare saved L past actions of shape (L), encoded as integers.
- 4. One-hot encode the actions as shape $(L, |\mathcal{A}^a|)$.
- 5. Normalize the action planes by the number of actions $|\mathcal{A}^a|$, shape remains the same.
- 6. Stack the L axis with the action axis, now shape $(L * |\mathcal{A}^a|)$.
- 7. Tile action planes $(L*|\mathcal{A}^a|)$ along the H and W dimensions, now shape $(H, W, L*|\mathcal{A}^a|)$
- 8. Stack the environment planes and actions planes, now shape $(H, W, L*(C_e + |\mathcal{A}^a|))$
- 9. The history is now represented as an image with height of H, width of W, and $L*(C_e+|\mathcal{A}^a|)$ channels

To process batched inputs from vectorized environments described in 5.3.2, all operations above are performed with an additional batch dimension B, yielding the final output with the shape $(B, H, W, L * (C_e + |\mathcal{A}^a|))$. We denote the channels of the final stacked history as $C_h = L * (C_e + |\mathcal{A}^a|)$, where the subscript h means the channel dimension for the representation function h.

Figure 10 illustrates this process with an example.

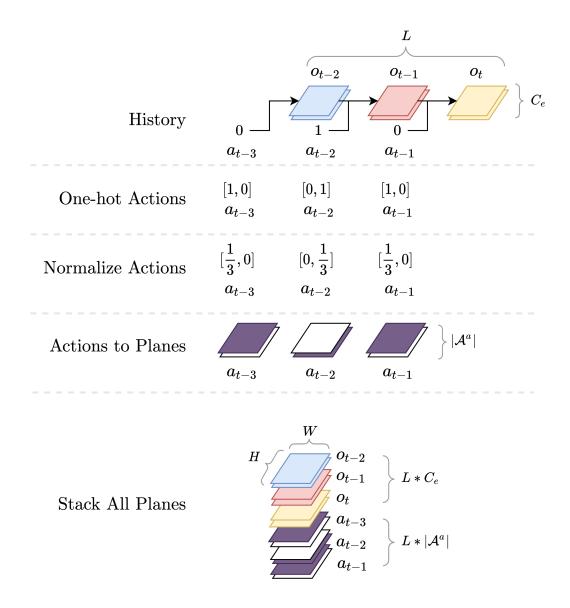


Figure 10: An example of history stacking. History: Partial observations and actions from the last 3 timesteps (L=3). Actions are integers and observations are images with 2 channels each. One-hot Actions: One-hot encodes L history actions into vectors. Normalize Actions: Diviv Actions to Planes: One-hot encodes actions into feature planes that has the same resolution (i.e., same width and height) as the observations, $|\mathcal{A}^a| = 2$. Stack Planes: Stack all planes together, creating an image with 12 channels and the same resolution as the observations.

5.3.5 Planner

The planner is the component that decides what actions to take based on the latest observations. We use the MuZero variant of MCTS described in 3.3 and 3.7 with the help from \mathbf{MCTX} by Danihelka et al. [9]. The planner \mathcal{P} takes a stacked history as its input (5.3.4), performs a search, collects search statistics, and outputs a action and search statistics

$$a_t, v_t^*, \mathbf{p}_t^* = \mathcal{P}(o_{t-L+1}, \dots, o_t, a_{t-L}, \dots, a_{t-1})$$
.

Here v_t^* is the search-updated value estimate of the root, \mathbf{p}_t^* is the search-updated action visits at the root, and a_t is action to take.

5.3.6 MooZi Neural Network

neural network specifical should go into experiment section

We used JAX, and Haiku to build the neural network [18, 15, 26]. We consulted other open-source projects that use neural networks to play games [12, 57, 55]. We implemented the neural-network model with two different architectures in our project, one is multilayer-perceptron-based and the other one is residual-blocks-based [22]. We primarily used residual-blocks-based model for experiments so we will describe the architecture in full details here.

Similar to MuZero described in section 3.7, the model had the representation function, the dynamics function, and the dynamics function. Additionally, we also trained the MooZi model with a self-consistency loss similar to that described by Ye et al. and de Vries et al. [57, 10]. We used an additional function, named as the **projection function** for this purpose. The learned model was used for two purposes during tree searches. The first one was to construct the root nodes using the representation function and the prediction function. We call this process the **initial inference**. The second one was to create edges and child nodes for a given node and action using the dynamics function and the prediction function. We call this process the **recurrent inference**.

This terminology is aligned with MuZero's pseudo-code and MCTX's real code

We implemented residual blocks using the same specification as He et al. [22]. One residual block was defined as follows:

- \bullet input x
- save a copy of x to x'
- apply a 2-D padded convolution on x, with kernel size 3 by 3, same channels
- apply batch normalization on x
- apply relu activation on x

- apply a 2-D padded convolution on x, with kernel size 3 by 3, same channels
- \bullet apply batch normalization on x
- add x' to x
- \bullet apply relu activation on x

The representation function h is parametrized as follows:

- input x of shape (H, W, C_h)
- apply a 2-D padded convolution on x, with kernel size 3 by 3, 32 channels
- \bullet apply batch normalization on x
- \bullet apply relu activation on x
- \bullet apply 6 residual blocks with 32 channels on x
- apply a 2-D padded convolution on x, with kernel size 3 by 3, 32 channels
- \bullet apply batch normalization on x
- \bullet apply relu activation on x
- output the hidden state head x_s

The prediction function f is parametrized as follows:

- \bullet input x
- apply a 2-D padded convolution on x, with kernel size 3 by 3, 32 channels
- \bullet apply batch normalization on x
- \bullet apply relu activation on x
- \bullet apply 1 residual block with 32 channels on x
- flatten x
- apply 1 dense layer with output size of 128 to obtain the value head x_v
- apply batch normalization on x_v
- apply relu activation on x_n
- apply 1 dense layer with output size of Z on x_v
- apply 1 dense layer with output size of 128 to obtain the policy head x_p
- apply batch normalization on x_p

- apply relu activation on x_p
- apply 1 dense layer with output size of A^a on x_p
- output the value head x_v and the policy head x_p

The dynamics function g is parametrized as follows:

- input x of shape (H, W, 32), a as an integer
- encode a as action planes of shape (H, W, A) (described in 5.3.4)
- \bullet append a to x
- apply a 2-D padded convolution on x, with kernel size 3 by 3, 32 channels
- \bullet apply batch normalization on x
- \bullet apply relu activation on x
- \bullet apply 1 residual block with 32 channels on x
- apply 1 residual block with 32 channels on x to obtain the hidden state head x_s
- apply a 2-D padded convolution on x_s , with kernel size 3 by 3, 32 channels
- apply batch normalization on x_s
- apply relu activation on x_s
- apply 1 dense layer with output size of 128 on x to obtain the reward head x_r
- apply batch normalization on x_r
- apply relu activation on x_r
- apply 1 dense layer with output size of Z on x_r
- \bullet output the hidden state head x_s and the reward head x_r

For convenience, the output specification is the same for both the initial inference and the recurrent inference. They both produce a tuple of $(\mathbf{x}, v, \hat{r}, \mathbf{p})$, where \mathbf{x} is the hidden state, v is the value prediction, \hat{r} is the reward prediction, and \mathbf{p} is the policy prediction. For the initial inference,

- input features $\psi_t = (o_{t-L+1}, \dots, o_t, a_{t-L}, \dots, a_{t-1})$
- obtain $\mathbf{x}_t^0 = h(\psi_t)$
- obtain v_t^0 , $\mathbf{p}_t^0 = f(\mathbf{x}_t^0)$
- set $\hat{r}_t^0 = 0$

• return $(\mathbf{x}_t^0, v_t^0, \hat{r}_t^0, \mathbf{p}_t^0)$

For the recurrent inference,

- input features \mathbf{x}_t^i, a_t^i
- obtain \mathbf{x}_t^{i+1} , $\hat{r}_t^{i+1} = g(\mathbf{x}_t^i, a_t^i)$
- obtain v_t^{i+1} , $\mathbf{p}_t^{i+1} = f(\mathbf{x}_t^{i+1})$
- return $(\mathbf{x}_t^{i+1}, v_t^{i+1}, \hat{r}_t^{i+1}, \mathbf{p}_t^{i+1})$

Moreover, we applied the invertible transformation ϕ described in section 3.8.6 to both the scalar reward targets and scalar value targets to create categorical representations with the same support size. The support we used for the transformation were integers from the interval [-5, 5], with a total size of 11. Scalars were first transformed using ϕ , then converted to a linear combination of the nearest two integers in the support. For example, for scalar $\phi(x) = 1.3$, the nearest two integers in the support are 1 and 2, and the linear combination is $\phi(x) = 1 * 0.7 + 2 * 0.3$, which means the target of this scalar is 0.7 for the category 1, and 0.3 for the category 2. We denote Φ for this process of applying ϕ then categorizing the resulting value into a support Z. Using the same example that $\phi(x) = 1.3$, assume the support is Z = [-2, -1, 0, 1, 2], |Z| = 5, then $\Phi(x) = [0, 0, 0, 0.7, 0.3]$, and $\Phi(x) \cdot Z = \phi(x) = 1.3$. For training, the value head and the reward head first produced estimations as logits of size |Z|. These logits were aligned with the scalar targets to produce categorization loss as described in the 5.3.8. For acting, the neural network additionally applied the softmax function to the logits to generated a distribution over the support. The linear combination of the distribution and their corresponding integer values were computed and fed through the inverse of the transformation, namely ϕ^{-1} , to produce scalar values. This means from the perspective of the planner (5.3.5), the scalar estimations made by the model were in same shape and scale as those produced by the environment.

5.3.7 Training Targets Generation

At each timestep t, the environment provides a tuple of data as described in section (5.3.1). The agent interacts with the environment by performing a tree search and taking action a_t . The search statistics of the tree search were also saved, including the updated value estimate of the root action \hat{v}_t , and the updated action probability distribution \hat{p}_t . These completes one **step sample** \mathcal{T}_t for timestep t, which is a tuple of $(o_t, a_t, b_t^{\text{first}}, b_t^{\text{last}}, r_t, m_t^{A_a}, \hat{v}_t, \hat{p}_t)$. Once an episode concludes $(b_T^{\text{last}} = 1)$, all recorded step samples are gathered and stacked together. This yields a final trajectory sample \mathcal{T} that has a similar shape to a step sample but with an extra batch dimension with the size of T. For example, o_t is stacked from shape (H, W, C_e) to shape (T, H, W, C_e) . The training workers described in 5.3.11 generate trajectories this way. The reanalyze rollout workers

generate trajectories with the same signature, but through statistics update described in using a vectorized mocked environment (see 5.3.10 and 5.3.2).

Each trajectory sample with T step samples were processed into T training targets. For each training target at timestep i, we create a training target as follows:

- Observations $o_{i-L+1}, \ldots, o_{i+1}$ where H is the history stacking size. The first H observations were used to create policy inputs as described in 5.3.4, and the pair of observation o_i, o_{i+i} were used to compute self-consistency loss described in 5.3.8.
- Actions $a_{i-L}, \ldots, a_{i+K-1}$. Similarly, The first H actions were used for policy input and the pair of actions at (a_{i-1}, a_i) were used for self-consistency loss. The actions a_i, \ldots, a_{i+K-1} were used to unroll the model during the training for K steps.
- Rewards r_{i+1}, \ldots, r_{i+K} as targets of the reward head of the dynamics function.
- Action probabilities $\mathbf{p}_i^*, \dots, \mathbf{p}_{i+K}^*$ from the statistics of K+1 search trees.
- Root values v_i^*, \dots, v_{i+K}^* , similarly, from the statistics of K+1 search trees.
- N-step return G_i^N, \ldots, G_{i+K}^N . Each N-step return was computed based on the formula

$$G_t^N = \sum_{i=0}^{N-1} \gamma^i r_{t+i+1} + \gamma^N v_{t+N}^*$$

• Importance sampling ratio $\rho = 1$. Placeholder value for future override based on replay buffer sampling weights (see 5.3.14).

Training targets were computed with minimum information necessary to be used in the loss function (5.3.8) so that the precomputed training targets take up the least memory.

5.3.8 Loss Computation

Our loss function is similar to that of 3.7, but with additional self-consistency loss, terminal action loss, and value loss coefficient

$$\mathcal{L}_{t}(\theta) = \left[\underbrace{\mathcal{L}^{p}(\mathbf{p}_{t}^{*}, \mathbf{p}_{t}^{0}) + \frac{1}{K} \sum_{k=1}^{K} \mathcal{L}^{p}\left(\mathbf{p}_{t+k}^{*}, \mathbf{p}_{t}^{k}\right)}_{1} + e^{v} \left(\mathcal{L}^{v}(G_{t}^{N}, v_{t}^{*}) + \frac{1}{K} \sum_{k=1}^{K} \mathcal{L}^{v}\left(G_{t+k}^{N}, v_{t+k}^{*}\right) \right)$$

$$\underbrace{2}$$

$$+ \underbrace{\sum_{k=1}^{K} \mathcal{L}^{r}\left(\hat{r}_{t}^{k}, r_{t+k}\right) + e^{s} \mathcal{L}_{t}^{s}(\mathbf{x}_{t}^{1}, \mathbf{x}_{t+1}^{0})}_{4}$$

$$\underbrace{+ e^{L_{2} \|\theta\|^{2}}_{5} \cdot \rho}_{1} \cdot \rho$$

To compute terms used in the loss function, we use the history observations o_{t-L+1}, \ldots, o_t and history actions a_{t-L}, \ldots, a_{t-1} to reconstruct the stacked frames as the input of the initial inference (5.3.4). We apply the initial inference to obtain $\mathbf{p}_t^0, v_t^0, \mathbf{x}_t^0$. We apply K consecutive recurrent inferences using actions a_t, \ldots, a_{t+K-1} to obtain $\mathbf{p}_t^1, \ldots, \mathbf{p}_t^K, v_t^1, \ldots, v_t^K, \mathbf{x}_t^1, \ldots, \mathbf{x}_t^K$. The policy loss 1 is the standard categorization loss using cross-entropy

$$\mathcal{L}^{p}(\mathbf{p}, \mathbf{q}) = -\sum_{p \in \mathbf{p}, q \in \mathbf{q}} p \log q$$

The policy targets $\mathbf{p}_{t+i}^*(i=0,1,\ldots,K)$ are action visits at the root of K+1 searches performed in the game (5.3.7). To compute the value loss 2 and the reward loss 3, we apply the scalar transformation 4 (3.8.6) that converts scalar values to categorizations, and use the same cross-entropy categorization loss

$$\mathcal{L}^{v}(p,q) = \mathcal{L}^{r}(p,q) = -\sum_{p \in \Phi(p), q \in \Phi(q)} p \log q$$

To compute the self-consistency loss (4), we reconstruct the initial inference for the next timestep $o_{t-L+2}, \ldots, o_{t+1}, a_{t-L+1}, \ldots, a_t$, and compute the cosine distance between the

projected one-step hidden state $\varrho(\mathbf{x}_t^1)$ of timestep t and the initial hidden state \mathbf{x}_{t+1}^0 of the next timestep t+1. Formally,

cosine distance
$$(\mathbf{a}, \mathbf{b}) = 1 - \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{a}\| \|\mathbf{b}\|}$$

$$(4) = \mathcal{L}^s(\mathbf{x}_t^1, \mathbf{x}_{t+1}^0) = 1 - \frac{\varrho(\mathbf{x}_t^1) \cdot \mathbf{x}_{t+1}^0}{\|\varrho(\mathbf{x}_t^1)\| \|\mathbf{x}_{t+1}^0\|}$$

Figure 11 illustrates the intuition behind this loss.

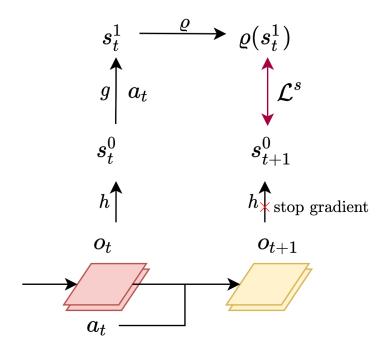


Figure 11: Self-consistency Loss Computation. The hidden state \mathbf{x}_t^1 after projection should be similar to the hidden state \mathbf{x}_{t+1}^0 . We assume the next timestep has more information, so we stop gradient from $\mathbf{x^0}_{t+1}$ to push the representation of the previous timestep towards the next timestep.

5 is a standard L_2 regularization loss to prevent network from overfitting, and coefficient c^{L_2} is used to control the strength of this regularization. The overall loss of a training target is scaled by its importance sampling ratio. We also use the gradient scaling described by Schrittwieser et al. that halves the gradient at the beginning of each dynamics function call [48].

5.3.9 Updating the Parameters

We use a standard **Adam** optimizer developed by Kingma and Ba [28]. We also clip the gradient as described by Pascanu, Mikolov, and Bengio [42]. The dynamics function g in our learned model is essentially an RNN, so we expect this gradient clipping trick to have a similar effect in our model. **Optax**, developed by Matteo Hessel et al., is a library for gradient manipulations implemented in JAX [36]. We use Optax's implementation for both the Adam optimizer and the gradient clipper. Moreover, we also use a target network that was used in DQN to stabilize training [38].

5.3.10 Reanalyze

In 3.7.1, we reviewed **MuZero Reanalyze**. In our project, we also implement a type of worker process that re-runs search on old trajectories with the latest neural network parameters. Given a trajectory sample \mathcal{T} , for each timestep t in the trajectory, the reanalyze process is as follows

- Use observations (o_{t-T+1}, \ldots, o_t) and actions $(a_{t-T}, \ldots, a_{t-1})$ to reconstruct the planner input.
- Feed the planner \mathcal{P} with the reconstructed input, obtaining the update action $\tilde{a_t}$, the updated policy target at the root $\tilde{\mathbf{p}_t^*}$, and the updated value target at the root $\tilde{v_t^*}$.
- Discard the updated action \tilde{a}_t since the action that got executed in the environment has to be the old action a_t to keep the trajectory consistent.
- Replace the old policy target \mathbf{p}_t^* with the updated policy target $\tilde{\mathbf{p}_t^*}$.
- Replace the old value target v_t^* with the updated policy target $\tilde{v_t^*}$.

Once the entire trajectory \mathcal{T} is processed, we obtain an updated trajectory $\tilde{\mathcal{T}}$ in which only the value targets and policy targets are replaced.

5.3.11 Training Worker

The main goal of **training workers** is to generate trajectories by interacting with environments for training purposes. For each worker, a vectorized environment is created as described in 5.3.2, a history stacker is created as described in 5.3.4, and a planner was created using MCTS configurations as described in 5.3.5. Each worker also has a delayed copy of the parameters similar to that in IMPALA (3.9.2 and [13]). Step samples and trajectory samples are collected as the planners giving actions and the vectorized environments taking the actions. Each worker is allocated with one CPU and a fraction of a GPU (usually 10%20% of a GPU) so neural network inferences could be done on GPU. Collected trajectory samples are returned as the final output of one run of the worker. See ?? for the pseudo-code of this process. The planner of these workers are configured to have more exploration to generate more diverse data. The exploration is

encouraged by setting a greater dirichlet_fraction, a greater dirichlet_alpha, and a greater temperature.

move these parameters into planner section

5.3.12 Testing Worker

The main goal of **testing workers** is to generate trajectories by interacting with environments for evaluation. These workers are similar to training workers and they hold the same type of data. The differences are: testing rollout workers only use a single environment, have less GPU allocation, and only ran once every other n training steps, where n is a configurable number (usually 5).

5.3.13 Reanalyze Worker

The main goal of **reanalyze workers** is to update search statistics using the reanalyze process described in 5.3.10, and push updated trajectories to the replay buffer.

5.3.14 Replay Buffer

The **replay buffer** processes trajectories into training targets and samples trajectories or training targets. Since most training targets are expected to be sampled more than once, the replay buffer precomputes the training targets for all received trajectory samples in the replay buffer with the process described in 5.3.7. The replay buffer also computes the value difference δ for each target, which is the difference between the predicted value from the search, and the bootstrapped N-step return (5.3.7)

$$\delta_i = |v_i^* - G_i^N|$$

We implemented three modes of sampling: uniform, proportional, and rank-based. In uniform sampling, every training target has equal probability of being drawn. The proportional sampling and rank-based sampling follows the same formula described by Schaul et al. [47]. However, instead of one-step temporal difference error, we use the δ error we described above. For each training target i, the replay buffer also computes the importance sampling ratio $\rho(i)$ based on the probability P(i) of it being drawn

$$\rho_i = \frac{1}{N \cdot P(i)}$$

Since the probabilities of targets depends on other targets as well, the importance sampling ratio of targets are not static, and have to be recomputed each time a batch is sampled from the replay buffer.

5.3.15 Parameter Server

The parameter server holds the central copy of the neural network parameters and updates the parameters. Once a batch of training targets is received by the parameter server, the loss is computed as described in 5.3.8.

6 System in Action

6.1 The Driver

```
start_training = False
trajectory_samples = []
parameter_server = make_parameter_server()
replay_buffer = make_replay_buffer()
training_worker = [make_train_worker() for i in range(num_train_workers)]
testing_worker = make_test_worker()
reanalyze_workers = [make_reanalyze_worker() for i in range(num_reanalyze_worker)]
for epoch in range(num_epochs):
    if not start_training:
        if start_training_condition_met():
            start_training = True
    # synchronize all workers parameters if conditions are met
    if (epoch % train_worker_update_period) == 0:
        for worker in training_worker:
            worker.set_parameters(parameter_server.get_parameters())
    if (epoch % reanalyze_worker_update_period) == 0:
        for worker in reanalyze_workers:
            worker.set_parameters(parameter_server.get_parameters())
    if (epoch % test_worker_eval_period) == 0:
        testing_worker.set_parameters(parameter_server.get_parameters())
    # process trajectories into training targets
    replay_buffer.process_trajectory_samples(trajectory_samples)
    \hbox{\it\# update parameters by sampling from replay buffer}
    if start_training:
        for i in range(num_updates_per_epoch):
            batch = replay_buffer.sample_batch(batch_size)
            parameter_server.update(batch)
    # generate train targets with training workers
    trajectory_samples.clear()
    for worker in training_worker:
        sample = worker.run()
        trajectory_samples.append(sample)
    # test with testing worker
    if (epoch % test_worker_eval_period) == 0:
        test_result = testing_worker.run()
    # update search statistics with reanalyze workers
    if start_training:
        for worker in reanalyze_workers:
            trajs_to_update = replay_buffer.get_trajectory_samples()
            worker.refill_trajectory(trajs_to_update)
            updated_trajs = worker.run()
            replay_buffer.add_trajs(updated_trajs)
```

Algorithm 3: The driver.

Algorithm 3 is the driver The driver starts by initializing all rollout workers, a parameter server, and a replay buffer. At the beginning of a training step, the driver performs lightweight tasks of all processes such as synchronizing parameters. During the training step, all processes perform their heavyweight tasks. Rollout workers interact with environments, the parameter server computes gradients, and the replay buffer process trajectories into training targets. The method calls made by the driver do not block. They schedule call events and return immediately rather than waiting for the methods to finish. The immediate return values of the calls are *promises* managed by Ray [16]. Actors execute their scheduled method calls sequentially once their concrete inputs are ready.

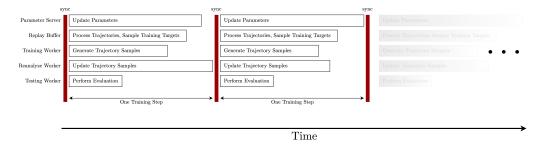


Figure 12: Timeline of training steps. The red bar indicates a synchronization barrier. The duration of each training step is decided by the last finished task.

7 Logging and Visualization

MooZi incorporates extensive logging and visualization utilities to help users understand its behavior better. All distributed process contains a dedicated log file that records all events within the process. Figure

add figure here

shows an example of the log files. MooZi uses **TensorBoard** to log informative scalars and vectors, including average returns, distribution of importance sampling ratios, replay buffer saturation status, gradient sizes, and much more [1]. Figure

add figure here

shows a screenshot of the TensorBoard. MooZi also provides utilities to visualize the behavior of the algorithm. Testing workers use the GIF maker tool to create animated records of evaluations. Figure

add figure here

shows an example of the GIF tiled as a sprite image.



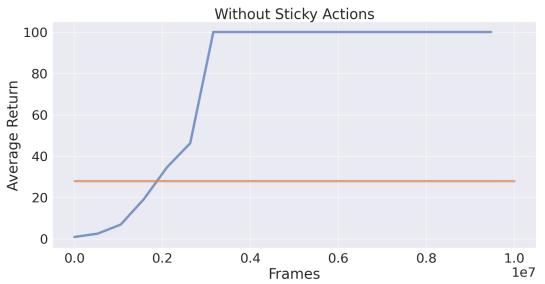


Figure 13: Sticky Actions

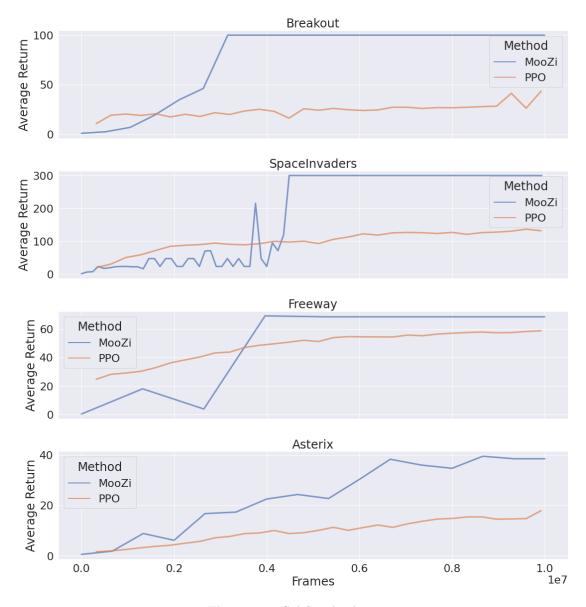


Figure 14: Sticky Actions

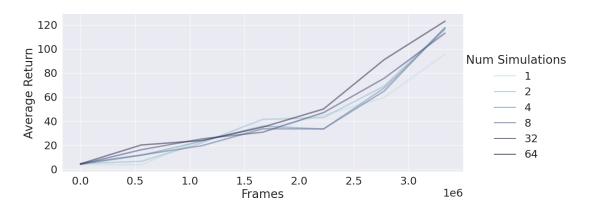


Figure 15: Sticky Actions

8 Things that went wrong

9 Conclusion

(3 pages)

9.1 Future Work

(1 page)

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