

On Monte Carlo Tree Search With Multiple Objectives



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Acknowledgements

TODO: acknowledgements here

Abstract

TODO: abstract here

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List of Abbreviations

CHVI	Convex Hull Value Iteration.
CHVS	Convex Hull Value Set.
CMAB	Contextual Multi-Armed Bandit (problem).
CZ	Contextual Zooming.
EMAB	Exploring Multi-Armed Bandit (problem).
MAB	Multi-Armed Bandit (problem).
MCTS	Monte Carlo Tree Search.
MCTS-1	A specific and common presentation of Monte Carlo Tree Search, presented in Section 2.4.
MDP	Markov Decision Process.
MENTS	Maximum ENtropy Tree Search.
MOMDP	Multi-Objective Markov Decision Process.
THTS	Trial-based Heuristic Tree Search.
THTS++	An extension of THTS used in this thesis.
UCB	Upper Confidence Bound (algorithm).
UCT	Upper Confidence Bound applied to Trees.

List of Notation

General Notation

$\mathbb{1}$	The indicator function, where $\mathbb{1}(A) = 1$ when A is true, and $\mathbb{1}(A) = 0$ when A is false.
\hat{A}	The hat notation is used to denote an estimate, i.e. \hat{A} is an estimate for some optimal value A^*
\bar{A}	The bar notation is used to denote sample averages, i.e. \bar{A} is a sample average of a number of samples A_1, \dots, A_k , or $\bar{A} = \frac{1}{n} \sum_{i=1}^k A_i$.
\tilde{A}	The tilde notation is used to denote a function approximator, such as a neural network.
\mathcal{A}	Calligraphic font is used to denote variables that are sets or tuples (ordered sets).
\mathbf{A}	Bolt font is used to denote vectors, and A_i is used to denote the i th component of the vector \mathbf{A} .
A	Typewriter text is used to refer to variables relating to an algorithm (or the analysis of an algorithm).
\mathcal{A}	The notations above will also be combined at times, so \mathcal{A} is used to denote a set that contains vectors.
\mathbb{E}	The expectation operator. $\mathbb{E}[f]$ denotes the expectation of a distribution f , and $\mathbb{E}_{x \sim f}[g(x)]$ denotes the expected value of $g(x)$ under the distribution f .
$x \sim f$	If $f : X \rightarrow [0, 1]$ specifies a probability distribution, then $x \sim f$ denotes that the variable x is sampled the distribution f .

(Multi-Objective) Markov Decision Processes (Defined in Sections 2.2 and 2.5)

\mathcal{A}	A (finite) set of actions.
a_t	The action at the t th timestep of a trajectory.

D	: The dimension of rewards in a MOMDP.
H	The finite-horizon time bound of an MDP.
\mathcal{M}	A Markov Decision Process, which is a tuple $\mathcal{M} = (\mathcal{S}, s_0, \mathcal{A}, R, p, H)$.
\mathbf{M}	A Multi-Objective Markov Decision Process, which is a tuple $\mathbf{M} = (\mathcal{S}, s_0, \mathcal{A}, \mathbf{R}, p, H)$.
p	The next-state transition distribution of an MDP. $p(s' s, a) : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$.
π	: A policy, mapping a state $s \in \mathcal{S}$ to a probability distribution over actions \mathcal{A} .
R	The reward function of an MDP: $R(s, a) : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$.
\mathbf{R}	The D dimensional reward function of a MOMDP: $\mathbf{R}(s, a) : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}^D$.
r_t	The reward at the t th timestep of a trajectory.
\mathcal{S}	A (finite) set of states.
$\text{Succ}(s, a)$	The set of successor states of a state-action pair (s, a) , with respect to an MDP: $\text{Succ}(s, a) = \{s' \in \mathcal{S} p(s' s, a) > 0\}$.
s_0	$s_0 \in \mathcal{S}$ is the initial starting state of an MDP.
s_t	The state at the t th timestep of a trajectory.
$\text{terminal}(s)$. .	Denotes if a state s is terminal or not. That is, if the transition distribution and reward function of the MDP is such that once reached, the state will never be left and no more reward will be received.
τ	A trajectory, or sequence, of states, actions and rewards that are sampled according to a policy π and an MDP \mathcal{M} : $\tau = (s_0, a_0, r_0, s_1, \dots, s_{H-1}, a_{H-1}, r_{H-1}, s_H)$.
τ	A multi-objective trajectory, of states, actions and rewards that are sampled according to a policy π and an MDP \mathbf{M} : $\tau = (s_0, a_0, \mathbf{r}_0, s_1, \dots, s_{H-1}, a_{H-1}, \mathbf{r}_{H-1}, s_H)$.
$\tau_{i:j}$	A truncated trajectory, starting at timestep i , and ending at timestep j : $\tau_{i:j} = (s_i, a_i, r_i, s_{i+1}, \dots, s_{j-1}, a_{j-1}, r_{j-1}, s_j)$.
$\tau_{i:j}$	A multi-objective truncated trajectory, starting at timestep i and ending at timestep j : $\tau_{i:j} = (s_i, a_i, \mathbf{r}_i, s_{i+1}, \dots, s_{j-1}, a_{j-1}, \mathbf{r}_{j-1}, s_j)$.

Reinforcement Learning (Section 2.3)

$J(\pi)$	The objective function for (standard) reinforcement learning: $J(\pi) = V^\pi(s_0; 0)$.
π^*	The optimal standard policy, that maximises the objective function $J(\pi)$.
Q^*	The optimal Q-value function. $Q^*(s, a; t)$ denotes the maximal expected value that can be achieved by any policy, starting from state $s_t = s$, with action $a_t = a$.
Q^π	The Q-value function of a policy π . $Q^\pi(s, a; t)$ denotes the expected cumulative reward that policy π will obtain, starting from state $s_t = s$, starting by taking action $a_t = a$.
V^*	The optimal value function. $V^*(s; t)$ denotes the maximal expected value that can be achieved by any policy, starting from state $s_t = s$.
V^π	The value of a policy π . $V^\pi(s; t)$ denotes the expected cumulative reward that policy π will obtain, starting from state $s_t = s$.

Maximum Entropy Reinforcement Learning (Section 2.3.1)

α	The temperature parameter, or, the coefficient of the entropy term in the maximum entropy (soft) objective.
\mathcal{H}	The Shannon entropy, of a probability distribution or policy.
$J_{\text{sft}}(\pi)$	The objective function for maximum entropy (soft) reinforcement learning: $J_{\text{sft}}(\pi) = V_{\text{sft}}^\pi(s_0; 0)$.
π_{sft}^*	The optimal soft policy, that maximises the soft objective function $J_{\text{sft}}(\pi)$.
Q_{sft}^*	The optimal soft Q-value function. $Q^*(s, a; t)$ denotes the maximal expected soft value that can be achieved by any policy, from state $s_t = s$ and taking action $a_t = a$.
Q_{sft}^π	The soft Q-value function of a policy π . $Q_{\text{sft}}^\pi(s, a; t)$ is the expected value of the policy from $s_t = s$, starting with action $a_t = a$, with an addition of the entropy of the policy weighted by the temperature α .
V_{sft}^*	The optimal soft value function. $V^*(s; t)$ denotes the maximal expected soft value that can be achieved by any policy, from state $s_t = s$.

V_{sft}^π The soft value of a policy π . $V_{\text{sft}}^\pi(s; t)$ is the expected value of the policy from $s_t = s$, with an addition of the entropy of the policy weighted by the temperature α .

Multi-Objective Reinforcement Learning (Section 2.5)

$CCS(\Pi)$ A convex coverage set of policies, which contains at least one policy that maximises the linear utility $u_{\text{lin}}(\cdot; \mathbf{w})$ for each weight vector \mathbf{w} .

$CCS_{\min}(\Pi)$ The minimal convex coverage set of policies, which has no redundant policies and for each policy in $CCS_{\min}(\Pi)$ there is some weight that it uniquely (with respect to $CCS_{\min}(\Pi)$) obtains the optimal linear utility.

$CH(\Pi)$ The undominated set of policies in Π (the set of all possible policies), with respect to the linear utility function u_{lin} . $CH(\Pi) = U(\Pi; u_{\text{lin}})$.

$CS(\Pi; u)$ A coverage set of policies, which contains at least one policy that maximises the utility $u(\cdot; \mathbf{w})$ for each weight vector \mathbf{w} .

cvx_prune An operation that takes an arbitrary set of vectors, and returns the subset that lie at the vertices of the geometric (partial) convex hull.

Δ^D The D dimensional simplex, or, the set of possible weightings over the D objectives of a MOMDP. $\Delta^D = \{\mathbf{w} \in \mathbb{R}^D | w_i > 0, \sum_i w_i = 1\}$.

Π The set of all possible policies in a MOMDP.

\mathbf{Q}^π The multi-objective Q-value function of a policy π . $Q^\pi(s, a; t)$ denotes the expected cumulative vector reward that policy π will obtain, starting from state $s_t = s$, starting by taking action $a_t = a$.

$U(\Pi; u)$ The undominated set of policies in Π (the set of all possible policies), with respect to the utility function u . Each policy in $U(\Pi; u)$ achieves a maximal utility for some weighting over the objectives.

u A utility function, mapping multi-objective values to scalar values, that depends on a weighting over objectives. The multi-objective value $\mathbf{V}^\pi(s, a; t)$ is mapped to $u(\mathbf{V}^\pi(s, a; t); \mathbf{w})$, where \mathbf{w} is a weighting over the objectives.

u_{lin}	The linear utility function: $u_{\text{lin}}(\mathbf{v}; \mathbf{w}) = \mathbf{w}^\top \mathbf{v}$.
\mathbf{V}^π	The multi-objective value of a policy π . $V^\pi(s; t)$ denotes the expected cumulative reward that policy π will obtain, starting from state $s_t = s$.
$\mathbf{Vals}(\Pi')$	The set of multi-objective values obtained by a set of policies Π' .
\mathbf{w}	A weighting over objectives that quantifies preferences over the multiple objectives, to be used in a utility function.

Trial Based Heuristic Tree Search (Section 2.4)

<code>backup_v</code>	Updates the values at a decision node in the backup phase of a trial THTS++ , using the decision node's children, the trajectory sampled for the trial and the heuristic value function.
<code>backup_q</code>	Updates the values at a chance node in the backup phase of a trial THTS++ , using the chance node's children, the trajectory sampled for the trial and the heuristic value function.
$H_{\text{THTS++}}$	The planning horizon used in THTS++ , with $H_{\text{THTS++}} \leq H$.
<code>mcts_mode</code> . . .	Specifies if THTS++ will sample a trajectory such that only one decision node is added to the search tree per trial. If not running in <code>mcts_mode</code> the THTS++ will sample a trajectory until the planning horizon $H_{\text{THTS++}}$.
$N(s)$	The number of visits at the decision node corresponding to state s .
$N(s, a)$	The number of visits at the chance node corresponding to state-action pair (s, a) .
<code>node(s)</code>	The decision node corresponding to the state s .
<code>node(s).chldrn</code>	The set of chance nodes that are children of <code>node(s)</code> .
<code>node(s).V</code> . . .	The set of variables stored at decision node <code>node(s)</code> , typically used for estimating values.
<code>node(s, a)</code> . . .	The chance node corresponding to the state-action pair (s, a) .
<code>node(s, a).chldrn</code>	The set of decision nodes that are children of <code>node(s, a)</code> .
<code>node(s, a).Q</code> . .	The set of variables stored at decision node <code>node(s, a)</code> , typically used for estimating Q-values.
π_{search}	The search policy used in THTS++ to sample a trajectory in the selection phase.

\hat{Q}_{init}	The heuristic action function used in THTS++, used to provide a Q-value estimate for any state-action pairs that aren't in the search tree.
<code>sample_context</code>	A function used in THTS++ that creates a context, or key-value story, and samples any initial values to be stored in the context.
<code>sample_outcome</code>	A function used in THTS++ to sample outcomes (successor states) from the environment (MDP).
\mathcal{T}	The THTS++ search tree. $\mathcal{T} \subseteq \mathcal{S} \cup \mathcal{S} \times \mathcal{A}$.
\hat{V}_{init}	The heuristic value function used in THTS++, used to initialise the value of a new decision node.

TODO: add MENTS, UCT, BTS, DENTS, and all of ch4 stuff

1

Introduction

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TODO: chapter structure (i.e. in the introduction section I give some background in the field(s), cover the main contributions of this thesis, etc, etc).

1.1 Overview

TODO: list

- Give some context around MCTS (and talk about exploration and exploitation), and why we might use it
 - Larger scale than tabular methods
 - Can do probability and theory stuff (and some explainability, by looking at stats in the tree the agent used)
 - Can use tree search with neural networks to get some of the above (and use for neural network training as in alpha zero)

- Argument from DENTS paper for exploration $>$ exploitation (in context of planning in a simulator)
- Give high level overview of Multi-Objective RL, and why it can be useful
- Give an idea of how my work fits into MCTS and MORL as a whole
- Discuss research questions/issues with current literature (i.e. introduce some of the ideas from contributions section below)

1.2 Contributions

TODO: Inline acronyms used, or make sure that they're defined before hand

Throughout this thesis, we will consider the following questions related to Monte Carlo Tree Search and Multi-Objective Reinforcement Learning:

Q1 - Exploration: When planning in a simulator with limited time, how can MCTS algorithms best explore to make good decisions?

Q1.1 - Entropy: Entropy is often used as an exploration objective in RL, but can it be used soundly in MCTS?

Q1.2 - Multi-Objective Exploration: How can Multi-Objective MCTS methods explore to find optimal actions for different objectives?

Q2 - Scalability: How can the scalability of (multi-objective) MCTS methods be improved?

Q2.1 - Complexity: MCTS algorithms typically run in $O(nAH)$, but are there algorithms that can improve upon this?

Q2.2 - Multi-Objective Scalability: With respect to the size of environments, how scalable are Multi-Objective MCTS methods?

Q2.3 - Curse of Dimensionality: With respect to the number of objectives, to what extent do Multi-Objective MCTS methods suffer from the curse of dimensionality?

Q3 - Evaluation: How can we best evaluate a search tree produced by a Monte Carlo Tree Search algorithm?

Q3.1 - Tree Policies: Does it suffice to extract a policy from a single search tree for evaluation? **TODO:** going to have to run some extra experiments for that, but I probably should do that for completeness anyway

Q3.2 - Multi-Objective Evaluation: Can we apply methods from the MORL literature to theoretically and empirically evaluate Multi-Objective MCTS?

TODO: some words about how below is the contributions we're making in this thesis and expand these bullets a bit more

- Max Entropy can be misaligned with reward maximisation (**Q1.1 - Entropy**)
- Boltzmann Search Policies - BTS and DENTS (**Q1.1 - Entropy**, and with extra results **Q3.1 - Tree Policies**)
- Use the alias method to make faster algorithms (**Q2.1 - Complexity**)
- Simple regret (**Q1 - Exploration**)
- Use of contexts in THTS to make consistent decisions in each trial (**Q1.2 - Multi-Objective Exploration**)
- Contextual regret introduced in CHMCTS (**Q2.2 - Multi-Objective Scalability**, **Q3.2 - Multi-Objective Evaluation**)
- Contextual Zooming and CHMCTS (designed for **Q1.2 - Multi-Objective Exploration**, runtimes cover **Q2.3 - Curse of Dimensionality**, results **Q3.2 - Multi-Objective Evaluation**)
- Simplex maps (**Q1.2 - Multi-Objective Exploration**, **Q2.2 - Multi-Objective Scalability**, **Q2.3 - Curse of Dimensionality**)
- Contextual Simple Regret (**Q3.2 - Multi-Objective Evaluation**)

TODO: Would like to do the comparing different types of eval, even if not listing it as a research question (compare giving it X seconds per decision and evaluating that policy (SLOW), and comparing policy extracted from the tree)

TODO: can make an argument that the best bound achieved by theory is given by letting temperature go to max. Which is consistent with the exploring bandits results

1.3 Structure of Thesis

TODO: a paragraph with a couple lines to a paragraph about each chapter. This is the high level overview/intro to the thesis paragraph. I.e. this section is “this is the story of my thesis in a page or two”

1.4 Publications

TODO: update final publication when submit

The work covered in this thesis also appears in the following publications:

- Painter, M; Lacerda, B; and Hawes, N. “Convex Hull Monte-Carlo Tree-Search.” In *Proceedings of the international conference on automated planning and scheduling. Vol. 30. 2020*, ICAPS, 2020.
- Painter, M; Baïoumy, M; Hawes, N; and Lacerda, B. “Monte Carlo Tree Search With Boltzmann Exploration.” In *Advances in Neural Information Processing Systems, 36, 2023*, NeurIPS, 2023.
- Painter, M; Hawes, N; and Lacerda, B. “Simplex Maps for Multi-Objective Monte Carlo Tree Search.” In *TODO, Under Review at conf_name*.

2

Background

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This chapter introduces the fundamental concepts that will be used throughout this thesis, in particular the **THTS++** schema is introduced in Section 2.4.2, in which monte carlo tree search algorithms will be defined. Section 2.1 begins with multi-armed bandit problems and decision theory, which provides a fundamental building block used in monte carlo tree search methods (Section 2.4). Sections 2.2 and 2.3 provide a framework for sequential decision making under uncertainty.

Section 2.4 introduces monte carlo tree search methods that can be used for solving problems in sequential decision making under uncertainty. Section 2.5 extends the frameworks to include multiple objectives. And Section 2.6 discusses sampling from categorical distributions efficiently.

2.1 Multi-Armed Bandits

This section introduces the K -armed bandit problem [22], which is a foundational problem considered in decision theory. In the multi-armed bandit (MAB) problem, an agent is tasked with deciding to pull one of K arms, and the decision typically needs to be made multiple times. For example, the MAB problem could be used in the context of clinical trials, where each “arm” corresponds to a treatment option. As such, the MAB problem is presented in rounds, where an arm is selected each round. In each round a random outcome is observed in form of a reward.

The distribution of rewards is unknown ahead of time, and so an agent needs to explore to gather information about what rewards can be obtained by pulling each arm, and if an agent does not explore then it may miss out on discovering the best strategy. Conversely, the agent should want to exploit, using the information that it has obtained, so that it gather high rewards. In the clinical trials example, exploitation is desirable so that patients receive the best treatment. The problem of balancing these two aspects is known as the *exploration-exploitation trade off*.

The remainder of this section will formalise the MAB problem, and give details of the widely used Upper Confidence Bound (UCB) algorithm [2]. Sections 2.1.1 and 2.1.2 considers two variations on the MAB problem that will be relevant in this thesis.

Figure 2.1 shows how the operation of a K -armed bandit problem proceeds. Formally, let $f(1), \dots, f(K)$ be the probability distributions for the rewards of each of the K arms, with expected values of $\mu(1), \dots, \mu(K)$ respectively. On the m th round, if the arm $x^m \in \{1, \dots, K\}$ is pulled, then a reward $y^m \sim f(x^m)$ is received. To specify a *strategy* σ , on each round m , a probability distribution σ^m is over $\{1, \dots, K\}$ is given, which is sampled to decide which arm to pull, i.e. $x^m \sim \sigma^m$.

Parameters: K probability distributions for the rewards of each arm $f(1), \dots, f(K)$.

- For each round $m = 1, 2, \dots$:
 - the agent selects an arm $x^m \sim \sigma^m$ to pull;
 - the agent receives a reward $y^m \sim f(x^m)$ from the environment;
 - if the environment sends a stop signal, then the game ends, otherwise the next round starts.

Figure 2.1: The procedure of a multi-armed bandit problem, following a strategy σ .

To assess algorithmic strategies for MAB problems, a quantity known as *regret* is commonly used, which compares the cumulative reward obtained, compared to the maximal expected reward that could be obtained with full knowledge of $\{f(i)\}$.

Definition 2.1.1. *The (cumulative) regret of strategy σ after n rounds in the MAB process is:*

$$\text{cum_regr}_{\text{MAB}}(n, \sigma) = n\mu^* - \sum_{m=1}^n y^m, \quad (2.1)$$

where $\mu^* = \max_i \mu(i)$.

To theoretically analyse algorithms for MAB problems, the quantity of expected regret, $\mathbb{E}[\text{cum_regr}_{\text{MAB}}(n, \sigma)]$ is considered. Lai and Robbins [18] show using information theory that there is a lower bound on the expected regret that an agent can achieve of $\Omega(\log n)$. And Auer [2] introduces the Upper Confidence Bound (UCB) algorithm, which achieves a matching upper bound of $O(\log n)$ on the expected regret.

To define the UCB strategy for pulling the arms, a few quantities need to be defined first. Let $N^m(x)$ be the number of times that arm x has been pulled after m rounds. And let $\bar{y}^m(x)$ be the average reward that has been received as a result of pulling arm x after m rounds. Mathematically:

$$N^m(x) = \sum_{i=1}^m \mathbb{1}[x^i = x], \quad (2.2)$$

$$\bar{y}^m(x) = \frac{1}{N^m(x)} \sum_{i=1}^m y^i \mathbb{1}[x^i = x]. \quad (2.3)$$

The strategy followed by the UCB algorithm on the m th round is given by:

$$x_{\text{UCB}}^m = \arg \max_{i \in \{1, \dots, K\}} \bar{y}^{m-1}(i) + b_{\text{UCB}} \sqrt{\frac{\log(m)}{N^{m-1}(i)}}, \quad (2.4)$$

$$\sigma_{\text{UCB}}^m(x) = \mathbb{1}[x = x_{\text{UCB}}^m], \quad (2.5)$$

where b_{UCB} is a bias parameter used to control how much the strategy explores. Additionally, each arm is pulled once in the first K rounds by the UCB strategy, to avoid division by zero in Equation 2.4. Alternatively, the division by zero can be considered to give a value of ∞ , to give the same effect.

2.1.1 Exploring Bandits

In the pure exploration problem for K -armed bandits [7], the format of each round is changed slightly. The agent still gets to pull an arm each round (according to the *exploration strategy* σ), but after it receives a reward on each round it is given the opportunity to output a *recommendation strategy* ψ . On the m th round, the recommendation strategy takes the form of ψ^m , a probability distribution over the K arms. In exploring multi-armed bandit (EMAB) problems, the emphasis is now on the algorithm being able to provide the best recommendations possible, rather than trying to exploit pulling the best arm each round. In essence, this separates the needs to explore and exploit, the agent needs to explore with its arm pulls, and output an exploiting recommendation at the end of each round. Figure 2.2 gives an overview of the EMAB problem.

The (*expected*) *instantaneous regret* for pulling an arm $x \in \{1, \dots, K\}$ is given by:

$$\text{inst_regr}(x) = \mu^* - \mu(x), \quad (2.6)$$

where again $\mu^* = \max_i \mu(i)$.

Under the exploring regime of EMABs, the performance of an algorithm can be analysed by considering the quantity of *simple regret* of the recommendation policy. The simple regret is the expected value of the instantaneous regret which would come from following the recommendation policy.

Parameters: K probability distributions for the rewards of each arm $f(1), \dots, f(K)$.

- For each round $m = 1, 2, \dots$:
 - the agent selects an arm $x^m \sim \sigma^m$ to pull;
 - the agent receives a reward $y^m \sim f(x^m)$ from the environment;
 - the agent outputs a recommendation distribution ψ^m , over the arms $\{1, \dots, K\}$;
 - if the environment sends a stop signal, then the game ends, otherwise the next round starts.

Figure 2.2: The procedure of an exploring multi-armed bandit problem, following an exploration strategy σ , and recommendation strategy ψ .

Definition 2.1.2. *The simple regret of following the exploration strategy σ and recommending a distribution ψ^m on the m th round is:*

$$\text{sim_regr}_{\text{EMAB}}(m, \sigma, \psi^m) = \mathbb{E}_{i \sim \psi^m}[\mu^* - \mu(i)]. \quad (2.7)$$

Bubeck et al. [7] analyse a range of exploration and recommendation strategies in their work. Two of the recommendation strategies considered are the *empirical best arm* (EBA) and *most played arm* (MPA):

$$x_{\text{EBA}}^m = \arg \max_{i \in \{1, \dots, K\}} \bar{y}^m(i), \quad (2.8)$$

$$\psi_{\text{EBA}}^m(x) = \mathbb{1}[x = x_{\text{EBA}}^m], \quad (2.9)$$

$$x_{\text{MPA}}^m = \arg \max_{i \in \{1, \dots, K\}} N^m(i), \quad (2.10)$$

$$\psi_{\text{MPA}}^m(x) = \mathbb{1}[x = x_{\text{MPA}}^m]. \quad (2.11)$$

In addition to the UCB strategy, a *uniform exploration strategy* is considered:

$$x_{\text{uniform}}^m = (m \bmod K) + 1, \quad (2.12)$$

$$\sigma_{\text{uniform}}^m(x) = \mathbb{1}[x = x_{\text{uniform}}^m]. \quad (2.13)$$

It is shown that exploring with UCB leads to a polynomial simple regret bound for both recommendation strategies: $\text{sim_regr}_{\text{EMAB}}(m, \sigma_{\text{UCB}}, \psi_{\text{EBA}}^m) = O(m^{-k_{\text{UCB}, \text{EBA}}})$

Parameters: the set of arms \mathcal{X} , the set of contexts \mathcal{W} and a mapping from $\mathcal{W} \times \mathcal{X}$ to probability distributions: $f(w, x)$.

- For each round $m = 1, 2, \dots$:
 - the agent receives a context $w^m \in \mathcal{W}$ from the environment;
 - the agent selects an arm $x^m \sim \sigma^m(w^m)$ to pull;
 - the agent receives a reward $y^m \sim f(w^m, x^m)$ from the environment;
 - if the environment sends a stop signal, then the game ends, otherwise the next round starts.

Figure 2.3: The procedure of a contextual multi-armed bandit problem, following a strategy σ .

and $\text{sim_regr}_{\text{EMAB}}(m, \sigma_{\text{UCB}}, \psi_{\text{MPA}}^m) = O(m^{-k_{\text{UCB,MPA}}})$ for some appropriate constants $k_{\text{UCB,EBA}}, k_{\text{UCB,MPA}} > 0$. It is also shown that exploring with the uniform strategy (and recommending the empirical best arm) leads to an exponential simple regret bound, $\text{sim_regr}_{\text{EMAB}}(m, \sigma_{\text{UCB}}, \psi_{\text{EBA}}^m) = O(e^{-k_{\text{uniform}}m})$ for an appropriate constant $k_{\text{uniform}} > 0$.

2.1.2 Contextual Bandits

In the contextual multi-armed bandit (CMAB) problem [15, 28], before an arm is chosen, the agent is provided with a context w . In the CMAB problem the set of arms, now \mathcal{X} , and the set of contexts, \mathcal{W} are compact sets (i.e. the sets are closed and bounded). The distribution of rewards now also depends on the context w and arm pulled x , and is written $f(w, x)$, with mean $\mu(w, x)$. The distribution of arms pulled on the m th round can now depend on the context: $\sigma^m(w)$. Figure 2.3 gives an overview of the CMAB problem.

Given this setup some further assumptions are required for the problem to be more tractable. Slivkins [28] make a fairly general assumption that some metric d over the similarity space $\mathcal{W} \times \mathcal{X}$ is known and is such that the following Lipschitz condition holds:

$$|\mu(x, y) - \mu(x', y')| \leq d((x, y), (x', y')). \quad (2.14)$$

For d to be a metric, the following conditions must hold for some arbitrary $z = (x, y), z' = (x', y'), z'' = (x'', y'')$ with $z \neq z' \neq z''$:

$$d(z, z) = 0, \quad (2.15)$$

$$d(z, z') > 0, \quad (2.16)$$

$$d(z, z') = d(z', z), \quad (2.17)$$

$$d(z, z'') \leq d(z, z') + d(z', z''). \quad (2.18)$$

Similar to MABs and EMABs, the notion of regret is used to analyse CMABs. Specifically, *contextual regret* is defined similarly to cumulative regret [15, 28], while taking into account the contexts drawn.

Definition 2.1.3. *The (cumulative) contextual regret of the strategy σ in the process given in Figure 2.3 is defined as:*

$$\text{ctx_regr}_{\text{CMAB}}(\pi, n) = \sum_{m=1}^n \mu^*(w^m) - y^m, \quad (2.19)$$

where $\mu^*(w) = \sup_i \mu(w, i)$.

Slivkins [28] also introduces the Contextual Zooming (CZ) algorithm. CZ runs over a fixed number of rounds T , and achieves the contextual regret of $O(T^{\frac{1+c}{2+c}} \log(T))$, where c is the (*Lebesgue*) *covering dimension* of the similarity space $\mathcal{W} \times \mathcal{X}$. For the purpose of this thesis the covering dimension (a notion about topological spaces), will always be equal to the typical notion of dimension. That is, if $\mathcal{W} \times \mathcal{X}$ has covering dimension c , then $\mathcal{W} \times \mathcal{X}$ can be mapped to a subspace of \mathbb{R}^c .

Throughout the CZ algorithm, a set of balls in the similarity space is maintained, called *active balls*. Let A^m denote the set of active balls at the start of the m th round. A ball with center (w, x) and radius r is given by $\{(w', x') \in \mathcal{W} \times \mathcal{X} \mid d((w, x), (w', x')) < r\}$.

The CZ algorithm operates using two rules each round m : the *selection rule* is used to select a relevant ball B^m from the set of active balls A^m ; then, an *activation rule* is optionally applied that adds a new ball with smaller radius.

Now the selection rule is described in more detail. Firstly, let $N^m(B)$ be the number of times that a ball $B \in A^m$ has been selected in the first m rounds, and $\bar{y}^m(B)$ the average reward received after m rounds when selecting ball B .

$$N^m(B) = \sum_{i=1}^m \mathbb{1}[B = B^i], \quad (2.20)$$

$$\bar{y}^m(B) = \frac{1}{N^m(B)} \sum_{i=1}^m y^i \mathbb{1}[B = B^i]. \quad (2.21)$$

Let $r(B)$ denote the radius of ball B and let $\text{dom}^m(B)$ be the domain of ball B on the m th round, which is the subset of B that excludes all balls of smaller radius, or:

$$\text{dom}^m(B) = B - \left(\bigcup_{B' \in A^m: r(B') < r(B)} B' \right). \quad (2.22)$$

The *confidence radius* $\text{conf}^m(B)$ of ball B on the m th round is:

$$\text{conf}^m(B) = 4 \sqrt{\frac{\log T}{1 + N^{m-1}(B)}}. \quad (2.23)$$

Let $\text{relevant}^m(w, A^m)$ denote the set of balls that are relevant for context w on the m th round, which is the set of balls that contain an arm x such that (w, x) is in the domain of the ball:

$$\text{relevant}^m(w, A^m) = \{B \in A^m \mid \exists x \in \mathcal{X}. (w, x) \in \text{dom}^m(B)\}. \quad (2.24)$$

The ball B^m selected on the m th round with context w^m can now be given as:

$$I^m(B) = \bar{y}^{m-1}(B) + r(B) + \text{conf}^m(B), \quad (2.25)$$

$$B^m = \max_{B \in \text{relevant}^m(w^m, A^m)} r(B) + \min_{B' \in A^m} (I^m(B') + d(B, B')), \quad (2.26)$$

where $d(B, B')$ is the distance between the centers of balls B, B' according to the metric d .

Once a ball has been selected, the arm sampled by CZ, x_{CZ}^m , is sampled randomly from the domain of ball B^m (from the set $\{x \in \mathcal{X} \mid (w^m, x) \in \text{dom}^m(B^m)\}$), which concludes the selection rule.

The activation rule is then used if the confidence radius from Equation (2.23) has shrunk to smaller than the radius of ball selected this round, i.e. if $\text{conf}^{m+1}(B^m) \leq r(B^m) < \text{conf}^m(B^m)$. In this case, a new ball B' is added to the set of active balls, with radius $r(B') = \frac{1}{2}r(B^m)$ and center (w^m, x^m) . If a new ball is added, then $A^{m+1} = A^m \cup \{B'\}$ and otherwise $A^{m+1} = A^m$.



Figure 2.4: An example MDP \mathcal{M} , where $s_0 = s_{\mathcal{M}}^1$, the finite horizon is $H = 2$, and terminal states are marked with a thicker border. Edges are appropriately marked with actions and rewards, or marked with transition probabilities.

2.2 Markov Decision Processes

In this section *Markov decision processes* (MDPs) are introduced, along with related definitions of *policies* and *trajectories*. MDPs give a mathematical framework for problems concerning sequential decision making under uncertainty, and in this thesis will be the framework used to model the environment that agents act in. An MDP contains, among other things, a set of states and actions. States are sampled according to a transition distribution which depends on the current state and current action being taken (the Markov assumption). Any time an action is taken from a state the agent receives an instantaneous reward, according to a reward function that depends on the state and action taken.

This thesis is concerned with discrete, finite, fully-observable and finite-horizon Markov decision processes, meaning that the state and action spaces are discrete and finite, and any *trajectories* (sequences of states, actions and rewards) are of a finite length.

Definition 2.2.1. A Markov decision process (MDP) is a tuple $\mathcal{M} = (\mathcal{S}, s_0, \mathcal{A}, R, p, H)$, where \mathcal{S} is a set of states, $s_0 \in \mathcal{S}$ is an initial state, \mathcal{A} is a set of actions, $R(s, a)$ is a reward function $\mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, $p(s'|s, a)$ is a next state transition distribution $\mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ and $H \in \mathbb{N}$ is a finite-horizon time bound.

An example MDP is shown in Figure 2.4. Notationally, it is convenient to define the set of successor states, that is the set of states that could be reached after

taking an action from the current state of the MDP:

Definition 2.2.2. *The set of successor states $\text{Succ}(s, a)$ of a state-action pair (s, a) , with respect to an MDP, is defined as:*

$$\text{Succ}(s, a) := \{s' \in \mathcal{S} | p(s'|s, a) > 0\}. \quad (2.27)$$

Additionally, throughout this thesis, MDPs will be defined with *terminal states*, which are states that once reached will never be left, and no more reward can be obtained.

Definition 2.2.3. *A state $s \in \mathcal{S}$ is a terminal state (or a trap state), if the transition distribution always returns the same state (i.e. $p(s|s, a) = 1$ for all actions a), and if no more reward is obtained from that state ($R(s, a) = 0$ for all a). The function `terminal`(s) returns a boolean in $\{\text{True}, \text{False}\}$ which will be used to denote if a state s is terminal or not.*

To define a strategy that an agent will follow in an MDP, an agent defines a *policy*. A policy maps each state in the state space to a probability distribution over the action space. To “follow” a policy, actions are sampled from the distribution. Often it is desirable to define deterministic policies, which always produce the same action when given the same state, and can be represented as *one-hot* distributions.

Definition 2.2.4. *A (stochastic) policy $\pi : \mathcal{S} \rightarrow (\mathcal{A} \rightarrow [0, 1])$ is a mapping from states to a probability distributions over actions and $\pi(a|s)$ is the probability of sampling action a at state s . The policy π must satisfy the conditions: for all $s \in \mathcal{S}$ we have $\sum_{a \in \mathcal{A}} \pi(a|s) = 1$ and for all actions $a \in \mathcal{A}$ that $\pi(a|s) \geq 0$.*

Additionally, a deterministic policy is defined as a one-hot policy, that is, the policy π is deterministic iff it can be written as $\pi(a|s) = \mathbb{1}[a = a']$ for some $a' \in \mathcal{A}$.

Moreover, the following notations are used for policies:

- $a \sim \pi(\cdot|s)$ denotes sampling an action a from the distribution $\pi(\cdot|s)$;
- $\pi(s) = a'$ is used as a shorthand to define the deterministic policy $\pi(a|s) = \mathbb{1}[a = a']$;

- $\pi(s)$ is used as a shorthand for the action $a' \sim \pi(\cdot|s)$ in the case of a deterministic policy.

Given an MDP \mathcal{M} and a policy π it is then possible to sample a sequence of states, actions and rewards, known as a *trajectory*. A trajectory *simulates* one possible sequence that could occur if an agent follows policy π in \mathcal{M} , and in Section 2.4 these simulations are used to incrementally build a search tree.

Definition 2.2.5. A trajectory τ , is a sequence of state, action and rewards, that is induced by a policy π and MDP \mathcal{M} pair. Let the trajectory be $\tau = (s_0, a_0, r_0, s_1, a_1, r_1, \dots, s_{H-1}, a_{H-1}, r_{H-1}, s_H)$, where $a_t \sim \pi(\cdot|s_t)$, $r_t = R(s_t, a_t)$ and $s_{t+1} \sim p(\cdot|s_t, a_t)$.

The following notations will also be used for trajectories:

- $\tau \sim \pi$ denotes a trajectory that is sampled using the policy π , where the MDP \mathcal{M} is implicit;
- $\tau_{i:j}$ denotes the truncated trajectory $\tau_{i:j} := (s_i, a_i, r_i, s_{i+1}, \dots, s_{j-1}, a_{j-1}, r_{j-1}, s_j)$, between the timesteps $0 \leq i < j \leq H$ inclusive;
- $\tau_{:j} := \tau_{0:j}$ denotes a trajectory that is truncated on only one end,
- given a trajectory τ , the following set notation is used, $s \in \tau$, $(s, a) \in \tau$ as a shorthand for $s \in \{s_i | i = 0, \dots, H\}$ and $(s, a) \in \{(s_i, a_i) | i = 0, \dots, H-1\}$ respectively,

and finally, when states, actions and rewards a timestep indexed (i.e. s_t, a_t, r_t), they will always correspond to a trajectory.

2.3 Reinforcement Learning

This section serves as a brief introduction to fundamental concepts in reinforcement learning, and motivates an alternative lens on reinforcement learning that this thesis will consider. The field of reinforcement learning considers an agent that has to learn how to make decisions by interacting with its environment (Figure 2.5).



Figure 2.5: An overview of reinforcement learning. In black depicts the standard agent-environment interface for reinforcement learning [29], where an agent can perform actions in an environment and is given feedback in the form of observations and rewards. In blue the environment is replaced by a simulated environment which the agent can use for planning, and is queried by a user for recommendations on how to act in the real environment.

The agent can take actions in the environment, receiving in return *observations* and *rewards*, which can be used to update internal state and used to make further decisions, and the goal of the agent is to maximise the rewards that it receives.

Classically the agent is considered to interact with its environment directly [29], and thus must make a trade-off between exploring new strategies and exploiting learned strategies. That is, reinforcement learning agents must consider the *exploration-exploitation trade-off* discussed in Section 2.1 too.

Also depicted in Figure 2.5 is a scenario where the agent is equipped with a simulator that it can use to plan and explore, and is either asked to recommend a strategy after a planning/learning phase, or is occasionally queried to recommend actions. This scenario more closely resembles how reinforcement learning is used in the modern era with greater amounts of compute power available, and interactions with the simulator occur at orders of magnitude quicker. Hence, in this scenario, the only significant real-world cost comes from following the recommendations output, to be used in the real-world environment. This changes the nature of the exploration-exploitation trade off, almost separating the two issues, where there is an emphasis on exploring during the planning phase, and the problem of providing good recommendations is concerned with pure exploitation. This

perspective on reinforcement learning motivates the research questions around exploration: **Q1 - Exploration.**

In this thesis, the environment will always take the form of an MDP (Definition 2.2.1), and observations will always be *fully-observable*, meaning that the agent is provided with full access to the states of the MDP.

Following on from Section 2.2, the remainder of this section defines *value functions* and the objectives of reinforcement learning and covers *Value Iteration*, a tabular dynamic programming approach to reinforcement learning. Finally Section 2.3.1 covers *maximum-entropy reinforcement learning*.

The value of a policy π is the expected cumulative reward that will be obtained by following the policy:

Definition 2.3.1. *The value of a policy π from state s at time t is:*

$$V^\pi(s; t) = \mathbb{E}_{\tau \sim \pi} \left[\sum_{i=t}^{H-1} r_i \middle| s_t = s \right]. \quad (2.28)$$

The Q-value of a policy π , from state s , with action a , at time t is:

$$Q^\pi(s, a; t) = R(s, a) + \mathbb{E}_{s' \sim p(\cdot | s, a)} [V^\pi(s'; t + 1)]. \quad (2.29)$$

From the definition of the values functions the optimal value functions can be defined by taking the maximum value over all policies:

Definition 2.3.2. *The Optimal (Q-)Value of a state(-action pair) is defined as:*

$$V^*(s; t) = \max_{\pi} V^\pi(s; t) \quad (2.30)$$

$$Q^*(s, a; t) = \max_{\pi} Q^\pi(s, a; t). \quad (2.31)$$

Value functions can also be used to define an objective function:

Definition 2.3.3. *The (standard) reinforcement learning objective function $J(\pi)$ is defined as:*

$$J(\pi) = V^\pi(s_0; 0). \quad (2.32)$$

The objective of (standard) reinforcement learning can then be stated as finding $\max_{\pi} J(\pi)$.

The *optimal policy* is the policy that maximises the objective function J , and can be shown to be deterministic [20]:

Definition 2.3.4. *The optimal (standard) policy π^* is the policy maximising the standard objective function:*

$$\pi^* = \arg \max_{\pi} J(\pi) \quad (2.33)$$

or equivalently, the optimal standard policy can be in terms of the optimal Q -value function:

$$\pi^*(s) = \arg \max_a Q^*(s, a). \quad (2.34)$$

It can be shown that the optimal (Q-)value functions satisfy the *Bellman equations* [5, 20]:

$$V^*(s; t) = \max_{a \in \mathcal{A}} Q^*(s, a; t), \quad (2.35)$$

$$Q^*(s, a; t) = R(s, a) + \mathbb{E}_{s' \sim p(\cdot|s, a)}[V^*(s'; t + 1)]. \quad (2.36)$$

The Bellman equations admit a *dynamic programming* approach which can be used to compute the optimal value functions, known as *Value Iteration* [5, 20]. In Value Iteration, a table of value estimates $\hat{V}(s; t)$ are kept for each s, t . Given any initial estimate of the value function \hat{V}^0 , the *Bellman backup* operations are:

$$\hat{V}^{k+1}(s; t) = \max_{a \in \mathcal{A}} \hat{Q}^{k+1}(s, a; t), \quad (2.37)$$

$$\hat{Q}^{k+1}(s, a; t) = \mathbb{E}_{s' \sim p(\cdot|s, a)}[R(s, a) + \hat{V}^k(s'; t + 1)]. \quad (2.38)$$

In each iteration of Value Iteration, these values are computed for all $s \in \mathcal{S}$, $a \in \mathcal{A}$ and $t \in \{0, 1, \dots, H\}$. The value estimates computed from the Bellman backups will converge to the optimal values in a finite number of iterations: $V^k \rightarrow V^*$.

2.3.1 Maximum Entropy Reinforcement Learning

In *maximum-entropy reinforcement learning*, the objective function is altered to include the addition of an entropy term. The addition of an entropy term is motivated by wanting to learn stochastic behaviours, that better explore large state spaces, and learn more robust behaviours under uncertainty by potentially learning multiple solutions rather than a single deterministic solution [10].

Let \mathcal{H} denote the (Shannon) entropy function [24]:

$$\mathcal{H}(\pi(\cdot|s)) = \mathbb{E}_{a \sim \pi(\cdot|s)}[-\log \pi(a|s)] = \sum_{a \in \mathcal{A}} \pi(a|s) \log \pi(a|s). \quad (2.39)$$

In the maximum entropy objective, the relative weighting of entropy terms is included using a coefficient α , called the *temperature*. In the maximum entropy objective, analogues of the value functions can be defined, which are typically referred to as *soft (Q-)values*, and similarly the maximum entropy objective is often referred to as the *soft objective*.

Definition 2.3.5. *The soft value of a policy π from state s at time t is:*

$$V_{\text{sft}}^{\pi}(s; t) = \mathbb{E}_{\tau \sim \pi} \left[\sum_{i=t}^{H-1} r_i + \alpha \mathcal{H}(\pi(\cdot|s_i)) \middle| s_t = s \right]. \quad (2.40)$$

The soft Q-value of a policy π , from state s , with action a , at time t is:

$$Q_{\text{sft}}^{\pi}(s, a; t) = R(s, a) + \mathbb{E}_{s' \sim p(\cdot|s, a)}[V_{\text{sft}}^{\pi}(s'; t + 1)]. \quad (2.41)$$

The optimal soft (Q-)values can be defined by taking the maximum over policies, similarly to the standard objective:

Definition 2.3.6. *The optimal soft (Q-)Value of a state(-action pair) is defined as:*

$$V_{\text{sft}}^*(s; t) = \max_{\pi} V_{\text{sft}}^{\pi}(s; t), \quad (2.42)$$

$$Q_{\text{sft}}^*(s, a; t) = \max_{\pi} Q_{\text{sft}}^{\pi}(s, a; t). \quad (2.43)$$

In maximum entropy reinforcement learning, the objective is to find a policy with maximal soft value.

Definition 2.3.7. *The maximum entropy (or soft) reinforcement learning objective function $J_{\text{sft}}(\pi)$ is defined as:*

$$J_{\text{sft}}(\pi) = V_{\text{sft}}^{\pi}(s_0; 0). \quad (2.44)$$

The objective of maximum entropy (or soft) reinforcement learning can then be stated as finding $\max_{\pi} J_{\text{sft}}(\pi)$.

The optimal soft policy is defined as the policy that maximises the soft objective function J_{sft} , and it can be computed from the optimal soft (Q-)values.

Definition 2.3.8. *The optimal soft policy π_{sft}^* is the policy maximising the soft objective function:*

$$\pi_{\text{sft}}^* = \arg \max_{\pi} J_{\text{sft}}(\pi). \quad (2.45)$$

Given V_{sft}^ and Q_{sft}^* the optimal soft policy is known to take the form [10]:*

$$\pi_{\text{sft}}^*(a|s; t) = \exp((Q_{\text{sft}}^*(s, a; t) - V_{\text{sft}}^*(s; t)) / \alpha). \quad (2.46)$$

Equations similar to the Bellman equations, aptly named the *soft Bellman equations*, can be defined for maximum entropy reinforcement learning. These equations differ to equations (2.35) and (2.36) by the replacement of the max operation with a *softmax* or *log-sum-exp* operation, and explain why the maximum entropy analogues are referred to as the *soft* versions of their standard reinforcement learning counterparts. The *soft Bellman equations* are [10]:

$$V_{\text{sft}}^*(s; t) = \alpha \log \sum_{a \in \mathcal{A}} \exp(Q_{\text{sft}}^*(s, a; t) / \alpha), \quad (2.47)$$

$$Q_{\text{sft}}^*(s, a; t) = R(s, a) + \mathbb{E}_{s' \sim p(\cdot|s, a)}[V_{\text{sft}}^*(s'; t + 1)]. \quad (2.48)$$

Analogous to standard reinforcement learning, the soft Bellman equations can be used in *soft Bellman backups* for a *Soft Value Iteration* algorithm [10]:

$$\hat{V}_{\text{sft}}^{k+1}(s; t) = \alpha \log \sum_{a \in \mathcal{A}} \exp\left(\frac{1}{\alpha} \hat{Q}_{\text{sft}}^{k+1}(s, a; t)\right), \quad (2.49)$$

$$\hat{Q}_{\text{sft}}^{k+1}(s, a; t) = R(s, a) + \mathbb{E}_{s' \sim p(\cdot|s, a)}[\hat{V}_{\text{sft}}^k(s'; t + 1)]. \quad (2.50)$$



Figure 2.6: Overview of one trial of MCTS-1, depicting the four commonly presented stages [6]. First, in the selection phase a search policy is used to sample a path down the tree. Next a new node is added to the search tree. Then the new node is initialised using a heuristic, often using a *simulation* using a *rollout policy* as depicted. Finally, values (triangles) are updated through *backups* along the path sampled in the selection phase.

2.4 Trial-Based Heuristic Tree Search and Monte Carlo Tree Search

When considering MDPs with large state-action spaces, using tabular dynamic programming methods becomes infeasibly slow. One approach for handling large state-action spaces is to use *heuristic methods*, that consider a subset of the state-action space and utilise heuristic estimates for the value of states. Often these heuristic methods build a *search tree* from the initial state of the MDP.

Monte Carlo Tree Search (MCTS) refers to heuristic algorithms that build a search tree using *Monte Carlo Trials*, where nodes are added to the tree based off randomly sampled trajectories. Two advantages of using MCTS methods in the modern day are: that they allow for statistical analysis, which can provide *probabilistic guarantees* for the performance of the algorithm; and they offer interpretability, as the search tree can be inspected post-hoc to identify why the algorithm made certain decisions. **TODO: consider adding interoperability refs when litrev'ed**

MCTS trials are commonly presented using four stages, selection, expansion, simulation/heuristic and backup phases [6], which are depicted in Figure 2.6. To

avoid confusion with the above definition of MCTS, this thesis will refer to this specific form of MCTS as MCTS-1. Each of the four phases of MCTS-1 are described in more detail below:

1. *Selection phase* - a *search policy* is used to traverse the search tree from the root node until it reaches a state not contained in the search tree;
2. *Expansion phase* - a new child node is added to the search tree;
3. *Simulation/Heuristic phase* - the new child node's value is initialised using a *heuristic*, often taking the form of a Monte Carlo return, obtained using a *simulation* with a *rollout policy*;
4. *Backup phase* - the value from the heuristic or simulation is used to backup values through the path traversed in the selection phase.

Trial-Based Heuristic Tree Search (THTS) [14] generalises heuristic tree search methods used for planning, such as Trial-Based Real Time Dynamic Programming [4] and LAO* [11]. However, THTS differs slightly from how MCTS-1 is presented above. In a THTS trial, after the expansion/heuristic phases are run, the trial “switches back to the selection phase and alternate between those phases”, until the planning horizon is reached. This is similar to the trial depicted in blue in Figure 2.8.

THTS++ [21] is introduced in Section 2.4.2, which is an open-source, parallelised extension of the THTS schema (including being able to implement MCTS-1 algorithms), and was built to facilitate the work in this thesis. Section 2.4.3 covers the Upper Confidence Bound applied to Trees (UCT) algorithm [16, 17], which is a commonly used MCTS algorithm, and Section 2.4.4 presents the Maximum ENtropy Tree Search (MENTS) algorithm [32], which is related to the algorithms introduced in Chapter 4 of this thesis.

2.4.1 Notation

To simplify notation in the presentation and analysis of THTS++ algorithms, this thesis assumes that states and state-action pairs have a one-to-one correspondence with nodes in the search tree. This assumption is purely to simplify notation for a clean presentation, and any results discussed in this thesis generalise to when this assumption does not hold.

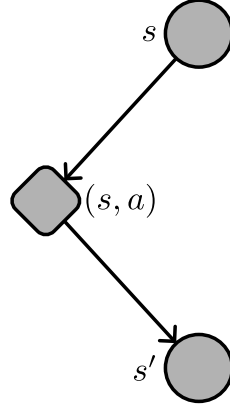
Specifically, this allows the notation for value functions to avoid explicitly writing the timestep parameter, so that $V^\pi(s)$ can be written instead of $V^\pi(s; t)$.

2.4.2 Trial Based Heuristic Tree Search

This subsection introduces THTS++ , which extends the Trial-Based Heuristic Tree Search (THTS) schema [14], and aims to provide a modular library which can implement any MCTS algorithm. The changes made to the original schema allow algorithms following the four-phase MCTS-1 trials described previously to be incorporated. Additionally, the notion of a per-trial *context* is added, which will be used in Chapters 5 and 6 for multi-objective MCTS algorithms. Additionally, beyond the scope of this thesis, contexts allow THTS++ to implement algorithms for *partially-observable* environments, such as Partially Observable Monte Carlo Planning [25]. The remainder of this section will be presented in the context of planning for fully-observable MDPs, but THTS++ generalises to partially-observable environments if *observation-action histories* are used in place of states.

In THTS++ trees consist of *decision nodes* and *chance nodes*. Decision nodes sample actions that can be taken by the agent, and chance nodes sample *outcomes* (MDP states) that depend on the action taken and the transition function of the MDP. As such, each decision node has an associated *state* and each chance node has an associated *state-action pair*. Figure 2.7 shows how decision and chance nodes will be depicted as circles and diamonds in diagrams.

A search tree \mathcal{T} is built using Monte Carlo *trials* and an overview of one trial in THTS++ is given in Figure 2.8. Each THTS++ trial is also split into four phases:



1. *Context sampling* - a *context* is sampled for the trial;
2. *Selection phase* - a trajectory is sampled using a *search policy*, any newly visited states (and state-action pairs) are added to \mathcal{T} as decision nodes (and chance nodes);
3. *Heuristic phase* - any new leaf nodes added in the selection phase are initialised using a *heuristic function*;
4. *Backup phase* - value estimates in the search tree are updated, along the path sampled in the selection phase.

Note that the selection and expansion phases of MCTS-1 are encapsulated by the selection phase of THTS++.

Definition 2.4.1. A search tree \mathcal{T} is a subset of the state and state-action spaces, that is $\mathcal{T} \subseteq \mathcal{S} \cup \mathcal{S} \times \mathcal{A}$, where for each $s \in \mathcal{T}$, there exists some truncated trajectory $\tau_{:h}$ such that $s_h = s$, each $s' \in \tau_{:h}$ is also in the tree, $s' \in \mathcal{T}$, and each $s', a' \in \tau_{:h}$ is also in the tree, $(s', a') \in \mathcal{T}$.

A *decision node* refers to any state that is in the search tree: $s \in \mathcal{T}$. A *chance node* refers to any state-action pair that is in the search tree: $(s, a) \in \mathcal{T}$. And a *node* is used to refer to any decision or chance node in the tree. Sometimes the

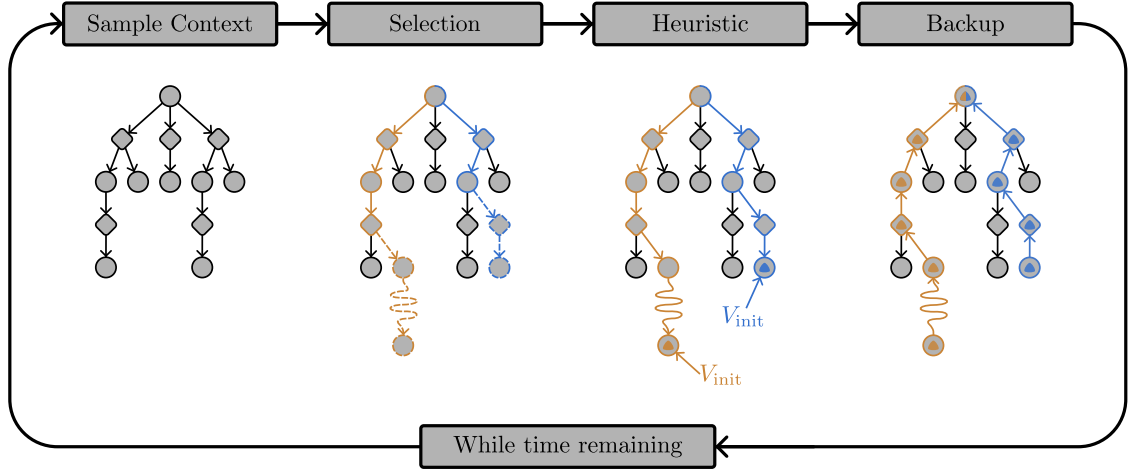


Figure 2.8: Overview of one trial of THTS++, where orange shows an example when `mcts_mode` is True, and blue shows an example when `mcts_mode` is False. From left to right: first a context is sampled, which stores any necessary per-trial state (not depicted) and the search tree at the beginning of the trial is shown; second shows the selection phase, where a trajectory is sampled and where dashed lines indicate any new nodes added; third shows that new leaf nodes are initialised using the \hat{V}_{init} heuristic function; and finally on the right, shows the backup phase, where the arrows directions are changed to show that information is being propagated back up the tree to update the values in the nodes (triangles).

notation $\text{node}(s)$ and $\text{node}(s, a)$ will be used to make it clear that a node is being discussed, rather than a state or state-action pair.

$N(s)$ and $N(s, a)$ denote the number of times $\text{node}(s)$ and $\text{node}(s, a)$ have been visited, or equivalently, the number of times s and (s, a) appear in trajectories sampled in THTS++ trials.

Each decision and chance node will generally store value estimates that are algorithm dependent. $\text{node}(s).V$ is used to denote the set of values stored at node $\text{node}(s)$, and $\text{node}(s, a).Q$ for the set of values stored at node $\text{node}(s, a)$.

Additionally, let $\text{node}(s).\text{chldrn}$ be a mapping from actions to the chance nodes that are children of $\text{node}(s)$. Likewise, $\text{node}(s, a).\text{chldrn}$ is a mapping from outcomes (successor states) to the decision nodes that are children of $\text{node}(s, a)$.

THTS++ introduces the idea of `mcts_mode` into the THTS schema. When `mcts_mode` is True, a single decision node is added to the search tree on each trial, similarly to MCTS-1. When it is False, the trajectory is sampled until a terminal state or the planning horizon is reached. These two modes of operation

are depicted in blue and orange respectively in Figure 2.8.

Definition 2.4.2. *When running in `mcts_mode`, the trajectory sampled in the selection phase is truncated, and will end if a state not in the search tree \mathcal{T} is reached, similarly to MCTS-1 [6]. When not running in `mcts_mode`, the trajectory is sampled until a terminal state is reached, or the planning horizon is reached, similarly to THTS [14].*

There are two main benefits to running an algorithm in `mcts_mode`. The first is that it uses significantly less memory, which can be a concern if using a large planning horizon H and the tree search is going to run for a long time. The second is that if `mcts_mode` is used with an informative heuristic function, then it allows the algorithm to avoid wasting resources (time and memory) on parts of the search tree that are not promising.

In contrast, when no informative heuristic is available, a random simulation is often used in MCTS-1 algorithms. In such cases, where memory allows, running with `mcts_mode` set to `False` can be beneficial, because states that would have been visited in the simulation phase of MCTS-1 are added to the tree and avoids throwing away potentially useful information.

THTS++ also introduces the notion of a *context* that is sampled for each trial. The context is passed to every subsequent function call in a trial of THTS++, and can be used to store temporary state. This context will go unused for the remainder of the chapter, but will be useful in Chapters 5 and 6 when *contextual tree search* is discussed.

Definition 2.4.3. *A context is an arbitrary key-value store that is used to store any relevant data that varies from trial to trial.*

To specify an algorithm in the THTS++ schema, the following need to be specified:

Value Estimates: What value estimates will be stored at each decision and chance node. That is, `node(s).V` and `node(s, a).Q` need to be defined;

Search policy: A policy π_{search} used to sample a trajectory for the trial, which can use values in the current search tree \mathcal{T} , and values from the heuristic action function (below);

Outcome Sampler: A function `sample_outcome` that samples outcomes according to the environment, given a current state and action. In this thesis, this will always sample a state from the transition distribution of the MDP: $s' \sim p(\cdot|s, a)$;

Heuristic value function: A function \hat{V}_{init} used as a heuristic to initialise values for new decision nodes added to the tree;

Heuristic action function: A function \hat{Q}_{init} used as a heuristic for Q-values when a state-action pair is not in the current search tree;

Backup functions: Two functions `backup_v` and `backup_q` which updates the values in decision and chance nodes respectively. These functions can use values from their children, from the sampled trajectory and from the heuristic value function;

Context sampler: A function `sample_context` which creates a context key-value store, and samples any initial values to be stored in the context;

MCTS mode: A boolean (which will also be denoted `mcts_mode`) specifying if THTS++ should operate in `mcts_mode`;

Planning horizon: A (problem dependent) planning horizon for the tree search $H_{\text{THTS++}}$, which is no longer than the horizon of the MDP, $H_{\text{THTS++}} \leq H$.

Figure 2.8 depicts a trial in THTS++, and pseudocode for running a trial is given in Listing 2.1. At the beginning of running a THTS++ algorithm, the search tree is initialised to $\mathcal{T} \leftarrow \{s_0\}$. When the components detailed above are provided, the operation of a trial in THTS++ is as follows:

- Firstly, a context is sampled using the `sample_context` function, which is available to be used by any other function in the trial.

- A trajectory is sampled $\tau_{:h} \sim \pi_{\text{search}}$ according to the search policy (which may use \hat{Q}_{init} as necessary) and `sample_outcome`.
 - If running in `mcts_mode`, then $\tau_{:h}$ is such that $s_t \in \mathcal{T}$ for $t = 0, \dots, h-1$ and $s_h \notin \mathcal{T}$, or $h = H_{\text{THTS++}}$, or s_h is terminal.
 - If not running in `mcts_mode`, then $h = H_{\text{THTS++}}$, or s_h is terminal.
- The search tree is updated to include any new nodes from the sampled trajectory, $\mathcal{T} \leftarrow \mathcal{T} \cup \tau_{:h}$.
- The heuristic value function is used to initialise the value of the new leaf node $\text{node}(s_h).v \leftarrow \hat{V}_{\text{init}}(s_h)$.
- Finally, for the backup phase, the `backup_q` and `backup_v` functions are used to update the values of $\text{node}(s_t, a_t).q$ and $\text{node}(s_t).v$ for $t = h-1, \dots, 0$.

2.4.3 Upper Confidence Bounds Applied to Trees (UCT)

Upper Confidence Bound applied to Trees (UCT) [16, 17] is a commonly used tree search algorithm, which is based on the Upper Confidence Bound (UCB) algorithm covered in Section 2.1. UCT is a good example of a common paradigm in tree search algorithms for sequential decision making, where each node in the tree is tasked with making a single decision in the sequence, and so adapts methods from the MAB literature. More specifically, UCT can be viewed as running UCB on a non-stationary MAB at every decision node, where it is non-stationary because the rewards obtained depend on the decisions that children make. The remainder of this subsection will outline how UCT can be defined using the `THTS++` schema given in Section 2.4.2.

In UCT `mcts_mode` is set to `True`. And at each decision node of UCT a sample average \bar{V}_{UCT} and \bar{Q}_{UCT} is used for a value estimate. The search policy that UCT then follows is given by:

$$\pi_{\text{UCT}}(s) = \arg \max_{a \in \mathcal{A}} \bar{Q}_{\text{UCT}}(s, a) + b_{\text{UCT}} \sqrt{\frac{\log(N(s))}{N(s, a)}}, \quad (2.51)$$

```

1  def run_trial(search_tree:  $\mathcal{T}$ ,
2              search_policy:  $\pi_{\text{search}}$ ,
3              heuristic_fn:  $\hat{V}_{\text{init}}$ ,
4              heuristic_action_fn:  $\hat{Q}_{\text{init}}$ ,
5              mcts_mode,
6              planning_horizon:  $H_{\text{THTS++}}$ ):
7      # context sampling
8      ctx = sample_context()
9      # simulation phase
10      $\tau_{:h}$  = sample_trajectory( $\mathcal{T}$ ,  $\pi_{\text{search}}$ ,  $\hat{Q}_{\text{init}}$ , mcts_mode,  $H_{\text{THTS++}}$ , ctx)
11      $\mathcal{T} \leftarrow \mathcal{T} \cup \tau_{:h}$ 
12     # heuristic phase
13     node( $s_h$ ).V  $\leftarrow \hat{V}_{\text{init}}(s_h, \text{ctx})$ 
14     # backup phase
15     for i in { $h-1, h-2, \dots, 1, 0$ }:
16         node( $s_i, a_i$ ).backup_q(node( $s_i, a_i$ ).chldrn,  $\tau_{:h}$ ,  $\hat{V}_{\text{init}}(s_h)$ , ctx)
17         node( $s_i$ ).backup_v(node( $s_i$ ).chldrn,  $\tau_{:h}$ ,  $\hat{V}_{\text{init}}(s_h)$ , ctx)
18
19 def sample_trajectory(search_tree:  $\mathcal{T}$ ,
20                     search_policy:  $\pi_{\text{search}}$ ,
21                     heuristic_action_fn:  $\hat{Q}_{\text{init}}$ ,
22                     mcts_mode,
23                     planning_horizon:  $H_{\text{THTS++}}$ ,
24                     ctx):
25     i = 0
26     while ((not mcts_mode or  $s_i \in \mathcal{T}$ )
27           and (i <  $H_{\text{THTS++}}$ )
28           and (not terminal( $s_i$ ))):
29          $a_i \sim \pi_{\text{search}}(\cdot | s_i, \text{ctx})$ 
30          $r_i \leftarrow R(s_i, a_i)$ 
31          $s_{i+1} \leftarrow \text{sample_outcome}(s_i, a_i, \text{ctx})$ 
32         i += 1
33     return ( $s_0, a_0, r_0, s_1, \dots, s_{i-1}, a_{i-1}, r_{i-1}, s_i$ )
34
35 def sample_outcome(s, a, ctx):
36      $s' \sim p(\cdot | s, a)$ 
37     return  $s'$ 

```

Listing 2.1: Psuedocode for running a trial in THTS++.

where b_{UCT} is a *bias* parameter that controls the amount of exploration UCT will perform. In Equation (2.51), when $N(s, a) = 0$ there is a division by zero, which is taken as ∞ , and ties are broken uniformly randomly. Note that like UCB (Section 2.1), this results in every action being taken once to obtain an initial value estimate, and as such, setting \hat{Q}_{init} is unnecessary for UCT.

There are two common approaches to implementing \hat{V}_{init} in UCT: the first consisting of using a function approximation \tilde{V} and setting $\hat{V}_{\text{init}} = \tilde{V}$ [26, 27, 19]

TODO: find another paper or two that is just an application of alphazero?, where \hat{V} aims to approximate the optimal value function V^* ; the second approach consists of using a *rollout policy* [6, 9, 13, 8]. When a rollout policy π_{rollout} is used, a Monte Carlo estimate $\hat{V}^{\pi_{\text{rollout}}}$ is used to estimate the value function $V^{\pi_{\text{rollout}}}$ and is used for \hat{V}_{init} .

Let $\tau_{:h} \sim \pi_{\text{UCT}}$, be the trajectory sampled in the selection phase of UCT, meaning that a decision node for s_h is added to the search tree, and needs to be initialised with \hat{V}_{init} . When using a rollout policy, the truncated trajectory is completed using the rollout policy, $\tau_{h:H} \sim \pi_{\text{rollout}}$, to provide the Monte Carlo estimate at s_h :

$$\hat{V}^{\pi_{\text{rollout}}}(s_h) = \sum_{i=h}^{H-1} r_i. \quad (2.52)$$

If no informative policy is available to be used for π_{rollout} , then uniformly random policy is often used [6, 1].

In UCT the backups `backup_v` and `backup_q` update the (sample average) value estimates. Letting heuristic value for the leaf node be $\tilde{r} = \hat{V}_{\text{init}}(s_h)$, they are computed as follows:

$$\bar{Q}_{\text{UCT}}(s_t, a_t) \leftarrow \frac{1}{N(s_t, a_t)} \left((N(s_t, a_t) - 1) \bar{Q}_{\text{UCT}}(s_t, a_t) + \tilde{r} + \sum_{i=t}^{h-1} r_i \right) \quad (2.53)$$

$$\bar{V}_{\text{UCT}}(s_t) \leftarrow \frac{1}{N(s_t)} \left((N(s_t) - 1) \bar{V}_{\text{UCT}}(s_t) + \tilde{r} + \sum_{i=t}^{h-1} r_i \right) \quad (2.54)$$

2.4.4 Maximum Entropy Tree Search

Maximum ENTropy Tree Search (MENTS) [32], in contrast to UCT, focuses on the maximum-entropy objective, and uses soft Bellman backups to update its value estimates. In its original presentation `mcts_mode` is set to True, and it uses the soft value estimates \hat{V}_{MENTS} and \hat{Q}_{MENTS} . The MENTS search policy is given by:

$$\pi_{\text{MENTS}}(a|s) = (1 - \lambda(s, \epsilon_{\text{MENTS}})) \rho_{\text{MENTS}}^k(a|s) + \frac{\lambda(s, \epsilon_{\text{MENTS}})}{|\mathcal{A}|} \quad (2.55)$$

$$\rho_{\text{MENTS}}(a|s) = \exp \left(\frac{1}{\alpha_{\text{MENTS}}} \left(\hat{Q}_{\text{MENTS}}(s, a) - \hat{V}_{\text{MENTS}}(s) \right) \right), \quad (2.56)$$

$$\lambda(s, x) = \min \left(1, \frac{x}{\log(e + N(s))} \right). \quad (2.57)$$



Figure 2.9: The decision-support scenario for multi-objective reinforcement learning [12].

where $\epsilon \in (0, \infty)$ is an exploration parameter, and α_{MENTS} is the temperature parameter used in MENTS for the maximum entropy objective (the coefficient of the entropy term in Equation (2.40)).

In MENTS the backups `backup_v` and `backup_q` update the soft value estimates and are updated using soft Bellman backups (Equations (2.49) and (2.50)) as follows:

$$\hat{Q}_{\text{MENTS}}(s_t, a_t) \leftarrow R(s_t, a_t) + \sum_{s' \in \text{Succ}(s, a)} \left(\frac{N(s')}{N(s_t, a_t)} \hat{V}_{\text{MENTS}}(s') \right), \quad (2.58)$$

$$\hat{V}_{\text{MENTS}}(s_t) \leftarrow \alpha \log \sum_{a \in \mathcal{A}} \exp \left(\frac{1}{\alpha} \hat{Q}_{\text{MENTS}}(s_t, a) \right). \quad (2.59)$$

In [32], the heuristic value function left as an arbitrary evaluation function, but is set using a function approximation $\hat{V}_{\text{init}} = \tilde{V}$ in experiments. The heuristic action function is set to zero, $\hat{Q}_{\text{init}}(s, a) = 0$, but they also suggest that if *policy network* $\tilde{\pi}$ is available, then the heuristic action function can alternatively be set to $\hat{Q}_{\text{init}}(s, a) = \log \tilde{\pi}(s|a)$.

2.5 Multi-Objective Reinforcement Learning

This thesis follows a utility based approach to multi-objective reinforcement learning similar to the review of Hayes et al. [12]. This work will specifically consider *linear utility* functions and the *decision support scenario* which is depicted in Figure 2.9. In the decision support scenario, an algorithm computes a *solution set* consisting of multiple *possibly optimal* solutions, from which a user then picks their most preferred option to be used. This scenario is useful when a user’s preferences over the multiple objectives is unknown or difficult to specify in advance.

This section defines the multi-objective counterparts to various definitions given in Section 2.2 and 2.3. Outside of this section, the prefix “multi-objective” may be dropped where it should be clear from context, however bold typeface will

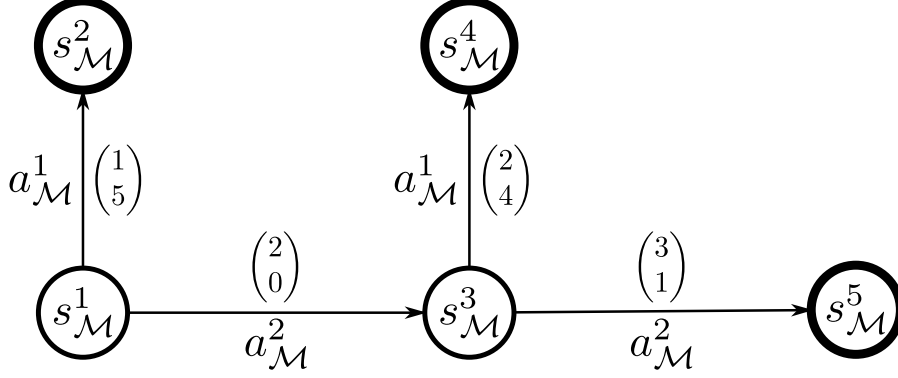


Figure 2.10: An example MOMDP \mathcal{M} , where $s_0 = s_{\mathcal{M}}^1$, the finite horizon is $H = 2$ and terminal states are marked with thicker borders. This particular MOMDP is deterministic, so all transition probabilities are one.

consistently be used to denote any vector variables or functions. In Section 2.5.1, a multi-objective extension of Value Iteration is given.

To specify problems with multiple objectives, the reward function of an MDP changed to give a vector of rewards, rather than a scalar reward:

Definition 2.5.1. A Multi-Objective Markov Decision Process (MOMDP) is a tuple $\mathcal{M} = (\mathcal{S}, s_0, \mathcal{A}, \mathbf{R}, p, H)$, where \mathcal{S} is a set of states, $s_0 \in \mathcal{S}$ is an initial state, \mathcal{A} is a set of actions, $\mathbf{R}(s, a)$ is a vector reward function $\mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}^D$, where D is the dimension of the rewards and the MOMDP, $p(s'|s, a)$ is a next state transition distribution $\mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ and $H \in \mathbb{N}$ is a finite-horizon time bound.

Now multi-objective trajectories are defined:

Definition 2.5.2. A multi-objective trajectory τ , is a sequence of state, action and vector rewards, that is induced by a policy π and MOMDP \mathcal{M} pair. Let the trajectory be $\tau = (s_0, a_0, \mathbf{r}_0, s_1, a_1, \mathbf{r}_1, \dots, s_{H-1}, a_{H-1}, \mathbf{r}_{H-1}, s_H)$, where $a_t \sim \pi(\cdot|s_t)$, $\mathbf{r}_t = \mathbf{R}(s_t, a_t)$ and $s_{t+1} \sim p(\cdot|s_t, a_t)$.

The notations used for single-objective trajectories (Definition 2.2.5) will also be used for multi-objective trajectories too. Such as, $\tau \sim \pi$ for sampling trajectories using policies, and $\tau_{i:j}$ for truncated trajectories.

Similarly, multi-objective variants of the (Q-)value of a policy are defined:

Definition 2.5.3. *The multi-objective value of a policy π from state s at time t is:*

$$\mathbf{V}^\pi(s; t) = \mathbb{E}_{\tau \sim \pi} \left[\sum_{i=t}^{H-1} \mathbf{r}_i \middle| s_t = s \right]. \quad (2.60)$$

The multi-objective Q-value of a policy π , from state s , with action a , at time t is:

$$\mathbf{Q}^\pi(s, a; t) = \mathbf{R}(s, a) + \mathbb{E}_{s' \sim p(\cdot | s, a)} [\mathbf{V}^\pi(s'; t + 1)]. \quad (2.61)$$

In the corresponding point of the single-objective reinforcement learning section (Section 2.3), the the optimal (Q-)value functions and the objective of single-objective reinforcement learning were defined. However, in a multi-objective setting there is no longer a *total ordering* over values, and so there maybe be multiple vectors that could be “optimal”. For example, consider two vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^2$ which are such that $u_1 > v_1$ and $u_2 < v_2$. To resolve this issue, a *utility function* or *scalarisation function* is used to map multi-objective values to scalar values.

Definition 2.5.4. *The (D -dimensional) Simplex consists of the set of D -dimensional vectors, whose entries are non-negative and sum to one. More formally, the D dimensional simplex is*

$$\Delta^D = \{\mathbf{w} \in \mathbb{R}^D | w_i \geq 0, \sum_i w_i = 1\}. \quad (2.62)$$

The elements of the D -dimensional Simplex will be referred to as weight vectors (or just weights) in this thesis, as they will be used to specify preferences over the D dimensions of the reward function.

Definition 2.5.5. *A utility function (or scalarisation function) $u : \mathbb{R}^D \times \Delta^D \rightarrow \mathbb{R}$ is used to map from a multi-objective value $\mathbf{v} \in \mathbb{R}^D$ and a weighting over the objectives $\mathbf{w} \in \Delta^D$ to a scalar value. That is, according to the utility function $u(\cdot; \mathbf{w})$ the multi-objective value \mathbf{v} is mapped to the scalar value $u(\mathbf{v}; \mathbf{w})$.*

Of particular interest in this thesis is the *linear utility function* where the scalar value takes the form of a dot-product:

Definition 2.5.6. The linear utility function u_{lin} is the utility function defined by:

$$u_{\text{lin}}(\mathbf{v}; \mathbf{w}) = \mathbf{w}^\top \mathbf{v}. \quad (2.63)$$

Equipped with a utility function and a weight vector any set of multi-objective values can be mapped to scalars and ordered. A policy is *possibly optimal*, or *undominated*, with respect to utility function u if it achieves a maximal utility for some weight $w \in \Delta^D$. In contrast, a policy is *dominated* if for every weight there is another policy that achieves a better utility.

Let Π be the set of all possible policies for a given MOMDP. When constructing a solution set, a subset of Π , it makes sense that it should not contain any dominated policies. This leads to the first notion of a solution set, called an *undominated set*, consisting of all undominated policies:

Definition 2.5.7. The undominated set of policies $U(\Pi; u) \subseteq \Pi$, with respect to a utility function u , is the set of policies for which there is a weight vector $\mathbf{w} \in \Delta^D$ where the utility (scalarised value) is maximised:

$$U(\Pi; u) = \left\{ \pi \in \Pi \mid \exists \mathbf{w} \in \Delta^D. \forall \pi' \in \Pi : u(\mathbf{V}^\pi(s_0; 0); \mathbf{w}) \geq u(\mathbf{V}^{\pi'}(s_0; 0); \mathbf{w}) \right\}. \quad (2.64)$$

In particular, the convex hull of policies $CH(\Pi)$ is the undominated set with respect to the linear utility function u_{lin} . That is $CH(\Pi) = U(\Pi; u_{\text{lin}})$.

Question: How do you feel about removing the timestep in the value functions in this section too? So it can be $\mathbf{V}^\pi(s)$ rather than $\mathbf{V}^\pi(s; t)$? I think it would make some definitions like undominated sets a bit cleaner. Alternatively, maybe I should write it $u_{\mathbf{w}}$.

When computing solutions sets, it is often useful to first compute the multi-objective values that could be obtained, and then later use the data structures used by the algorithm to read out the selected policy. This thesis will refer to the set of values obtained by a set of policies as a *value set*:

Definition 2.5.8. The (multi-objective) value set with respect to a set of policies $\Pi' \subseteq \Pi$ is defined as $\mathbf{Vals}(\Pi') = \{\mathbf{V}^\pi(s_0; 0) \mid \pi \in \Pi'\}$.

Undominated sets often have an infinite cardinality, and as such are infeasible to compute. However, in undominated sets there are often many redundant policies that obtain the same scalarised values. Instead of computing an undominated set, it is more feasible to compute a *coverage sets* which contain at least one policy that maximises the scalarised value given any weight vector \mathbf{w} :

Definition 2.5.9. A set $CS(\Pi; u) \subseteq U(\Pi)$, is a coverage set with respect to a utility function u , if for every weight vector $\mathbf{w} \in \Delta^D$, there is a policy $\pi \in CS(\Pi; u)$ that maximises the value of $u(\cdot; \mathbf{w})$. That is, for $CS(\Pi; u)$ to be a coverage set, the following statement must be true:

$$\forall \mathbf{w} \in \Delta^D. \exists \pi \in CS(\Pi; u). \forall \pi' \in \Pi : u(\mathbf{V}^\pi(s_0; 0); \mathbf{w}) \geq u(\mathbf{V}^{\pi'}(s_0; 0); \mathbf{w}). \quad (2.65)$$

Again, in particular, any set $CCS(\Pi)$ is a convex coverage set if it is a coverage set with respect to the linear utility function u_{lin} .

Note that it is still possible for there to be multiple coverage sets. Algorithms that compute convex coverage sets typically compute a unique minimal convex coverage set that contains no redundant policies, that is, each policy has some weight for which it uniquely gives an optimal solution in the set.

Definition 2.5.10. A set $CCS_{\min}(\Pi) \subseteq CH(\Pi)$ is minimal if the following holds

$$\forall \pi \in CCS_{\min}(\Pi). \exists \mathbf{w} \in \Delta^D. \forall \pi' \in CCS_{\min}(\Pi) - \{\pi\}. u_{\text{lin}}(\mathbf{V}^\pi(s_0; 0); \mathbf{w}) > u_{\text{lin}}(\mathbf{V}^{\pi'}(s_0; 0); \mathbf{w}). \quad (2.66)$$

Now the geometry of convex coverage sets is considered, to see how something like $\mathbf{Vals}(CCS_{\min}(\Pi))$ can be computed. Firstly, any multi-objective values that obtain the same linear utility will lie on a hyperplane, whose normal is the weight vector used in the linear utility function (see (a) in Figure 2.11). As a result, the values of the convex hull, $\mathbf{Vals}(CH(\Pi))$ lie on a *geometric (partial) convex hull* (see (b) in Figure 2.11). Moreover, any points in $\mathbf{Vals}(CH(\Pi))$ that lie on the edge of the geometric convex hull are redundant, as the values corresponding to the neighbouring vertices of geometric convex hull will always achieve the same or greater utility (see (c) in Figure 2.11).



Figure 2.11: The geometry of convex coverage sets, shown with $D = 2$. In each images the points depicted correspond to a value set $\mathbf{Vals}(\Pi')$, for some set of policies Π' . (a) demonstrates that values $(\mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4)$ obtaining the same utility lie on a hyperplane. Moving in the direction of the weight vector increases the utility (\mathbf{u}_5) and likewise moving in the opposite direction decreases utility (\mathbf{u}_1); (b) circles correspond to values that are on the convex hull, so form the set $\mathbf{Vals}(CH(\Pi'))$, the blue circles form the minimal convex coverage set, $\mathbf{Vals}(CCS_{\min}(\Pi'))$, and triangles are not part of the convex hull. All of the unfilled shapes would be pruned by `cvx_prune`(Equation (2.67)); (c) shows a magnification of (b) with additional labels, it shows that the value \mathbf{v}_2 is redundant because one of \mathbf{v}_1 or \mathbf{v}_3 will achieve an equal or greater utility. Additionally, it shows \mathbf{w}_2 and \mathbf{w}_4 which are weights that the values \mathbf{v}_1 and \mathbf{v}_3 uniquely maximise the utility within $\mathbf{Vals}(\Pi')$

Because of the ambiguity between the convex hull of policies, and the geometric convex hulls of values, this thesis will refer to any value set that forms a geometric convex hull as a *convex hull value set* (CHVS) and will refer to the set $\mathbf{Vals}(CCS_{\min}(\Pi))$ as the *optimal convex hull value set*. Question: should I make this paragraph a definition to emphasise it a bit more?

Given a value set, the `cvx_prune` operation removes any vectors that are dominated or redundant. That is, for every vector that remains after the pruning operation, there is some weight for which it *uniquely* gives the maximal utility for. Given set of vectors \mathbf{V} it is defined as:

$$\text{cvx_prune}(\mathbf{V}) = \{\mathbf{v} \in \mathbf{V} \mid \exists \mathbf{w} \in \Delta^D. \forall \mathbf{v}' \in \mathbf{V} - \{\mathbf{v}\}. \mathbf{w}^\top \mathbf{v} > \mathbf{w}^\top \mathbf{v}'\}. \quad (2.67)$$

Note that the `cvx_prune` operator computes the values of a minimal convex coverage set, that is, for some set of policies Π' the `cvx_prune` operation satisfies

$\text{cvx_prune}(\mathbf{Vals}(\Pi')) = \mathbf{Vals}(CCS_{\min}(\Pi'))$. cvx_prune can be implemented using *linear programming* [23], and an example of its operation on a set of vectors can be seen in (b) of Figure 2.11, where cvx_prune would prune all points but the blue circles.

TODO: Not sure where to put this PF stuff, cant see where to put it in to make it flow well. Also proof read

Another commonly used solution set is the *Pareto front*, which is defined using a *strict partial ordering* over vectors, known as *Pareto domination*, as opposed to using utility. An example is shown in Figure 2.12.

Definition 2.5.11. *The Pareto front $PF(\Pi) \subseteq \Pi$ is defined as:*

$$PF(\Pi) = \{\pi \in \Pi \mid \nexists \pi' \in \Pi. \mathbf{V}^{\pi'}(s_0; 0) \succ_P \mathbf{V}^{\pi}(s_0; 0)\}, \quad (2.68)$$

where the Pareto domination relation is defined as:

$$\mathbf{v} \succ_P \mathbf{v}' \iff (\forall i. v_i \geq v'_i) \wedge (\exists j. v_j > v'_j). \quad (2.69)$$

The Pareto front can be related to the previously defined solution sets if *mixture policies* are allowed, where a mixture policy between π and π' will follow each policy with some probability. Specifically, if Π is closed with respect to mixture policies, then the Pareto front is a convex coverage set.

2.5.1 Convex Hull Value Iteration

TODO: Should we also be defining undominated set/coverage sets for a given $(s; t)$?
As in just add them as a param? As kind of using them in this sect as if we did

Convex Hull Value Iteration (CHVI) [3] is a tabular dynamic programming algorithm similar to Value Iteration (Section 2.3) that will compute optimal convex hull value sets. In CHVI the value estimates of Value Iteration are replaced by CHVSs, which are estimates of the optimal CHVS. These estimates will be denoted $\hat{\mathbf{V}}_{\text{CHVI}}(s; t)$ and $\hat{\mathbf{Q}}_{\text{CHVI}}(s, a; t)$.

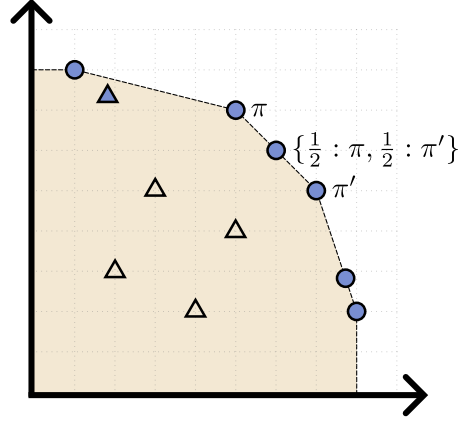


Figure 2.12: An example Pareto front, where the circles correspond to a convex coverage set, and the filled blue points denote the Pareto front. Two points are marked with their corresponding policies π and π' , and a mixture policy is shown, denoted $\{\frac{1}{2} : \pi, \frac{1}{2} : \pi'\}$ that follows each of π and π' with probability $\frac{1}{2}$.

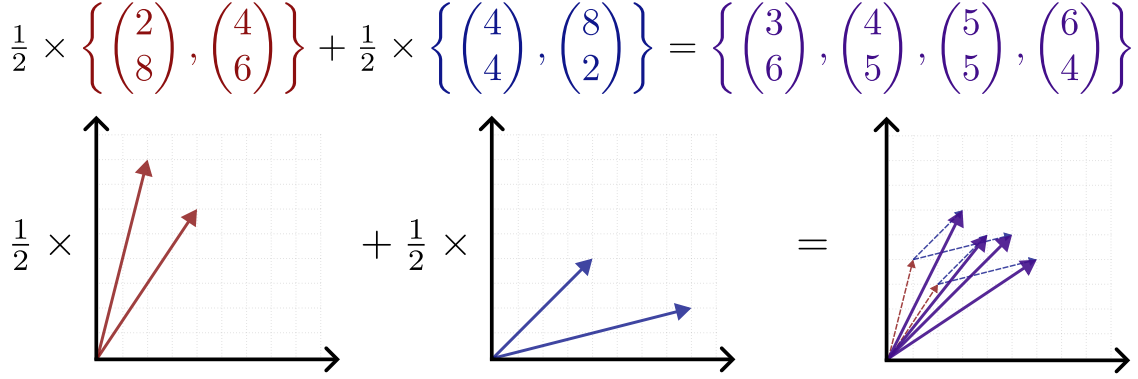


Figure 2.13: An example of arithmetic over vector sets. Two vector sets are shown in red and blue, which are multiplied by $\frac{1}{2}$ using Equation (2.70), and then added using Equation (2.71). On the right the resulting vector set is shown in purple, which are the sum of appropriately scaled red and blue vectors.

Firstly, to define a multi-objective version of Value Iteration, an arithmetic over vector sets needs to be defined. An example of the following arithmetic is given in Figure 2.13. Given the vector sets \mathcal{U} and \mathcal{V} , define multiplication by a scalar s , addition with a vector \mathbf{x} and addition between sets as follows:

$$\mathbf{x} + s\mathcal{V} = \{\mathbf{x} + s\mathbf{v} | \mathbf{v} \in \mathcal{V}\} \quad (2.70)$$

$$\mathcal{U} + \mathcal{V} = \{\mathbf{u} + \mathbf{v} | \mathbf{u} \in \mathcal{U}, \mathbf{v} \in \mathcal{V}\}. \quad (2.71)$$

Now to define the multi-objective Bellman backups used in CHVI, let $\hat{\mathcal{V}}_{\text{CHVI}}^0(s; t) =$

$\{\mathbf{0}\}$, where $\mathbf{0} = (0, \dots, 0) \in \mathbb{R}^D$. The CHVI backups are then:

$$\hat{\mathbf{V}}_{\text{CHVI}}^{k+1}(s; t) = \text{cvx_prune} \left(\bigcup_{a \in \mathcal{A}} \hat{\mathbf{Q}}_{\text{CHVI}}^{k+1}(s, a; t) \right), \quad (2.72)$$

$$\hat{\mathbf{Q}}_{\text{CHVI}}^{k+1}(s, a; t) = \mathbb{E}_{s' \sim p(\cdot | s, a)} [\mathbf{R}(s, a) + \hat{\mathbf{V}}_{\text{CHVI}}^k(s'; t + 1)]. \quad (2.73)$$

This again parallels the Bellman backups use in single-objective Value Iteration, where the max operation is replaced by the `cvx_prune` operation over the set of achievable values from the current state s : $\bigcup_{a \in \mathcal{A}} \hat{\mathbf{Q}}_{\text{CHVI}}^{k+1}(s, a; t)$.

Once the algorithm has terminated, and a weight \mathbf{w} is provided, a policy can be extracted by computing scalar Q-values from the CHVSs [3]:

$$Q_{\mathbf{w}}(s, a; t) = \max_{\mathbf{q} \in \hat{\mathbf{Q}}_{\text{CHVI}}(s, a; t)} \mathbf{w}^\top \mathbf{q}, \quad (2.74)$$

$$\pi_{\text{CHVI}}(s; t, \mathbf{w}) = \arg \max_{a \in \mathcal{A}} Q_{\mathbf{w}}(s, a; t). \quad (2.75)$$

If the user would rather select a particular value from the CHVS, say $\mathbf{v} \in \hat{\mathbf{V}}_{\text{CHVI}}(s_0; 0)$, rather than provide a weight, one can be computed. Let \mathbf{v}_\perp be a *reference point*, defined at each index as:

$$(v_\perp)_i = \min\{v'_i | \mathbf{v}' \in \hat{\mathbf{V}}_{\text{CHVI}}(s_0; 0)\}. \quad (2.76)$$

The vector that runs from \mathbf{v}_\perp to \mathbf{v} provides an appropriate weighting over objectives for which \mathbf{v} will produce the largest utility out of $\hat{\mathbf{V}}(s_0; 0)$, as is demonstrated in Figure 2.14. Hence, to extract a policy that achieves the value \mathbf{v} the weight \mathbf{w} should be set to:

$$\mathbf{w} = \frac{\mathbf{v} - \mathbf{v}_\perp}{\|\mathbf{v} - \mathbf{v}_\perp\|_2}, \quad (2.77)$$

and then follow $\pi_{\text{CHVI}}(s; t, \mathbf{w})$ as defined in Equation (2.75).

2.6 Sampling From Catagorical Distributions

Question: Maybe heres a good time to ask about some notation stuff. So I used m in MABs section, and I reuse it here. Is that ok? I was trying to keep as much notation unique as possible, but noticed I've reused a couple variables. I was hoping its ok because I'm using them "locally".

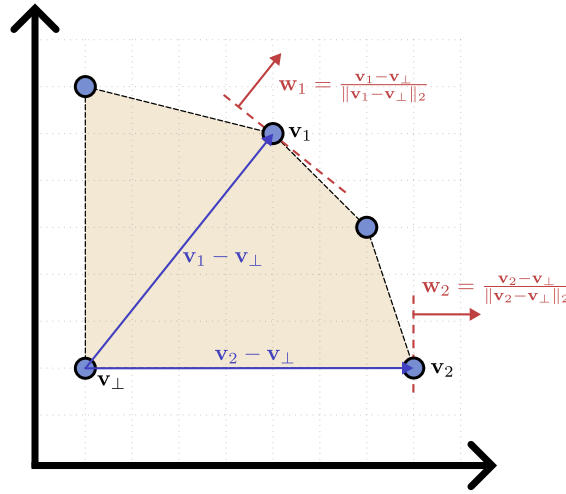


Figure 2.14: A visualisation, reusing the convex hull from Figure 2.11, demonstrating how to compute a weight vector that can be used to extract a specific value from a vector set. The hyperplane running through \mathbf{v}_i with normal $\mathbf{w}_i = \frac{\mathbf{v}_i - \mathbf{v}_\perp}{\|\mathbf{v}_i - \mathbf{v}_\perp\|_2}$ is tangential to the geometric convex hull. Hence \mathbf{v}_i is the optimal value for the weight \mathbf{w}_i and following the CHVI policy in Equation (2.75) will give the desired value \mathbf{v}_i .

```

1 def sample_catagorical(f):
2     threshold ~ Uniform(0,1)
3     i = 0
4     accumulated_mass = 0
5     while (accumulated_mass < threshold):
6         i += 1
7         accumulated_mass += f(i)
8     return i

```

Listing 2.2: Psuedocode for naively sampling from a catagorical distribution.

Some of the work in this thesis will involve sampling from catagorical distributions, and sometimes it will be helpful to do so efficiently, as in Chapter 4. Let $f : \{C_1, \dots, C_m\} \rightarrow [0, 1]$ be the probability mass function of a catagorical distribution with m categories. Suppose that we want to sample $c \sim f$. A naive method to sample from f will take $O(m)$ time, where a continuous uniform random value is sampled, $u \sim \text{Uniform}(0, 1)$, and f is linearly scanned until a probability mass of u has been passed. See Listing 2.2 for psuedocode of the naive method.

However, the *alias method* [31, 30] can instead be used to sample from a catagorical distribution. The alias method uses $O(m)$ preprocessing time to construct an *alias table*, and after can sample from f , using the table, in $O(1)$ time. An alias table consists of m entries, accounting for an m th of the probability mass


```

1 def sample_from_alias_table(alias_table):
2     index ~ Uniform({1, ..., m})
3     (c0, c1, thrsh) = alias_table[index]
4     u ~ Uniform(0, 1)
5     if (u <= thrsh):
6         return c0
7     return c1

```

Listing 2.3: Psuedocode for sampling from an alias table.

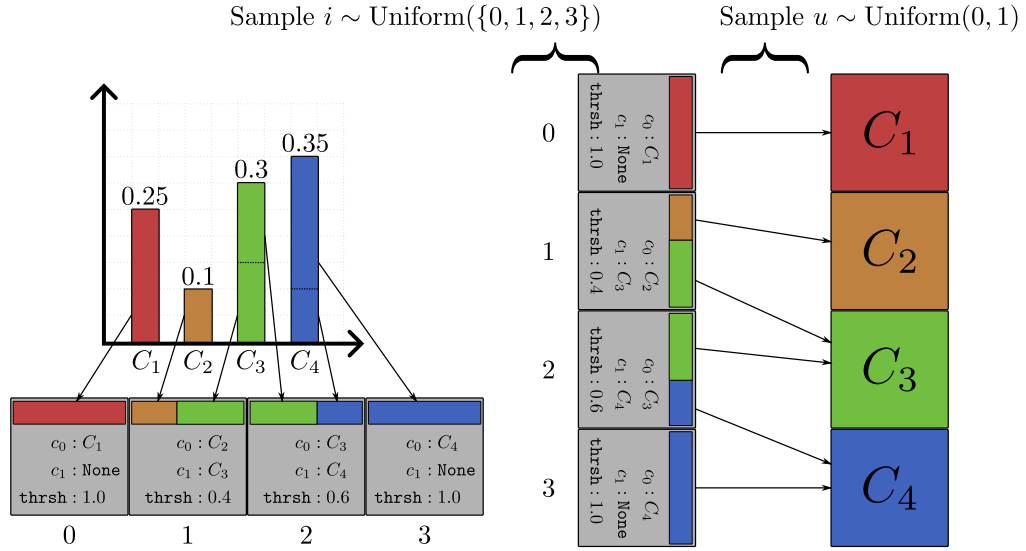


Figure 2.15: Example of building and sampling from an alias table, on a distribution with four categories. Left: shows how the probability mass is split into the four entries of the table. Right: shows how two random variables can be used to sample from the table in $O(1)$ time, where i is used to index into the table, and u is used to compare with thrsh and decide which of the two arrows from the entry to follow.

of f . Each entry takes the form (c_0, c_1, thrsh) , where $c_0, c_1 \in \{C_1, \dots, C_m\}$ are categories and $\text{thrsh} \in [0, 1]$ gives the ratio of the $\frac{1}{m}$ probability mass to assign to c_0 and c_1 . Sampling from the alias table can be performed by sampling two random numbers, one to index into the table and one to compare against thrsh , from which $c \sim f$ can be returned by looking it up in the table. Listing 2.3 gives psuedocode for sampling from an alias table, and Figure 2.15 visualises the construction and sampling of an alias table.

Vose [30] proves that an alias table can always be constructed from an arbitrary catagorical distribution, such that the probability of sampling any catagory from the alias table is identical to the probability of sampling it from the original probability mass function.

```

1  def build_alias_table(f):
2      # lists of categories and mass remaining
3      small = []
4      big = []
5
6      # fill big and small lists
7      for c in f:
8          if f(c) >  $\frac{1}{m}$ :
9              big.append((c, f(c)))
10             else:
11                 small.append((c, f(c)))
12
13     # construct alias table
14     alias_table = []
15     while len(small) > 0:
16         # create entry
17         c0, c0_mass_remaining = small.pop()
18         if mass_remaining ==  $\frac{1}{m}$ :
19             alias_table.append((c0, None, 1.0))
20             continue
21         c1, c1_mass_remaining = big.pop()
22
23         # add entry to table (accounting for 1/mth of total mass)
24         thrsh = m * c0_mass_remaining
25         alias_table.append((c0, c1, thrsh))
26
27         # put c1 back in lists appropriately
28         c1_mass_remaining -= c0_mass_remaining
29         if c1_mass_remaining >  $\frac{1}{m}$ :
30             big.append((c1, c1_mass_remaining))
31         else:
32             small.append((c1, c1_mass_remaining))
33
34     return alias_table

```

Listing 2.4: Psuedocode for constructing an alias table.

Psuedocode for constructing an alias table is given in Listing 2.4, following [31, 30]. An alias table can be constructed by keeping two sets of categories, one set for “big” categories that currently have more than $\frac{1}{m}$ mass to be added to the table, and one for “small” catagories that have at most $\frac{1}{m}$ mass left to be added to the table. To create a new entry in the table, take one category from the small set, and take a category from the big set to complete the remainder of the $\frac{1}{m}$ mass that the small set didn’t fill. After creating a new entry, move the big category to the little set if it no longer has more than $\frac{1}{m}$ mass to be added.

3

Literature Review

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TODO: currently this is a copy and paste of what I originally wrote for background chapter 2. Deleted parts which are irrelevant for litreview here (and vice versa for the background section).

TODO: I'm also going to use this as a space to paste papers I should write about as they come up while writing later chapters

3.1 Multi-Armed Bandits

TODO: Maybe dont need to cover this in litrev, but should talk about exploring bandits, UCT and contextual bandits either in background or in litrev

TODO: linUCB for contextual bandits think this is the linucb paper: <https://arxiv.org/pdf/1003>

Designing multi-objective multi-armed bandits algorithms: a study - Madalina

M. Drugan and Ann Nowe

TODO: MAB book

Talk about Exp3?

3.2 Reinforcement Learning

TODO: Intro should say that look at Sutton and Barto and something else for deep RL, for a more complete overview. Here we will just discuss papers that consider entropy in their work, as that's the most relevant part for this thesis.

TODO: list

- Talk about entropy and some of that work (probably a subsection)

TODO: In the entropy bit talk add this, removed from ch2: Note that there are other forms of entropy, such as relative and Tsallis entropy, which can be used in place of Shannon entropy (TODO cite). For the work considered in this thesis, the other forms of entropy can be used by replacing the definition of \mathcal{H} by the relevant definition.

TODO: talk about some deep learning methods here

3.3 Trial-Based Heuristic Tree Search and Monte-Carlo Tree Search

TODO: talk about UCT, and multiarmed bandits. Specifically that the theoretical lower bound is $\log T$ and UCT achieves $\log T$ lower bound. Define cumulative regret here.

3.3.1 Trial Based Heuristic Tree Search

TODO: THTS paper, talk about the differences that the paper has to our presentation of THTS++

TODO: cut from ch2: Finally we will briefly point out the differences between THTS++ and the original THTS schema in subsection

TODO: talk about how these methods are still relevant with deep learning because of algorithms that use both, such as alpha zero

3.3.2 Monte-Carlo Tree Search

TODO: list

- Talk about the things that are ambiguous from literature (e.g. people will just say UCT, which originally presented doesn't run in `mcts_mode`, but often assumed it does)
- Should talk about multi-armed bandits here?

<https://inria.hal.science/inria-00164003/document>

<https://pdf.sciencedirectassets.com/271585/1-s2.0-S0004370211X0005X/1-s2.0-S000437021100052X/main.pdf?X-Amz-Security-Token=IQoJb3JpZ2luX2VjEOP>

TODO: removed from ch2, this can be litrev: add polynomial UCT here? and or prioritised UCT from alpha go here?

TODO: removed from ch2: add stuff about regret here, give the $O(\log n)$ bound for UCT, and also talk about the papers that

3.3.3 Maximum Entropy Tree Search

TODO: MENTS, RENTS and TENTS

3.4 Multi-Objective Reinforcement Learning

TODO: list

- Should talk about multi-objective and/or contextual multi-armed bandits here?
- Bunch of the work covered in recent MORL survey [12]
- Mention some deep MORL stuff, say that this work (given AlphaZero) is adjacent work

TODO: removed from ch2: comment here or in literature review about there being more types of scalarization function that aren't necessarily weighted by a weight, and ESR vs SER stuff

TODO: talk about more of the MORL survey, including some of the other motivating scenarios

TODO: Talk about the better way of doing CHVI? <https://www.jmlr.org/papers/volume13/lizotte12a> and Efficient reinforcement learning with multiple reward functions for randomized controlled trial analysis. Also by Lizotte. But also say that its approximate for $D > 2$ and so we stick with the slower one? But the CHVS operations can be computed more efficiently in $D = 2$ using this stuff. Did it for the python implementation.

TODO: also need to talk about the MO sequential decision survey. Define Pareto Front. Say that the Pareto Front "Definition 3 If the utility function u is any monotonically increasing function, then the Pareto Front (PF) is the undominated set [Roijers et al., 2013]:"

TODO: need to talk about this because some prior/related work uses PF rather than CH

TODO: cover some inner loop and outer loop things? Roijers computing CCS work? See what MORL survey says about it

TODO: Maybe talk about the *witness algorithm* for Partially Observable MDPs as its very similar to CHVI stuff

Ann Nowe papers:

<https://www.jmlr.org/papers/volume15/vanmoffaert14a/vanmoffaert14a.pdf>

<https://arxiv.org/pdf/2402.07182>

<https://www.ifaamas.org/Proceedings/aamas2024/pdfs/p1611.pdf>

TODO: Go through Roijers and Ann Nowe and Mykel Kochenderfer

TODO: Deep MORL things in MO-gymnasium

TODO: Some of the outer and inner loop things - prism, computing convex coverage sets

3.5 Multi-Objective Monte Carlo Tree Search

TODO: I think this whole section can just go in litrev

TODO: list

- Define the old methods (using the CH object methods, so clear that not doing direct arithmetic)
- Mention that old method could be written using the arithmetic of CHMCTS (but they don't)
- TODO: write about & make sure its implemented - its because just updating for 1 is more efficient in deterministic, and say that the additions can be implemented as updating for 1 value when deterministic
- Different flavours copy UCT action selection, but with different variants
- Link back to contributions and front load our results showing that all of the old methods don't explore correctly

TODO: There has been some prior work in multi-objective MCTS which we will outline here

TODO: Write out implementations of prior works using THTS

TODO: define pareto front

TODO: perez algorithms

TODO: <https://ieeexplore.ieee.org/document/8107102>

TODO: <https://www.roboticsproceedings.org/rss15/p72.pdf> TODO: <https://arxiv.org/abs/211>

TODO: <https://proceedings.mlr.press/v25/wang12b/wang12b.pdf>

TODO: <https://ifmas.csc.liv.ac.uk/Proceedings/aamas2021/pdfs/p1530.pdf> TODO: <https://link.springer.com/article/10.1007/s10458-022-09596-0>

TODO: Some stuff we wrote that didnt use in ch2. Might want to talk about it with eval:

Moreover, in the case of MCTS algorithms, by having the user select a preferred policy, it implicitly forces the user to chose a preference over the objectives, as the

policy corresponds to a weight vector that it is optimal for. As MCTS algorithms are often used in an online fashion, where planning is interleaved with execution, this implicitly selected weight can be used for any online execution needed, effectively reducing the multi-objective problem into a single-objective problem.

4

Monte Carlo Tree Search With Boltzmann Exploration

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This chapter discusses MCTS algorithms for planning in single-objective environments whose search policies take the form of Boltzmann distributions. Primarily, this chapter aims to answer question **Q1.1 - Entropy**, while laying the foundation to answer **Q1.2 - Multi-Objective Exploration** in Chapter 6.

Figure 4.1 gives the exploration setting for reinforcement learning, where the agent is only assessed on the recommendations that it provides, and is not penalised

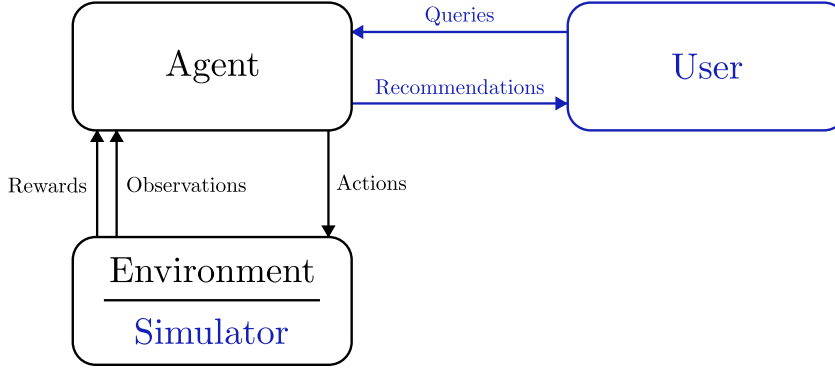


Figure 4.1: **TODO:** update fig to just be the blue version. Exploration setting in reinforcement learning (**TODO:** reproduced and edited from fig 2.5), **BD:** where the agent aims to discover the optimal policy and has a larger emphasis on exploration to find better solutions rather than exploiting.

for considering poor actions in the simulator.

This chapter will also consider how entropy can be used as an auxiliary secondary objective to encourage exploration. Entropy is already used widely in the reinforcement literature **TODO:** cites, ppo, sac etc, ref ch3, and is often cited for its **BD:** exploration, and robustness to uncertainty, and robustness to simulator/environment differences, and robustness to noise.

When considering the maximum entropy reinforcement learning objective (**TODO:** ref), the optimal policy (equation (**TODO:** ref)) naturally takes the form of a Boltzmann policy. Notably, MENTS (Section 2.4.4), and RENTS and TENTS (Section **TODO:** ref litrev) are existing MCTS algorithms for the maximum entropy setting (Section 2.3.1), so will be discussed further in this chapter, along with UCT (Section **TODO:** ref), and used as baseline algorithms.

Section 4.1 discusses limitations of existing MCTS algorithms in this exploration setting, motivating the work covered in the remainder of the chapter. Additionally, the planning framework is defined so that the algorithms can be theoretically analysed using *simple regret*.

In Section 4.2 the *Boltzmann Tree Search* and *Decaying Entropy Tree Search* algorithms are defined.

Section 4.3 considers some theoretical MDPs, which are used to empirically demonstrate the limitations of the existing MCTS algorithms, and are used for

constructive proofs of some theorems.

Results on grid world and the game of Go are given in section 4.4.

Finally, in Section 4.5 the main theoretical analysis and proofs are given.

TODO: add sect 4.6 if actually use that.

TODO: one paragraph for ch overview? Or make other descriptions longer?

Or make it bullet points?

TODO: After finished writing, do another pass through neurips paper and check no results/writing missing from thesis that really should be included. (Thinking about some of the frozen lake plots in the appendix when writing this.)

4.1 Introduction and Motivation

UCT TODO: ref BD: is designed in the traditional reinforcement learning setting (todo ref Fig 2.5), minimising the cumulative regret (todo ref), and so UCT makes a trade off between exploration and exploitation. As such, UCT will frequently choose the same action to exploit, which results in it getting stuck in local optima when BD: rewards are sparse or not informative.

To see this consider two grid world MDPs which differ only in the reward function. TODO: state space is (x,y,time), actions are cardinal directions etc. The first reward function is to use a constant cost of $R_1(s, a) = -1$, and the second is a sparse version where the time cost is only revealed at the end $R_2((x, y, t), (x_a, y_a)) = -(t + 1)\mathbb{1}[(x, y) + (x_a, y_a) == G]$. TODO: clean and actually define goal state, and name better than R1 and R2

TODO: make diagram

TODO: something that says although this example can be solved by using the more sensible reward, it's just to highlight the issue of exploration.

TODO: would like to have figs showing the best path found by UCT in both cases AND showing the number of trials (one step of branches) where it explored.

Although the issues in the above toy problem can be resolved by using the simpler constant reward R_1 , the example serves to highlight that UCT performs best when provided with a dense and informative reward.

As we are considering the exploration setting given in Figure 4.1, this example shows in the sparse reward setting that UCT will use most of its available computation time exploiting the same sub-optimal solution that it has already found. As the objective is to provide the best recommendations to the user, it would be desirable to better utilise this computation time exploring alternative solutions.

TODO: reword this sect, not super hapy with it

TODO: some comment somewhere that although it does seem a little unfair to compare UCT in a scenario for which it was not designed, in practise it is used in these cases

This example is extended upon in Section TODO: ref where the performance of algorithms discussed in this chapter are compared on mixtures of these two rewards.

Now that some limitations of UCT have been discussed, lets now consider the maximum entropy objective. When using the maximum entropy objective it is often argued that the standard objective can be recovered by setting $\alpha = 0$, or setting α to an infitesimally small values ($0 < \alpha \ll 1$). TODO: add refs TODO: add the words “temperature” somewhere

However, in practise setting α to some tiny value will nullify any advantages that can be obtained from using entropy to promote exploration. Considering the other extreme, if we allowed a very large value of α (or let $\alpha \rightarrow \infty$), then maximising entropy becomes the dominant objective and the ‘optimal’ policy will be a uniformly random one. Thus there is some tradeoff that needs to be made. When using a maximum entropy method the temperature parameter needs to be tuned: which intuitively should be made as large as possible, so as to obtain as much benefit from entropy exploration; while keeping it small enough such that policy acts as desired (i.e. it maximises the standard objective).

TODO: supp expr on gridworld shortest path problem, where vary alpha value

In Figure TODO: ref, the performance of MENTS (TODO: ref) on the above gridworld problem with sparse reward is considered (Figure TODO: ref). As the value of α is increased from zero, it can be seen the shortest path is found with fewer and fewer trials initially. Then, above a threshold value of TODO: quote value, MENTS

can gain more “reward” by acting randomly and optimising for entropy, largely ignoring the rewards from the MDP. This example empirically demonstrates an issue with using the maximum-entropy objective, where the temperature parameter needs to be finely tuned to a sweet-spot for it to be effective.

More concretely, consider the policy $\pi_{\text{eval}}(s) = \arg \max_{a'} \pi_{\text{sft}}^*(a'|s)$ that would be followed at test time with the maximum entropy objective. In the following, the maximum entropy objective will be said to be *misaligned* with the standard objective when $\pi_{\text{eval}}(s) \neq \pi^*(s)$.

Building off this intuition, in Section [TODO: ref](#), an MDP is constructed such that the temperature parameter needs to be made prohibitively small (i.e. little to no benefit is gained from the entropy rewards) to avoid the maximum entropy objective from being missaligned.

While only MENTS has been discussed, the issue lies predominantly from mixing entropy into the scalar objective, and as such similar issues arise no matter the form of entropy considered. [TODO: basically saying RENTS and TENTS dont fix this problem](#)

Now *simple regret* is defined, which will be used motivate and analyse the algorithms developed. The simple regret of a policy is the difference between the value of the policy and optimal value of the policy ([TODO: ref the equation below](#)). By definition, the optimal policy achieves a simple regret of zero, and an MCTS algorithm is considered *consistent* if it’s expected simple regret tends to zero. In plain english, an algorithm is consistent if left to run forever it would eventually output an optimal policy. An implication of consistency is that if an algorithm can be run for longer, then it is expected to improve on its solution.

[TODO: Talk about the setup we’re using. Probably want to try motive similarly to DENTS paper, and recall the diagram from 2.3. TODO: Say that in fig below that normally step 3 is not considered](#)

[TODO: make this a proper def](#) Simple regret of a policy ψ is then defined as

$$\text{sim_regr}(s, \psi) = V^*(s) - V^\psi(s). \quad (4.1)$$

Parameters: An MDP \mathcal{M} .

- For each round $m = 1, 2, \dots$:
 1. the agent produces a search policy π^m to follow;
 2. the environment samples a trajectory $\tau \sim \pi^m$ (including rewards $r_t = R(s_t, a_t)$ for each s_t, a_t pair in τ);
 3. the agent produces a recommendation policy ψ^m ;
 4. if the environment sends a stop signal, then the game ends, otherwise the next round starts.

Figure 4.2: The procedure of an exploring planning problem for MDPs. **TODO:** Make this sound better. **TODO:** Also make ch2 MAB figs use enumerate?

TODO: make this a proper def An agent, that produces recommendation policies ψ^1, ψ^2, \dots is said to be *consistent* if $\mathbb{E}[\text{sim_regr}(s, \psi^m)] \rightarrow 0$ as $m \rightarrow \infty$.

Returning to the discussion around UCT and MENTS now that simple regret and consistency has been defined. It can be shown the UCT is always consistent **TODO:** ref?, although MDPs can be constructed where it requires a hyperexponential amount of time to find the optimal policy. Whereas, the consistency of MENTS depends on if the temperature parameter is sufficiently small for the optimal soft policy to not be misaligned with the standard optimal policy. Moreover, the threshold for the temperature parameter is dependent on the MDP, and so needs to be tuned on every MDP instance separately.

From the discussion in this section, the following properties are desired from the MCTS algorithms:

- define algorithms that are as simple to implement as UCT and MENTS;
- able to utilise dense and informative rewards (UCT ✓, MENTS ✓);
- effectively explore when rewards are sparse, or have sparse components (UCT ✗, MENTS ✓);
- are consistent, for parameters independent of the environment (UCT ✓, MENTS ✗). **TODO:** something like can get a reasonable result without

having to tune params on each env. Maybe “doesn't require parameter tuning on every environment”

As such, this chapter will consider how entropy can be used as an additional secondary objective, while still focusing on performing well in the standard objective. TODO: place this better. Want it to say, that because the issue lies in the maximum entropy objective, we're going to start by stripping MENTS of the maximum entropy objective and then consider how it can be reintroduced in a consistent way.

4.2 Boltzmann Search

TODO: list

- Recall MENTS
- Define BTS using THTS functions
- Define DENTS using THTS functions
- Discuss alias method variant (and complexity analysis) in a subsection?

TODO: would like to read more about the exp3 stuff before submitting this ch TODO: <https://tor-lattimore.com/downloads/book/book.pdf> - bandits book
 TODO: exp3 paper: <http://rob.schapire.net/papers/AuerCeFrSc01.pdf> TODO: add to future work ideas to adapt BTS to use exp3 type stuff, and the thing gradient update covered in the Sutton and Barto book (todo get link and page ref to RL book where talk about that) TODO: moved already

This section defines two algorithms Boltzmann Tree Search and Decaying ENTropy Tree Search in the THTS++ schema.

4.2.1 Boltzmann Tree Search

TODO: define BTS in thtsp

TODO: Define with variable alpha, change proofs to say for fixed alpha get regret bound. And add theorem that

Our first approach, put simply, replaces the use of soft values in MENTS with *Bellman* values. We call this algorithm *Boltzmann Tree Search* (BTS). The search policy π_{BTS} and backups for the n th trial are given by:

This section introduces the *Boltzmann Tree Search* (BTS) algorithm, presented in terms of the THTS++ schema [TODO: ref](#). BTS promotes exploration through the stochastic Boltzmann search policy, like MENTS [TODO: ref](#), while using backups that optimise for the standard objective, like UCT [TODO: ref](#). Unlike MENTS, the temperature parameter generalised to a function $\alpha_{\text{BTS}}(x) > 0$, which allows the temperature to vary with the number of times that a node has visited. BTS uses Bellman value estimates at each node \hat{V}_{BTS} and \hat{Q}_{BTS} . The search policy is defined by:

$$\pi_{\text{BTS}}(a|s) = (1 - \lambda(s, \epsilon_{\text{BTS}}))\rho_{\text{BTS}}(a|s) + \frac{\lambda(s, \epsilon_{\text{BTS}})}{|\mathcal{A}|}, \quad (4.2)$$

$$\rho_{\text{BTS}}(a|s) \propto \exp\left(\frac{1}{\alpha_{\text{BTS}}(N(s))} (\hat{Q}_{\text{BTS}}(s, a))\right). \quad (4.3)$$

$$\lambda(s, x) = \min\left(1, \frac{x}{\log(e + N(s))}\right) \quad (4.4)$$

where $\epsilon_{\text{BTS}} \in (0, \infty)$ is an exploration parameter and $\alpha_{\text{BTS}}(x)$ is the search temperature schedule. [TODO: Add a comment about defining rho as taking the max when N\(s\) is zero?](#) And given a trajectory $\tau = (s_0, a_0, r_0, \dots, s_{h-1}, a_{h-1}, r_{h-1}, s_h)$ the value estimates are updated for $t = h - 1, \dots, 0$:

$$\hat{Q}_{\text{BTS}}(s_t, a_t) \leftarrow R(s_t, a_t) + \sum_{s' \in \text{Succ}(s_t, a_t)} \left(\frac{N(s')}{N(s_t, a_t)} \hat{V}_{\text{BTS}}(s') \right), \quad (4.5)$$

$$\hat{V}_{\text{BTS}}(s_t) \leftarrow \max_{a \in \mathcal{A}} \hat{Q}_{\text{BTS}}(s_t, a). \quad (4.6)$$

In line with the THTS++ schema, the values of $\hat{V}_{\text{BTS}}(s)$ and $\hat{Q}_{\text{BTS}}(s, a)$ are initialised using the arbitrary functions \hat{V}_{init} and \hat{Q}_{init} , which for example can be set to a constant value or be the output from a neural network. [TODO: check all of the above definition is in line with thtspp definition](#)

When BTS needs to recommend a policy, it can use it's Q-value estimates:

$$\psi_{\text{BTS}}(s) = \arg \max_{a \in \mathcal{A}} \hat{Q}_{\text{BTS}}(s, a). \quad (4.7)$$

Alternatively, the node visit counts can be used in the recommendation policy

$$\mathbf{mv}_{\text{BTS}}(s) = \arg \max_{a \in \mathcal{A}} N(s, a). \quad (4.8)$$

TODO: Find better notation for this?

As BTS uses Bellman backups, it can be guaranteed that the BTS recommendation policy converges to the optimal standard policy. **TODO:** make this sound better given we're also talking about most visited recommendation policy now.

TODO: Work out how best to add the AR-BTS stuff?

Additionally, this search policy can still be used with average returns. The following is a summary of the definitions for *Boltzmann Tree Search with Average Returns* (AR-BTS), which uses the value estimates of $\hat{V}_{\text{AR-BTS}}$ and $\hat{Q}_{\text{AR-BTS}}$ at each node, and temperature schedule $\alpha_{\text{AR-BTS}}(x) > 0$:

$$\pi_{\text{AR-BTS}}(a|s) = (1 - \lambda(s, \epsilon_{\text{AR-BTS}}))\rho_{\text{AR-BTS}}(a|s) + \frac{\lambda(s, \epsilon_{\text{AR-BTS}})}{|\mathcal{A}|}, \quad (4.9)$$

$$\rho_{\text{BTS}}(a|s) \propto \exp \left(\frac{1}{\alpha_{\text{AR-BTS}}(N(s))} \left(\hat{Q}_{\text{AR-BTS}}(s, a) \right) \right). \quad (4.10)$$

where $\epsilon_{\text{AR-BTS}} \in (0, \infty)$ is an exploration parameter and $\alpha_{\text{AR-BTS}}(x)$ is the search temperature schedule. Given a trajectory $\tau = (s_0, a_0, r_0, \dots, s_{h-1}, a_{h-1}, r_{h-1}, s_h)$ and the leaf node value estimate $\tilde{r} = \hat{V}_{\text{init}}(s_h)$, the value estimates are updated for $t = h - 1, \dots, 0$:

$$\hat{Q}_{\text{AR-BTS}}(s_t, a_t) \leftarrow \frac{1}{N(s_t, a_t)} \left((N(s_t, a_t) - 1)\hat{Q}_{\text{AR-BTS}}(s_t, a_t) + \tilde{r} + \sum_{i=t}^{h-1} r_i \right) \quad (4.11)$$

$$\hat{V}_{\text{AR-BTS}}(s_t) \leftarrow \frac{1}{N(s_t)} \left((N(s_t) - 1)\hat{V}_{\text{AR-BTS}}(s_t) + \tilde{r} + \sum_{i=t}^{h-1} r_i \right). \quad (4.12)$$

Similarly to BTS, either the Q-value estimates can be used for a recommendation policy or the most visited child node can be used:

$$\psi_{\text{AR-BTS}}(s) = \arg \max_{a \in \mathcal{A}} \hat{Q}_{\text{BTS}}(s, a), \quad (4.13)$$

$$\mathbf{mv}_{\text{AR-BTS}}(s) = \arg \max_{a \in \mathcal{A}} N(s, a). \quad (4.14)$$

TODO: Still find better notation for this?

In Section **TODO: ref** convergence results about BTS and AR-BTS are given, which are summarised below:

- BTS is consistent and converges for any setting of parameters;
- if $\alpha_{\text{BTS}}(x) \geq L > 0$: BTS converges with an theoretical exponential rate;
- if $U \geq \alpha_{\text{AR-BTS}}(x)$ and $\alpha_{\text{AR-BTS}}(x) \rightarrow 0$: AR-BTS converges;

noting that these results are independent of all of the other parameters, including which of the two recommendation policies are used.

TODO: Add theorems here? Or just reference theorems?

TODO: Is the upper bound needed for arbts? Revisit these after having written the proofs up.

4.2.2 Decaying ENtropy Tree Search

TODO: add label TODO: define DENTS in thtspp

Decaying ENtropy Tree Search (DENTS) extends the BTS algorithm by introducing *entropy estimates*. In DENTS nodes have a secondary entropy value estimate, $\bar{\mathcal{H}}_{V,D}$ and $\bar{\mathcal{H}}_{Q,D}$, which are monte carlo estimates the entropy of the search policy rooted from the relevant node. By keeping a separate estimate for entropy, DENTS is able to use entropy in it's search policy, and discard it for recommendations.

Given a trajectory $\tau = (s_0, a_0, r_0, \dots, s_{h-1}, a_{h-1}, r_{h-1}, s_h)$, the entropy values are updated as follows for $t = h - 1, \dots, 0$:

$$\bar{\mathcal{H}}_{V,D}(s_t) \leftarrow \mathcal{H}(\pi_D(\cdot|s_t)) + \sum_{a \in \mathcal{A}} \pi_D(a|s_t) \bar{\mathcal{H}}_{Q,D}(s_t, a), \quad (4.15)$$

$$\bar{\mathcal{H}}_{Q,D}(s_t, a_t) \leftarrow \sum_{s' \in \text{Succ}(s_t, a_t)} \frac{N(s')}{N(s_t, a_t)} \bar{\mathcal{H}}_{V,D}(s'), \quad (4.16)$$

where \mathcal{H} is the Shannon entropy function. TODO: sentence about how the entropy values are initialised $\bar{\mathcal{H}}_{V,D}(s) \leftarrow 0$.

The entropy values are used as an exploration bonus in the search policy, and are weighted by a non-negative function $\beta_D(x) \geq 0$. Generally this will be set to a function such that $\beta_D(x) \rightarrow 0$ as $x \rightarrow \infty$ and will achieve better theoretical

performance in this case. The DENTS search policy π_D is defined follows:

$$\pi_D(a|s) = (1 - \lambda(s, \epsilon_D))\rho_D(a|s) + \frac{\lambda(s, \epsilon_D)}{|\mathcal{A}|}, \quad (4.17)$$

$$\rho_D(a|s) \propto \exp\left(\frac{1}{\alpha_D(N(s))} \left(\hat{Q}_D(s, a) + \beta(N(s))\bar{\mathcal{H}}_{Q,D}(s, a)\right)\right). \quad (4.18)$$

And finally, given the the trajectory τ the Bellman value estimates for DENTS, \hat{V}_D and \hat{Q}_D are updated identically to BTS for $t = h - 1, \dots, 0$:

$$\hat{Q}_D(s_t, a_t) \leftarrow R(s_t, a_t) + \sum_{s' \in \text{Succ}(s_t, a_t)} \left(\frac{N(s')}{N(s_t, a_t)} \hat{V}_{\text{BTS}}(s') \right), \quad (4.19)$$

$$\hat{V}_D(s_t) \leftarrow \max_{a \in \mathcal{A}} \hat{Q}_{\text{BTS}}(s_t, a), \quad (4.20)$$

TODO: also give the recommendation policies

TODO: Write about AR-DENTS here? My brain is getting bored copying and slightly editing things. this is just copying dents and then copying the value backups from ar-bts

Section TODO: ref also provides convergence results about DENTS and AR-DENTS are given, which are summarised below:

- When using the TODO: default? Bellman? recommendation policy:
 - DENTS is consistent and converges for any setting of parameters;
 - if $\alpha_D(x) \geq L > 0$: DENTS converges with an theoretical exponential rate;
 - if $U \geq \alpha_{\text{DENTS}}(x)$ and $\alpha_{\text{AR-BTS}}(x) \rightarrow 0$: AR-BTS converges;
- When using the most visited recommendation policy, the same results hold, but additionally requires $\beta_D(x) \rightarrow 0$.

TODO: Add theorems here? Or just reference theorems?

TODO: Double check these after having written up the proofs. Particularly the differences between using the two different recommendation policies.

4.2.3 Advantages of Stochastic Search Policies

Using a stochastic search policy in MCTS (or THTS++) provides more benefits than just encouraging exploration through randomly sampled actions. In particular, the Alias Method (Section 2.6) can be used to trade off using the most up to date policy for computational speed. Moreover, when prior knowledge (in the form of a policy prior) is available **TODO: cite alphago etc**, it can naturally be integrated into the search using a *mixture policy*.

TODO: add ref to Q2.1 - Complexity

The Alias Method in MCTS

When using the Alias Method in THTS++ an alias table **TODO: capitalise?** is constructed at every decision node. This table can be updated every $\lambda|\mathcal{A}|$ visits to the node, for an arbitrary $\lambda \in \mathbb{R}_{>0}$, giving an amortised complexity of $O(1)$. **TODO: just say constant amortised complexity?** $O(O(1) + \frac{|\mathcal{A}|}{\lambda|\mathcal{A}|}) = O(O(1) + \frac{1}{\lambda}) = O(1)$. **TODO: probably dont need to do that maths.** In THTS++ the value of the λ can be varied to adjust the trade off between The value of lambda can be varied to adjust the trade off between up-to-dateness and sampling speed. For the remainder **TODO: find a better way of saying this**, $\lambda = 1$ will be considered **TODO: but all of the results still hold**. Note that when a new decision node is constructed and added to the tree, there will still be a cost of $O(|\mathcal{A}|)$ to construct the new alias table.

Although this will always lead to quite a significant computational speedup, in the case where `mcts_mode`, the computational speedup is also asymptotic. **TODO: where this paragraph go?**

In the following, the computational complexity to run n trials is considered.

First consider the computational complexity of running UCT: at each decision node visited on a trial, the maximum over $|\mathcal{A}|$ values is computed **TODO: this is worded poorly**, on each trial at most $H_{\text{THTS++}}$ decision nodes will be visited. Hence, the computational complexity of running n trials of UCT is $O(nH_{\text{THTS++}}|\mathcal{A}|)$.

TODO: copy out appendix C stuff, cleaning up above and below as needed

Finally, considering the case when THTS++ is not running in `mcts_mode`, the asymptotic complexity is still $O(nH_{\text{THTS++}}|\mathcal{A}|)$, as each trial is sampled until the planning horizon $H_{\text{THTS++}}$

TODO: Talk about co

TODO: add label TODO: write about alias sampling

Encorporating Prior Knowledge Through Mixture Policies

Let π be some THTS++ search policy, and supposed that we have access to another policy $\tilde{\pi}$ with prior knowledge, such as a neural network. Then a new search policy π_{mix} can be naturally be defined using a mixture of π and $\tilde{\pi}$.

TODO: some comment about just using the same mixing function as before ... because? .. it lets it tend towards the correct thing

The mixture policy is defined by:

$$\pi_{\text{mix}}(a|s) = (1 - \lambda(s, \epsilon_{\text{mix}}))\pi(a|s) + \lambda(s, \epsilon_{\text{mix}})\tilde{\pi}(a|s), \quad (4.21)$$

where λ is the same function as defined in equation (TODO: ref), and $\epsilon_{\text{mix}} \in (0, \infty)$ weights the amount to use the prior knowledge by. TODO: word better.

TODO: are there theoretical results? Maybe we can show that for arbitrary function that it doesnt change anything. It should be the same as mixing in the uniform. Also another good reason to use the same function, because then the proof is basically the same thing as before.

TODO: write about using $\tilde{\pi}$, \tilde{Q} , \tilde{V} ? TODO: talk about grid world and how Qinit need to be able to handle costs

TODO: discuss the MENTS intiialisation here? : MENTS suggests using $\tilde{\pi}$ as TODO: their description However, this may still lead to issues in for example in grid world problems. TODO: talk about

4.2.4 Things still missing in this section

Defining the average reward versions of the algorithms

TODO: Talking about the OG DENTS algorithm and why that didn't work? I feel like its a reasonable question

4.3 Toy Environments

TODO: list

- Define D-chain stuff from the paper
- Define the D-chain with entropy trap
- Front load some results still

TODO: (commented out below this), original writing in the motivation section, which talked about the d-chain environment.

4.4 Empirical Results

TODO: list

- DChain
- GridWorlds
- Go

- Get some better results using hyperparam optimise - want a dense env where the (not entropy) temp decay fn gets optimised to something that decays a lot - want a sparse env where the temp decay fn gets optimised to something flat (or basically flat)

TODO: TWO: would like to have experiments which vary the proportion of the sparse reward. So have FL(λ), where λ specifies the ratio between the dense and sparse rewards. Then investigate what happens as vary λ . So this is the grid world experiments run again,

4.5 Theoretical Results

TODO: list

- add theoretical results

Should we try to add a result about most visited? Where will be concentration bounds around the number of visits being proportional to the values. So think can bootstrap those proofs.

- Generalise the AR proof to say that for decaying search functions still work (as long as they are bounded) - Have a result that using most visited is theoretically sound

The Neurips paper proof section was structured as follows:

1. First, in Section ?? we revisit MCTS as a stochastic process, defining some additional notation that was not useful in the main body of the paper, but will be for the following proofs;
2. Second, in Section ?? we introduce preliminary results, that will be useful building blocks for proofs in later Theorems;
3. Third, in Section ?? we show some general results about soft values that will also be useful later;
4. Fourth, in Section ?? simple regret is then revisited, and we show that any bounds on the simple regret of a policy are equivalent to showing bounds on the simple regret of an action;
5. Fifth, in Section ?? we show in a general way, that if a value function admits a concentration inequality, then the corresponding Q-value function admits a similar concentration inequality;
6. Sixth, in Section ?? we show concentration inequalities for MENTS about the optimal soft values, and give bounds on the simple regret of MENTS, provided the temperature parameter is sufficiently small;
7. Seventh, in Sections ?? and ?? we also provide concentration inequalities around the optimal standard values for BTS and DENTS, and give simple regret bounds, irrespective of the temperature paramters;

8. Finally, in Section ?? we consider results that are relevant for the algorithms using average returns from Section ??.

TODO: above is note taking and below is me starting to write the proofs stuff

TODO: Some comment about using a policy of the form XXX will be referred to a Boltzmann MCTS Process.

4.5.1 MCTS As A Stochastic Process

Now the MENTS, BTS and DENTS are written as a stochastic process, where values are indexed (with a superscript) by the number of times that the corresponding node has been visited. For completeness and reference, the stochastic processes for TODO: UCT?, MENTS, BTS and DENTS are given below.

When reasoning about a *MCTS stochastic process* the following notations will be helpful.

- The search policy used on the m th trial is π^m , and if the process were stopped after m trials, the recommendation policy that the algorithm would output is denoted ψ^m . Where if the process is run for n trials, then m ranges from 1 to n .
- The m trajectory sampled is $\tau^m = (s_0^m, a_0^m, \dots, s_{h-1}^m, a_{h-1}^m, s_h^m)$ TODO: add reward, also make it h subscript m instead of h?, and is sampled using the search policy $\tau^m \sim \pi^m$ (that is $a_i^m \sim \pi^m(\cdot | s_i^m)$ and $s_{i+1}^m \sim p(\cdot | s_i^m, a_i^m)$). TODO: comment that k th trial is run until h where s subscript h is terminal in some thtspp sense. Comment about how the superscripts on s a and r will be used when necessary, but not always
- The search tree after m trials is denoted \mathcal{T}^m , the initial search tree is $\mathcal{T}^0 = \{s_0\}$, and $\mathcal{T}^k = \mathcal{T}^{k-1} \cup \tau^k$.

When making arguments that apply to multiple algorithms the general policies π and ψ will be used, and when making arguments about specific algorithms the subscripts will be used, such as π_{BTS} . Note that superscript is used to index

with respect to the trial, and superscript with parenthesis is used to denote the number of visits.

In the proofs of following sections, it will be useful to write the number of times state s was visited in the first m trials as $N(s, m)$, and the number of times action a was selected from state s in the first m trials as $N(s, a, m)$. Additionally, it will be useful to write these quantities in terms of indicator random variables.

Let $T(s_t, m)$ (and $T(s_t, a_t, m)$) be the set of trajectory indices that s_t was visited on (and action a_t selected) in the first m trials, that is: **TODO: this can avoid using s subscript t**

$$T(s_t, m) = \{i | i \leq m, s_t^i = s_t\} \quad (4.22)$$

$$T(s_t, a_t, m) = \{i | i \leq m, s_t^i = s_t, a_t^i = a_t\}. \quad (4.23)$$

This allows the counts $N^m(s_t)$, $N^m(s_t, a_t)$ and $N^m(s_{t+1})$ (with $s_{t+1} \in \text{Succ}(s_t, a_t)$) to be written as sums of indicator random variables in the following ways:

$$N(s_t, m) = \sum_{i=1}^m \mathbb{1}[s_t^i = s_t] = |T(s_t, m)|, \quad (4.24)$$

$$N(s_t, a_t, m) = \sum_{i=1}^m \mathbb{1}[s_t^i = s_t, a_t^i = a_t] = |T(s_t, a_t, m)|, \quad (4.25)$$

$$N(s_t, a_t, m) = \sum_{i \in T(s_t, m)} \mathbb{1}[a_t^i = a_t], \quad (4.26)$$

$$N(s_{t+1}, m) = \sum_{i \in T(s_t, a_t, m)} \mathbb{1}[s_{t+1}^i = s_{t+1}]. \quad (4.27)$$

Additionally, the assumption that for any two states $s, s' \in \mathcal{S}$ **TODO: double check use calligraphic S for state space?** that $s = s'$ if and only if the trajectories leading to them are identical is made. This assumption is purely to simplify notation, so that nodes in the tree have a one-to-one correspondence with states (or state-action pairs). **TODO: move this up**

TODO: do we do anything at all with the UCT process?

The MENTS Process

Below is a complete summary of the MENTS process, for reference. On the m th trial, the MENTS process follows the search policy:

TODO: make ments section in ch2 use consistent definitions of alphaments, lambdaments and so on

$$\pi_{\text{MENTS}}^m(a|s) = (1 - \lambda^m(s, \epsilon_{\text{MENTS}}))\rho_{\text{MENTS}}^m(a|s) + \frac{\lambda^m(s, \epsilon_{\text{MENTS}})}{|\mathcal{A}|}, \quad (4.28)$$

$$\rho_{\text{MENTS}}^m(a|s) = \exp\left(\frac{1}{\alpha_{\text{MENTS}}} \left(\hat{Q}_{\text{MENTS}}^{(N(s,a,m-1))}(s, a) - \hat{V}_{\text{MENTS}}^{(N(s,m-1))}(s)\right)\right). \quad (4.29)$$

$$\lambda^m(s, x) = \min\left(1, \frac{x}{\log(e + N(s, m - 1))}\right), \quad (4.30)$$

where $\epsilon_{\text{MENTS}} \in (0, \infty)$ is an exploration parameters, and α_{MENTS} is the temperature parameter.

The m th trajectory is sampled using the search policy: $\tau^m \sim \pi_{\text{MENTS}}^m$. Letting $\tau^m = (s_0, a_0, r_0, \dots, s_{h-1}, a_{h-1}, r_{h-1}, s_h)$, the MENTS value estimates are computed using backups for $t = h - 1, \dots, 0$: TODO: either add the superscript m into every s and a, or update words to say implicit

$$\hat{V}_{\text{MENTS}}^{(N(s_t, m))}(s_t) = \alpha_{\text{MENTS}} \log \sum_{a \in \mathcal{A}} \exp\left(\frac{1}{\alpha_{\text{MENTS}}} \hat{Q}_{\text{MENTS}}^{(N(s_t, a, m))}(s_t, a)\right), \quad (4.31)$$

$$\hat{Q}_{\text{MENTS}}^{(N(s_t, a_t, m))}(s_t, a_t) = R(s_t, a_t) + \sum_{s' \in \text{Succ}(s, a)} \left(\frac{N(s', m)}{N(s_t, a_t, m)} \hat{V}_{\text{MENTS}}^{(N(s', m))}(s')\right). \quad (4.32)$$

TODO: also want something about initialisation and everything in line with tht-spp

TODO: recommendation policies and some comment about it being the soft values used?

$$\psi_{\text{MENTS}}^m(s) = \arg \max_{a \in \mathcal{A}} \hat{Q}_{\text{MENTS}}^{(N(s, a, m))}(s, a), \quad (4.33)$$

$$\mathbf{mv}_{\text{MENTS}}^m(s) = \arg \max_{a \in \mathcal{A}} N(s, a, m). \quad (4.34)$$

The DENTS Process

TODO: this whole sections math is pretty mess and a struggle to fit onto one line at a time. Maybe it suffices to just wordily describe the values of the suffixed values?

Follow policy: TODO: add more wordy things. Some things we said here before were: (1) defining beta $\beta : \mathbb{R} \rightarrow [0, \infty)$ be a bounded function; TODO: (2) defined

epsilon as exploration policy; (3) in Neurips we defined the propto version of rho and also the full version saying “becasue we need to reason about the search policy we give the exact form,” for the moment I’ve kept both. I think just copy the full version where relevent in the proofs.

$$\pi_D^m(a|s) = (1 - \lambda^m(s, \epsilon_D))\rho_D^m(a|s) + \frac{\lambda^m(s, \epsilon_D)}{|\mathcal{A}|}, \quad (4.35)$$

$$\rho_D^m(a|s) \propto \exp\left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a, m-1))}(s, a) + \beta_D(N(s, m))\bar{\mathcal{H}}_{Q,D}^{(N(s, a, m-1))}(s, a)\right)\right). \quad (4.36)$$

$$\rho_D^m(a|s) = \frac{\exp\left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a, m-1))}(s, a) + \beta_D(N(s, m))\bar{\mathcal{H}}_{Q,D}^{(N(s, a, m-1))}(s, a)\right)\right)}{\sum_{a' \in \mathcal{A}} \exp\left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a', m-1))}(s, a') + \beta_D(N(s, m))\bar{\mathcal{H}}_{Q,D}^{(N(s, a', m-1))}(s, a')\right)\right)}. \quad (4.37)$$

$$\lambda^m(s, x) = \min\left(1, \frac{x}{\log(e + N(s, m-1))}\right), \quad (4.38)$$

The m th trajectory is sampled using the search policy: $\tau^m \sim \pi_{\text{MENTS}}^m$. Letting $\tau^m = (s_0, a_0, r_0, \dots, s_{h-1}, a_{h-1}, r_{h-1}, s_h)$, the DENTS value and entropy estimates are computed using backups for $t = h-1, \dots, 0$: TODO: either add the superscript m into every s and a , or update words to say implicit

$$\hat{Q}_D^{(N(s_t, a_t, m))}(s_t, a_t) = R(s_t, a_t) + \sum_{s' \in \text{Succ}(s_t, a_t)} \left(\frac{N(s', m)}{N(s_t, a_t, m)} \hat{V}_D^{(N(s', m))}(s')\right), \quad (4.39)$$

$$\hat{V}_D^{(N(s_t, m))}(s_t) = \max_{a \in \mathcal{A}} \hat{Q}_D^{(N(s_t, a, m))}(s_t, a), \quad (4.40)$$

$$\bar{\mathcal{H}}_{Q,D}^{(N(s_t, a_t, m))}(s_t, a_t) = \sum_{s' \in \text{Succ}(s_t, a_t)} \frac{N(s', m)}{N(s_t, a_t, m)} \bar{\mathcal{H}}_{V,D}^{(N(s', m))}(s'), \quad (4.41)$$

$$\bar{\mathcal{H}}_{V,D}^{(N(s_t))}(s_t) = \mathcal{H}(\pi_D^m(\cdot|s_t)) + \sum_{a \in \mathcal{A}} \pi_D^m(a|s_t) \bar{\mathcal{H}}_{Q,D}^{(N(s_t, a, m))}(s_t, a). \quad (4.42)$$

TODO: also want something about initialisation and everything in line with tht-spp

TODO: recommendation policies word stuff

$$\psi_D^m(s) = \arg \max_{a \in \mathcal{A}} \hat{Q}_D^{(N(s, a, m))}(s, a), \quad (4.43)$$

$$\mathbf{mv}_D^m(s) = \arg \max_{a \in \mathcal{A}} N(s, a, m). \quad (4.44)$$

TODO: From the neurips, also wrote the following (everything left in this subsection is copied and cleaned up, but probably needs a proof read) Let $\hat{V}_{\rho,D}^{(N(s))}(s)$ be defined as the value:

$$\hat{V}_{\rho,D}^{(N(s))}(s) = \alpha_D(N(s, m)) \log \left[\sum_{a' \in \mathcal{A}} \exp \left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a'))}(s, a') + \beta_D(N(s, m)) \bar{\mathcal{H}}_{Q,D}^{(N(s, a'))}(s, a') \right) \right) \right], \quad (4.45)$$

and notice that the value of $\exp(\hat{V}_{\rho,D}^{(N(s, m))}(s) / \alpha_D(N(s, m)))$ is equal to the denominator in Equation (4.37), and so by rearranging we can write ρ_D^m as

$$\rho_D^m(a|s) = \exp \left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a, m))}(s, a) + \beta_D(N(s, m)) \bar{\mathcal{H}}_{Q,D}^{(N(s, a, m))}(s, a) - \hat{V}_{\rho,D}^{(N(s, m))}(s) \right) \right), \quad (4.46)$$

and subsequently, the full DENTS policy can be written as:

$$\pi_D^m(a|s) = (1 - \lambda(s, m)) \exp \left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a, m))}(s, a) + \beta_D(N(s, m)) \bar{\mathcal{H}}_{Q,D}^{(N(s, a))}(s, a) - \hat{V}_{\rho,D}^{(N(s))}(s) \right) \right) \quad (4.47)$$

The AR-DENTS Process

The (AR-)BTS process.

The (AR-)BTS process is a special case of the (AR-)DENTS process when $\beta_D(x) = 0$. As such, results about BTS will be corollaries from proofs about the (AR-)DENTS process.

4.5.2 Preliminaries - Exp

TODO: This section contains things related to exponential bounds, which might move to appendix This subsection contains lemmas that will be useful in multiple times and are used to avoid repeating the same argument multiple times.

Firstly it will be that the union of exponentially unlikely events is also exponentially unlikely, and that the intersection of exponentially likely events is exponentially likely. Although this is a special case of the union bound TODO: ref? TODO: it is stated here so that it can be referenced, because this fact is

used regularly TODO: Some comment about how this is just a special case of the union bound (and ref that?) and also

Lemma 4.5.1. *Let A_1, \dots, A_ℓ be some events that satisfy for $1 \leq i \leq \ell$ the inequality $\Pr(\neg A_i) \leq C_i \exp(-k_i)$ then:*

$$\Pr\left(\bigcup_{i=1}^{\ell} \neg A_i\right) \leq C \exp(-k), \quad (4.48)$$

$$\Pr\left(\bigcap_{i=1}^{\ell} A_i\right) = 1 - \Pr\left(\bigcup_{i=1}^{\ell} \neg A_i\right) \geq 1 - C \exp(-k), \quad (4.49)$$

where $C = \sum_{i=1}^{\ell} C_i$ and $k = \min_i k_i$.

Proof outline. Lemma 4.5.1 is a consequence of the union bound, using $\exp(k_i) \leq \exp(k)$ and simplifying. Inequality (4.49) is just a negation of Inequality (4.48). \square

The following two lemma's show that the MENTS and DENTS processes always have a minimum probability of picking any action. TODO: not in good headspace writing up these two lemmas. Do a clean up, double checking maths and that have eliminated using 'we' and so on

Lemma 4.5.2. *For any MENTS process there exists some $\pi^{\min} > 0$, for any state $s_t \in \mathcal{S}$, for all $a_t \in \mathcal{A}$ and any number of trials $m \in \mathbb{N}$, such that $\pi_{\text{MENTS}}^m(a_t|s_t) \geq \pi^{\min}$.*

Proof outline. TODO: Fix N having to be N(s,m) not N(s) etc Define the Q^{\min} function as follows:

$$Q^{\min}(s_t, a_t) = \min_{s_{t+1}, a_{t+1}, \dots, s_H, a_H} \sum_{i=t}^H \min(0, Q_{\text{sft}}^{\text{init}}(s_i), R(s_i, a_i)). \quad (4.50)$$

TODO: clean up with respect to init function

And define the V^{\max} function as:

$$V^{\max}(s_t) = \alpha_{\text{MENTS}} \log \sum_{a \in \mathcal{A}} \exp(Q^{\max}(s_t, a) / \alpha_{\text{MENTS}}), \quad (4.51)$$

$$Q^{\max}(s_t, a_t) = R(s_t, a_t) + \max_{s_{t+1} \in \text{Succ}(s_t, a_t)} V^{\max}(s_{t+1}). \quad (4.52)$$

Via induction, it is possible to show that $Q^{\min}(s_t, a_t) \leq \hat{Q}_{\text{MENTS}}^{(N(s_t, a_t, m))}(s_t, a_t)$ and $V^{\max}(s_t) \geq \hat{V}_{\text{MENTS}}^{(N(s_t, m))}(s_t)$ for any arbitrary s_t, a_t and m . Now, define π^{\min} as:

$$\pi^{\min} = \inf_{\lambda \in [0, 1]} \min_{(s, a) \in \mathcal{S} \times \mathcal{A}} (1 - \lambda) \exp \left(\left(Q^{\min}(s, a) - V^{\max}(s) \right) / \alpha \right) + \frac{\lambda}{|\mathcal{A}|}. \quad (4.53)$$

Because the value of an exponential is positive, as is $1/|\mathcal{A}|$, it follows that $\pi^{\min} > 0$. Recall the MENTS policy (Equation (4.28)). By the monotonicity of the exponential function, it follows that for any $s_t \in \mathcal{S}, a_t \in \mathcal{A}, n \in \mathbb{N}$:

$$\pi_{\text{MENTS}}^m(a_t | s_t) = (1 - \lambda(s_t, m)) \exp \left(\left(\frac{1}{\alpha_{\text{MENTS}}} \left(\hat{Q}_{\text{MENTS}}^{(N(s_t, a_t, m))}(s_t, a_t) - \hat{V}_{\text{MENTS}}^{(N(s_t, m))}(s_t) \right) \right) \right) + \frac{\lambda(s_t, m)}{|\mathcal{A}|} \quad (4.54)$$

$$\geq (1 - \lambda(s_t, m)) \exp \left(\left(Q^{\min}(s_t, a_t) - V^{\max}(s_t) \right) / \alpha \right) + \frac{\lambda(s_t, m)}{|\mathcal{A}|} \quad (4.55)$$

$$\geq \pi^{\min}. \quad (4.56)$$

□

TODO: this lemma requires $\beta_D(x) < U$ for all x , or β_D is bounded. AND it requires $\alpha_D(x) < U'$ so α_D to be bounded.

Lemma 4.5.3. *For any DENTS process there exists some $\pi^{\min} > 0$, for any state $s_t \in \mathcal{S}$, for all $a_t \in \mathcal{A}$ and any number of trials $m \in \mathbb{N}$, such that $\pi_D^m(a_t | s_t) \geq \pi^{\min}$.*

Proof outline. This proof outline follows similar reasoning to Lemma 4.5.2. The same definition for Q^{\min} can be used:

$$Q^{\min}(s_t, a_t) = \min_{s_{t+1}, a_{t+1}, \dots, s_H, a_H} \sum_{i=t}^H \min(0, Q_{\text{sft}}^{\text{init}}(s_i), R(s_i, a_i)). \quad (4.57)$$

TODO: clean up with respect to init function

However, the definition of V^{\max} from Equation (4.51) needs to be altered to:

$$V^{\max}(s_t) = \max_{a \in \mathcal{A}} Q^{\max}(s_t, a) \quad (4.58)$$

$$Q^{\max}(s_t, a_t) = R(s_t, a_t) + \max_{s' \in \text{Succ}(s_t, a_t)} V^{\max}(s') \quad (4.59)$$

$$V_{\rho}^{\max}(s_t) = \alpha \log \sum_{a \in \mathcal{A}} \exp \left((Q^{\max}(s_t, a) + \beta_{\max} H \log |\mathcal{A}|) / \alpha \right), \quad (4.60)$$

TODO: clean up the use of alpha in this one. Should be alpha dents, and need to work out if should be using a sup or inf or whatever. Maybe just put a sup outside it. TODO: H was the horizon, make that consistent with what we've defined before (above and in below paragraph) where $\beta_{\max} = \sup_{x \in \mathbb{R}} \beta(x)$. Similarly to the MENTS process case, it can be shown by induction that $Q^{\min}(s_t, a_t) \leq \hat{Q}_D^{(N(s_t, a_t, m))}(s_t, a_t)$ and $V_\rho^{\max}(s_t) \geq V_\rho^{N(s_t, m)}(s_t)$, where the latter implicitly uses that $0 \leq \mathcal{H}_Q^{N(s_t, a_t)}(s_t, a_t) \leq (H - t) \log |\mathcal{A}| \leq H \log |\mathcal{A}|$ TODO: using well-known properties of entropy (left was what was originally written. Consider rewording this entire paragraph tho).

Define π^{\min} similarly to Equation (4.53), with the updated definition of V_ρ^{\max} :

$$\pi^{\min} = \inf_{\lambda \in [0, 1]} \min_{(s, a) \in \mathcal{S} \times \mathcal{A}} (1 - \lambda) \exp \left(\left(Q^{\min}(s, a) - V_\rho^{\max}(s) \right) / \alpha_{\max} \right) + \frac{\lambda}{|\mathcal{A}|}. \quad (4.61)$$

where $\alpha_{\max} = \sum_x \alpha_D(x)$ TODO: double check this is right. Recalling the DENTS policy (Equation (4.47)), and using similar reasoning to before, as well as $\beta_D(N(s, m)) \bar{\mathcal{H}}_{Q, D}^{(N(s, a))}(s, a) \geq 0$, the result follows:

$$\pi_D^m(a_t | s_t) = (1 - \lambda(s, m)) \exp \left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a, m))}(s, a) + \beta_D(N(s, m)) \bar{\mathcal{H}}_{Q, D}^{(N(s, a))}(s, a) - \hat{V}_{\rho, D}^{(N(s, a))}(s) \right) \right) \quad (4.62)$$

$$\geq (1 - \lambda(s, m)) \exp \left(\frac{1}{\alpha_D(N(s, m))} \left(\hat{Q}_D^{(N(s, a))}(s, a) - \hat{V}_{\rho, D}^{(N(s))}(s) \right) \right) + \frac{\lambda(s, m)}{|\mathcal{A}|} \quad (4.63)$$

$$\geq (1 - \lambda(s, m)) \exp \left(\left(Q^{\min}(s_t, a_t) - V_\rho^{\max}(s_t) \right) / \alpha_{\max} \right) + \frac{\lambda(s, m)}{|\mathcal{A}|} \quad (4.64)$$

$$\geq \pi^{\min}. \quad (4.65)$$

□

Additionally, Hoeffding's inequality will be useful to bound the difference between a sum of indicator random variables and its expectation.

Theorem 4.5.4. *Let $\{X_i\}_{i=1}^k$ be indicator random variables (i.e. $X_i \in \{0, 1\}$), and $S_k = \sum_{i=1}^k X_i$. Then Hoeffding's inequality for indicator random variables states for any $\varepsilon > 0$ that:*

$$\Pr(|S_k - \mathbb{E}S_k| > \varepsilon) \leq 2 \exp \left(-\frac{2\varepsilon^2}{k} \right). \quad (4.66)$$

Proof. This is a specific case of Hoeffding's inequality. See **TODO: add cite** for proof. \square

TODO: here here here. Next time = consider just defining a logsumexp function, and define the temp to have at zero it equal to max. Also finish writing up the preliminaries

4.5.3 Consistency Of Boltzmann MCTS Processes

Because the search temperature is now decayed, we need to show that the exploration term in the search policies leads to actions being sampled infinitely often.

TODO: This lemma restated means that Boltzmann search policies will select all actions infinitely often. **TODO:** Check the variables in this proof are consistent with the definitions of $N(s,a,m)$ etc

Lemma 4.5.5. *Let ρ^m be an arbitrary policy, and the following policy: **TODO:** handle when epsilon is greater than one? I think its just let ell be large enough argument*

$$\pi^m(a) = (1 - \lambda(m))\rho^m(a) + \lambda(m)\frac{1}{|\mathcal{A}|}, \quad (4.67)$$

with $\lambda(m) = \min(1, \epsilon/\log(e + m))$, where $\epsilon \in (0, \infty)$. Let $a^m \sim \pi^m$ be the m th sampled action, and let $M(a, m)$ be the number of times action a was selected in the first m samples, i.e. $M(a, m) = \sum_{i=1}^m \mathbb{1}[a^i = a]$. Then for all $a \in \mathcal{A}$ we have $M(a, m) \xrightarrow{a.s.} \infty$ as $m \rightarrow \infty$.

Proof. First consider that if $M(a, m) \not\rightarrow \infty$ then it is logically equivalent to say that there exists some ℓ such that from a^ℓ onwards that there is some action which is never sampled again. To prove the result, argue by contradiction, and suppose that there is some $\ell \in \mathbb{N}$ and $b \in \mathcal{A}$ such that:

$$\Pr\left(\bigcap_{m=\ell}^{\infty} a^m \neq b\right) > 0. \quad (4.68)$$

However, from the definition of equation (4.67) it must be that:

$$\Pr(a^m = b) \geq \frac{\lambda(m)}{|\mathcal{A}|} = \frac{\epsilon}{|\mathcal{A}| \log(e + m)}. \quad (4.69)$$

And so using this lower bound to work out the probability of never sampling action b again after the first $\ell - 1$ samples gives:

$$\Pr\left(\bigcap_{m=\ell}^{\infty} a^m \neq b\right) = \lim_{k \rightarrow \infty} \prod_{m=\ell}^k \Pr(a^m \neq b) \quad (4.70)$$

$$\leq \lim_{k \rightarrow \infty} \prod_{m=\ell}^k \left(1 - \frac{\epsilon}{|\mathcal{A}| \log(e + k)}\right) \quad (4.71)$$

$$\leq \lim_{k \rightarrow \infty} \left(1 - \frac{\epsilon}{|\mathcal{A}| \log(e + k)}\right)^{k-\ell} \quad (4.72)$$

$$= 0, \quad (4.73)$$

which is in contradiction to inequality (4.68) that was assumed. Inequality (4.72) holds because the factors in the product are increasing with respect to m . To see why the final limit equality (4.73) holds, consider the simpler function $f(x) = (1 - 1/\log(x))^x$. Taking logarithms and applying L'Hopital's rule [TODO: cite?](#) generously gives:

$$\lim_{x \rightarrow \infty} \log f(x) = \lim_{x \rightarrow \infty} x \log \left(1 - \frac{1}{\log(x)}\right) \quad (4.74)$$

$$= \lim_{x \rightarrow \infty} \frac{\log \left(1 - \frac{1}{\log(x)}\right)}{x^{-1}} \quad (4.75)$$

$$= \lim_{x \rightarrow \infty} \frac{\frac{1}{x \log(x)(\log(x)-1)}}{-x^{-2}} \quad (4.76)$$

$$= \lim_{x \rightarrow \infty} \frac{-x}{\log(x)(\log(x)-1)} \quad (4.77)$$

$$= \lim_{x \rightarrow \infty} \frac{-x}{2 \log(x) - 1} \quad (4.78)$$

$$= \lim_{x \rightarrow \infty} \frac{-x}{2} \quad (4.79)$$

$$= -\infty. \quad (4.80)$$

And thus $\lim_{x \rightarrow \infty} f(x) = \lim_{y \rightarrow -\infty} e^y = 0$.

[TODO: cut this down maybe, its a little excessive showing all of the working out?](#)

Hence, by contradiction, it must be the case that $\Pr(M(a, m) \not\rightarrow \infty) = 0$, or rather that $\Pr(M(a, m) \rightarrow \infty) = 1$ which is the desired result. \square

TODO: Can we also say that if its $(1 - 1/o(x))$ to the x , then it will generally hold, so x to the power of 0.99 could equally be used. And also any polynomial of $\log(x)$ could be used

TODO: Words about the consequences of this lemma?

In direct consequence of Lemma 4.5.5, every reachable state (and state-action pair) will be visited infinitely often in a Boltzmann MCTS Process.

Corollary 4.5.5.1. *For any Boltzmann MCTS Process (i.e. a MCTS algorithm using a search policy of the form $\pi^m(a) = (1 - \lambda(m))\rho^m(a) + \lambda(m)\frac{1}{|A|}$), all reachable states from the root node are visited infinitely often. Specifically, for any reachable $s \in \mathcal{S}$ it must be that $N(s, m) \xrightarrow{as} \infty$ and $N(s, a, m) \xrightarrow{as} \infty$ as $m \rightarrow \infty$. TODO: handle reachability somewhere better? just make some assumption at the start of the theory section saying we assume all s are reachable?*

Proof outline. This is a direct consequence of Lemma 4.5.5 when applied inductively at each node. \square

TODO: Theorem that show that values in AR-BTS and AR-DENTS converge

TODO: Theorem that shows if backups converge to the optimal, then guaranteed to converge and simple regret tends to 0 which is the result.

TODO: Theorem to show that most visited policy will also converge. Say that from the point of values converging it will add exp many additional trials for the. Essentially, if converges after K trials, then each action visited $M(a)$ many times is a constant start. And then $N(a) \approx \text{new}(a) + M(a)$ will converge by law of large numbers, and should do exp fast. Basically need to do some DKW and (strong?) law of large numbers stuff. Its just a bit bothersome because the sum is not identically distributed, as each action sampled from a diff distribution.

4.6 Full Results

TODO: there's a lot of figures for the D-chain environment, work out how to best fit them in? Or put them in this separate section?

5

Convex Hull Monte Carlo Tree Search

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5.1 Introduction

TODO: list

- high level overview of CHMCTS work
- discuss how CHMCTS answers the research questions from introduction chapter
- moving into multi-objective land now
- Comment about CHVI and prior MOMCTS work motivating this

5.2 Contextual Tree Search

TODO: list

- Discuss need for context when doing multi-objective tree Search
 - Use an example env where left gives (1,0) and right gives (0,1), optimal policy picks just left or just right, but hypervolume based methods wont
 - Use previous work on these examples and show they dont do well bad
- Discuss how UCT = running a non-stationary UCB at each node, so given above discussion, there is work in contextual MAB
- Introduce contextual regret here

5.3 Contextual Zooming for Trees

TODO: list

- Give contextual zooming for trees algorithm
- Discussion on the contextual MAB to non-stationary contextual MAB stuff (CZT is to CZ what UCT is to UCB) (and what theory carry over)

5.4 Convex Hull Monte Carlo Tree Search

TODO: list

- Give convex hull monte carlo tree search
- Contextual zooming with the convex hull backups

TODO: Repeat definition of cprune, and add to abbreviations there

5.5 Results

TODO: list

- Results from CHMCTS paper
- Get same plots from C++ code, but compare expected utility, rather than the confusing hypervolume ratio stuff

6

Simplex Maps for Multi-Objective Monte Carlo Tree Search

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6.1 Introduction

TODO: list

- high level overview of simplex maps work
- discuss how simplex maps answer the research questions from introduction chapter
- staying in multi-objective land now
- Motivated by CHMCTS being slow

6.2 Simplex Maps

TODO: list

- Define simplex map interface
- Give details on how to efficiently implement the interface with tree structures
- (Good diagram is everything here I think)

6.3 Simplex Maps in Tree Search

TODO: list

- Come up with better title for section
- Use simplex maps interface to create algorithms from the dents work
- Give a high level idea of what δ parameter is (used in theory section)

6.4 Theoretical Results

TODO: list

- Convergence can build ontop of DENTS results
- Runtime bounds (better than $O(2^D)$ which is what using convex hulls has)
- Simplex map has a diameter δ (i.e. the furthest away a new context could be from a point in the map)
- Bounds can then come from that diameter (which is a parameter of the simplex map/algorithm) and DENTS results

6.5 Empirical Results

TODO: list

- Results from MO-Gymnasium
- Compare algorithms using expected utility

7

Conclusion

Contents

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TODO: Something about we'll conclude by looking back at contributions and possible future work.

7.1 Summary of Contributions

TODO: go through each of the research questions and contributions, and write about how the work answers the research questions

7.2 Future Work

TODO: outline some avenues of potential future work

Appendices



List Of Appendices To Consider

- Multi Armed Bandits, maybe
- MMaybe from of the things in background are more appropriate as appendices?

B

Go Parameter Tuning

TODO: Edit this down correctly for thesis and change ch title?

B.0.1 Additional Go details, results and discussion

Recall from Appendix ?? that we initialised values with the neural networks as $Q^{\text{init}}(s, a) = \log \tilde{\pi}(a|s) + B$ and $V^{\text{init}}(s) = \tilde{V}(s)$, where B is a constant (adapted from Xiao [TODO: fixcites](#)). For these experiments we set a value of $B = \frac{-1}{|\mathcal{A}|} \sum_{a \in \mathcal{A}} \log \tilde{\pi}(a|s)$. Initialising the values in such a way tends to lead to the values of $Q^{\text{init}}(s, a)$ being in the range $[-20, 20]$, to account for this, we scaled the results of the game to 100 and -100 , which means that any parameters selected are about 100 times larger than they would be if we had not have used this scaling.

In these experiments we used a recommendation policy that recommends the action that was sampled the most, i.e. $\psi(s) = \max_a N(s, a)$, as this tends to be more robust to any noise from neural network outputs.

To select each parameter we ran a round robin tournament where we varied the value of one parameter. The agent that won the most games was used to select the parameter moving forward, and in the case of a tie we used the agent which won the most games. If the winning agent had the largest or smallest value, then we ran another tournament adjusting the values accordingly.

Black \ White	3	1	0.3	0.1	0.03
3	-	7-8	9-6	12-3	12-3
1	15-0	-	12-3	15-0	15-0
0.3	13-2	11-4	-	14-1	15-0
0.1	14-1	10-5	11-4	-	15-0
0.03	13-2	5-10	8-7	13-2	-

Table B.1: Results for round robin to select the temperature parameter α for BTS. The value of 1.0 won all four of its matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	3-12	4-11	3-12	1-14
1	14-1	-	8-7	9-6	7-8
0.3	14-1	8-7	-	7-8	11-4
0.1	15-0	11-4	9-6	-	9-6
0.03	14-1	8-7	4-11	8-7	-

Table B.2: Results for round robin to select the temperature parameter α_{init} for AR-BTS. The value of 0.1 won all four of its matches so was selected.

We tuned all of these algorithms using the game of 9x9 Go with a komi of 6.5, and giving each algorithm 2.5 seconds per move. For our final results we used the same parameters on 19x19 Go with a komi of 7.5, giving each algorithm 5.0 seconds per move.

Parameter selection for Go and supplementary results

In this section we work through the process used to select parameters for the Go round robin tournament used in Section ???. Predominantly parameters were chosen by playing out games of Go between agents. The parameters used for PUCT were copied from Kata Go and Alpha Go Zero [TODO: fix cites](#)

Initially we set the values of $\epsilon, \epsilon_{\bar{\lambda}}$ to 0.03, 1.0. In Tables B.1 and B.2 we give results of tuning the search temperature for BTS and AR-BTS. For AR-BTS we tried different values of α_{init} in $\alpha(m) = \alpha_{\text{init}}/\sqrt{m}$.

We then tuned the weighting of the prior policy $\epsilon_{\bar{\lambda}}$. In Tables B.3 and B.4 we give results of tuning the prior policy weight for BTS and AR-BTS.

Following that, we then tuned MENTS exploration parameter ϵ . In Tables B.5 and B.6 we give results of tuning the exploration parameter for BTS and AR-BTS. Although we selected the lowest value we tried here, we note that with such a value

Black \ White	10	5	3	2	1
10	-	5-10	3-12	1-14	3-12
5	14-1	-	12-3	11-4	11-4
3	15-0	15-0	-	12-3	12-3
2	15-0	12-3	12-3	-	10-5
1	15-0	14-1	12-3	9-6	-

Table B.3: Results for round robin to select the weighting of the prior policy $\epsilon_{\tilde{\lambda}}$ for BTS. The value of 2.0 won the most matches so was selected.

Black \ White	3	2	1	0.75	0.5
3	-	14-1	9-6	13-2	14-1
2	12-3	-	12-3	15-0	10-5
1	12-3	13-2	-	11-4	13-2
0.75	11-4	10-5	12-3	-	14-1
0.5	11-4	13-2	9-6	7-8	-

Table B.4: Results for round robin to select the weighting of the prior policy $\epsilon_{\tilde{\lambda}}$ for AR-BTS. The value of 1.0 won the most matches so was selected.

that a random action would have been sampled very few times, so the result of the hyperparameter selection was essentially that ϵ should be as low as possible.

Then we tuned the (fixed and constant) search temperatures for MENTS, AR-MENTS, RENTS, AR-RENTS, TENTS and AR-TENTS in tables B.7, B.8, B.9, B.10, B.11 and B.12.

Finally, we considered entropy temperatures of the form $\beta(m) = \beta_{\text{init}}/\sqrt{m}$ for DENTS and AR-DENTS, and tuned the value of β_{init} , in Tables B.13 and B.14 for DENTS and AR-DENTS respectively.

After tuning all of the algorithms, we compared each algorithm to their AR version in table B.15, and the AR versions universally outperformed their counterparts. We used all of the selected parameters in 19x19 Go to run our final

Black \ White	0.1	0.03	0.01	0.003	0.001
0.1	-	12-3	10-5	8-7	7-8
0.03	9-6	-	8-7	13-2	12-3
0.01	11-4	9-6	-	7-8	12-3
0.003	13-2	9-6	11-4	-	11-4
0.001	12-3	11-4	8-7	9-6	-

Table B.5: Results for round robin to select the exploration parameter ϵ for BTS. The value of 0.003 won the most matches so was selected.

Black \ White	0.1	0.03	0.01	0.003	0.001
0.1	-	12-3	14-1	12-3	13-2
0.03	15-0	-	11-4	14-1	14-1
0.01	15-0	11-4	-	13-2	13-2
0.003	15-0	14-0	14-1	-	13-2
0.001	14-1	14-1	14-1	15-0	-

Table B.6: Results for round robin to select the exploration parameter ϵ for AR-BTS. The value of 0.001 won the most matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	9-6	9-6	11-4	10-5
1	11-4	-	11-4	9-6	10-5
0.3	9-6	7-8	-	11-4	6-9
0.1	4-11	4-11	0-15	-	4-11
0.03	2-13	2-13	0-15	0-15	-

Table B.7: Results for round robin to select the temperature parameter α for MENTS. The value of 1.0 won the most matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	2-13	1-14	3-12	5-10
1	14-1	-	11-4	13-2	15-0
0.3	15-0	12-3	-	12-3	14-1
0.1	15-0	9-6	9-6	-	15-0
0.03	15-0	8-7	9-6	14-1	-

Table B.8: Results for round robin to select the temperature parameter α for AR-MENTS. The value of 0.3 won the most matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	7-8	9-6	10-5	9-6
1	13-2	-	12-3	11-4	12-3
0.3	10-5	11-4	-	10-5	5-10
0.1	3-12	2-13	1-14	-	3-12
0.03	3-12	0-15	0-15	0-15	-

Table B.9: Results for round robin to select the temperature parameter α for RENTS. The value of 1.0 won the most matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	4-11	2-13	9-6	3-12
1	15-0	-	12-3	13-2	13-2
0.3	15-0	13-2	-	14-1	15-0
0.1	15-0	10-5	13-2	-	15-0
0.03	13-2	13-2	12-3	14-1	-

Table B.10: Results for round robin to select the temperature parameter α for AR-RENTS. The value of 0.3 won the most matches so was selected.

Black \ White	300	100	30	10	3
300	-	3-12	5-10	7-8	9-6
100	6-9	-	9-6	12-3	12-3
30	8-7	7-8	-	9-6	11-4
10	0-15	2-13	2-13	-	6-9
3	1-14	1-14	2-13	5-10	-

Table B.11: Results for round robin to select the temperature parameter α for TENTS. The value of 30.0 won the most matches so was selected.

Black \ White	30	10	3	1	0.3
30	-	14-1	15-0	14-1	14-1
10	15-0	-	13-2	15-0	15-0
3	15-0	14-1	-	14-1	15-0
1	15-0	15-0	14-1	-	15-0
0.3	15-0	15-0	14-1	15-0	-

Table B.12: Results for round robin to select the temperature parameter α for AR-TENTS. The value of 3.0 won the most matches so was selected.

Black \ White	0.1	0.03	0.01	0.003	0.001
0.1	-	10-5	12-3	8-7	11-4
0.1	13-2	-	11-4	13-2	10-5
0.1	12-3	11-4	-	10-5	11-4
0.1	7-8	13-2	13-2	-	10-5
0.1	13-2	13-2	11-4	11-4	-

Table B.13: Results for round robin to select the initial entropy temperature β_{init} for DENTS. The value of 0.3 won the most matches so was selected.

Black \ White	3	1	0.3	0.1	0.03
3	-	11-4	12-3	12-3	14-1
1	13-2	-	11-4	13-2	13-2
0.3	14-1	13-2	-	13-2	14-1
0.1	12-3	12-3	12-3	-	11-4
0.03	12-3	13-2	13-2	14-1	-

Table B.14: Results for round robin to select the initial entropy temperature β_{init} for AR-DENTS. The value of 0.3 won the most matches so was selected.

Black \ White	MENTS	AR-MENTS	BTS	AR-BTS	DENTS	AR-DENTS
MENTS	-	0-25				
AR-MENTS	25-0	-				
BTS			-	16-9		
AR-BTS			22-3	-		
DENTS					-	21-4
AR-DENTS					22-3	-
Black \ White	RENTS	AR-RENTS	TENTS	AR-TENTS		
RENTS	-	2-23				
AR-RENTS	24-1	-				
TENTS			-	8-17		
AR-TENTS			23-2	-		

Table B.15: Results for the matches of each algorithm against its AR version.

experiments given in Table ??.

Finally, we also ran AR-BTS against Kata Go directly limiting each algorithm to 1600 trials. KataGo beat AR-BTS by 31-19, confirming that the additional exploration is outweighed by the information contained in the neural networks, and in Go the Boltzmann search algorithms gain their advantage via the Alias method and being able to run more trials quickly.

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