Doing Better Than UCT:
Rational Monte Carlo Sampling in Trees

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Abstract

UCT, a state-of-the art algorithm for Monte Carlo tree sampling (MCTS), is based on UCB, a sampling policy for the Multi-armed Bandit Problem (MAB) that minimizes the accumulated regret. However, MCTS differs from MAB in that only the final choice, rather than all arm pulls, brings a reward, that is, the simple regret, as opposite to the cumulative regret, must be minimized. This ongoing work aims at applying meta-reasoning techniques to MCTS, which is non-trivial. We begin by introducing policies for multi-armed bandits with lower simple regret than UCB, and an algorithm for MCTS which combines cumulative and simple regret minimization and outperforms UCT. We also develop a sampling scheme loosely based on a myopic version of perfect value of information. Finite-time and asymptotic analysis of the policies is provided, and the algorithms are compared empirically.

1 Introduction and definitions

Monte-Carlo tree sampling, and especially a version based on the UCT formula [4] appears in numerous search applications, such as [3]. Although these methods are shown to be successful empirically, most authors appear to be using the UCT formula "because it has been shown to be successful in the past", and "because it does a good job of trading off exploration and exploitation". While the latter statement may be correct for the multi-armed bandit and for the UCB method [1], we argue that it is inappropriate for search. The problem is not that UCT does not work; rather, we argue that a simple reconsideration from basic principles can result in schemes that outperform UCT. This is demonstrated both theoretically and empirically.

In the Multi-armed Bandit problem we have a set of K arms. Each arm can be pulled multiple times. When the ith arm is pulled, a random reward X_i from an unknown stationary distribution is returned. The reward is bounded between 0 and 1.

The simple regret of a sampling policy for the Multi-armed Bandit Problem is the expected difference between the best expected reward μ_* and the expected reward μ_j of the arm with the best sample mean $\overline{X}_j = \max_i \overline{X}_i$:

$$\mathbb{E}[R] = \sum_{j=1}^{K} \Delta_j \Pr(\overline{X}_j = \max_i \overline{X}_i) \tag{1}$$

where $\Delta_j = \mu_* - \mu_j$. Strategies that minimize the simple reward are called pure exploration strategies [2].

Such strategies are used to select the best arm, and, by extension, the best action in Monte Carlo tree search. Monte Carlo tree search is used to solve Markov Decision Processes (MDP) approximately.

1

An MDP is defined by the set of states S, the set of actions A, the transition table $T(s, a, s')$, the reward table $R(s, a, s')$, the initial state s and the goal state t: (S, A, T, R, s, t) [5]. Monte Carlo tree search explores an MDP by *rollouts*—trajectories from the current state to a state in which a termination condition is satisfied (either the goal state, or a cutoff state for which the reward is evaluated approximately). The UCB algorithm (that attempts to minimize the cumulative regret) [1] had been extended into the tree search sampling scheme known as UCT [4].

UCT-driven search achieves good results in many search problems. At each search step, the algorithm allocates Monte Carlo rollouts to choose the best action, thereby (approximately) minimizing the cumulative regret. The core issue is that in search (especially for adversarial search and for "games against nature" - optimizing behavior under uncertainty) the goal is typically to either find a good (or optimal) strategy, or even to find the best first action of such a policy. Once such an action is discovered, it is not beneficial to further sample that action, "exploitation" is thus meaningless for search problems. Finding a good first action is closer to the pure exploration variant, as seen in the selection problem [2, 6]. In the selection problem, it is much better to minimize the *simple* regret. However, the simple and the cumulative regret cannot be minimized simultaneously; moreover, [2] shows that in many cases the smaller the cumulative regret, the greater the simple regret.

UCT performance can thus be improved by combining UCB with a sampling scheme that minimizes the simple regret of selecting an action at the current root node. Indeed, the algorithm must select an action with the minimum regret *given the assumption that after performing the selected action the algorithm performs optimally*, which corresponds to maximizing the value of partial information [5]. Therefore, an improved allocation scheme would

- maximize the value of partial information by sampling actions to minimize the **simple** regret of the selection at the current root node, and

- as the goal of sampling in deeper tree nodes is estimating the value of a node, rather than selection, it makes sense to minimize the **cumulative** regret of the rollouts from the second step onwards.

The ultimate goal of this ongoing work is "optimal" sampling in the meta-reasoning sense. Nevertheless, this task is daunting for the following reasons:

- Defining the cost of a sample is not easy, and even if we simply use time-cost as an approximation, we get an intractable meta-reasoning problem.

- Applying the standard myopic and subtree independence assumptions, we run into serious problems. Even in the standard selection problem [6], we get a non-concave utility function and premature stopping of the algorithm. This is due to the fact that the value of information of a single measurement (analogous to a sample in MCTS) is frequently less than its time-cost, even though this is not true for multiple measurements. When applying the selection problem to MCTS, the situation is exacerbated. The utility of an action is usually bounded, and thus in many cases a single sample may be insufficient to change the current best action, *regardless* of its outcome. As a result, we frequently get a *zero* "myopic" value of information for a single sample.

As the ultimate task is extremely difficult to achieve, and even harder to analyze, we begin with simple schemes more amenable to analysis. We then develop a crude value of information (VOI) based scheme. Although the latter is a somewhat ad-hoc attempt to estimate value of information of a sample, it already appears (empirically) to do better than UCT as well as better than all the simpler schemes we propose.

2 Main Results

2.1 Doing better than UCB

1. The ε-greedy allocation scheme has exponential convergence rate of the simple regret $\mathbb{E}r$:

$$\mathbb{E}r_\varepsilon \leq \sum_{j=1}^{K} \Delta_j \left(\frac{n\varepsilon}{K} + \frac{4\sqrt{e}}{\Delta_j^2} \right) e^{-\Delta_j^2 n\varepsilon/8K} \tag{2}$$

2. The UCB allocation scheme exhibits polynomial convergence rate:

$$\mathbb{E}r_{ucb} \leq 2 \sum_{j=1}^{K} \Delta_j n^{\frac{-\alpha\Delta_j^2}{8}} \tag{3}$$

3. A tighter upper regret bound for the ε-greedy allocation scheme depends on ε. The lowest bound is achieved for $\varepsilon = \frac{1}{2}$, and for a large number of arms the bound for the $\frac{1}{2}$-greedy scheme approaches the square of the bound for uniform sampling.

4. Another improved allocation scheme for minimizing the simple regret, called **UQB** here, is obtained by substituting $\sqrt{\cdot}$ instead of $\log(\cdot)$ into the formula for UCB and has a superpolynomial convergence rate.

Proofs and derivations for the above statements are in the full paper, removed for brevity.

2.2 Doing better than UCT

The **two-stage** Monte Carlo tree search sampling scheme selects an action at the current root node according to an algorithm that minimizes the simple regret, such as $\frac{1}{2}$-greedy or UQB, and then selects actions according to UCB. Such two-stage outperforms the UCT sampling scheme that selects actions based on UCB only.

Such sampling scheme is significantly less sensitive to the tuning of the exploration factor (C_p in [4]) of UCT, since the conflict [2] between the need for a larger value of C_p on the first step (simple regret) and a smaller value for the rest of the rollout (cumulative regret) is resolved. In fact, a sampling scheme that uses UCB at all steps but a larger value of C_p for the first step than for the rest of the steps, outperforms UCT. The pseudocode of the two-stage rollout is in Algorithm 1.

3 Empirical Evaluation

The results were empirically verified on Multi-armed Bandit instances (Section 3.1), on search trees (Section 3.2), and on the sailing domain (Section 3.3), as defined in [4]. The experiments confirmed the hypotheses. The algorithms used in the experiments are:

RND: uniform random samping;

UCT: Upper Confidence Bounds applied to Trees [4];

**GCT:** UCT with the first step replaced with $\frac{1}{2}$-greedy sampling;

QCT: UCT with the first step replaced with UQB.

Algorithm 1 Two-stage Monte-Carlo tree search sampling

1: **procedure** Rollout(node, depth=1)
2:     **if** IsLeaf(node, depth) **then**
3:         **return** 0
4:     **else**
5:         **if** depth=1 **then**
6:             action ← FirstAction(node)   ▷ minimizes simple regret, e.g. $\frac{1}{2}$-greedy
7:         **else**
8:             action ← NextAction(node)   ▷ UCB — minimizes cumulative regret
9:         **end if**
10:        next-node ← NextState(node, action)
11:        reward ← TransitionReward(node, action, next-node)
12:             + Rollout(next-node, depth+1)   ▷ call Rollout recursively
13:        UpdateStats(node, action, reward)
14:     **end if**
15: **end procedure**

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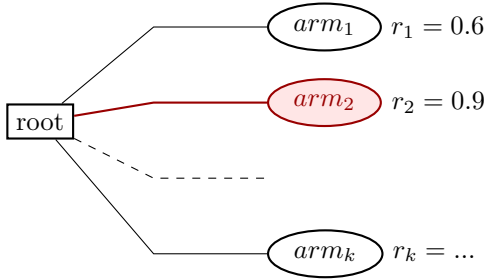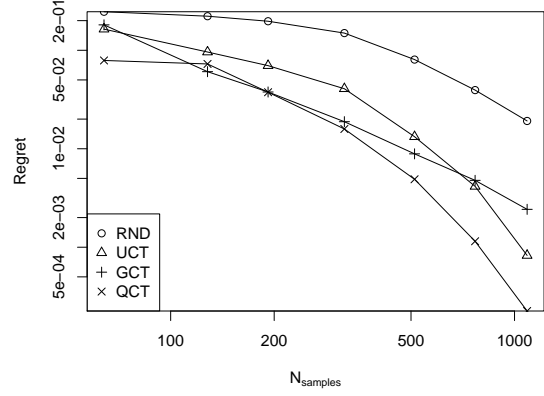
a. search tree   b. regret vs. number of samples

Figure 1: Simple regret in MAB

3.1   Simple regret in multi-armed bandits

Figure 3.1 presents a comparison of simple regret minimization algorithms for Multi-armed bandits. Figure 3.1.a shows the search tree corresponding to a problem instance. Each arm returns a random reward drawn from a Bernoulli distribution. The search selects an arm and compares the expected reward, unknown to the algorithm during the sampling, to the expected reward of the best arm.

Figure 3.1.b shows the regret vs. the number of samples, averaged over 10^4 experiments for randomly generated instances of 32 arms.

For smaller numbers of samples, $\frac{1}{2}$-greedy achieves the best performance; for large number of samples, QCT outperforms GCT. QCT is better than UCT everywhere except for very small numbers of samples. A combination of GCT and QCT dominates UCT over the whole range.

3.2   Monte Carlo tree search

The second set of experiments was performed on randomly generated trees crafted in such a way that uniform random sampling selects a direction at the root randomly. The degree of the root is a parameter of the tree generator. The degree of all nodes at distance 1 from the root is 2, and all nodes at distance 2 from the roots are leaves. The average reward of two children of each node at distance 1
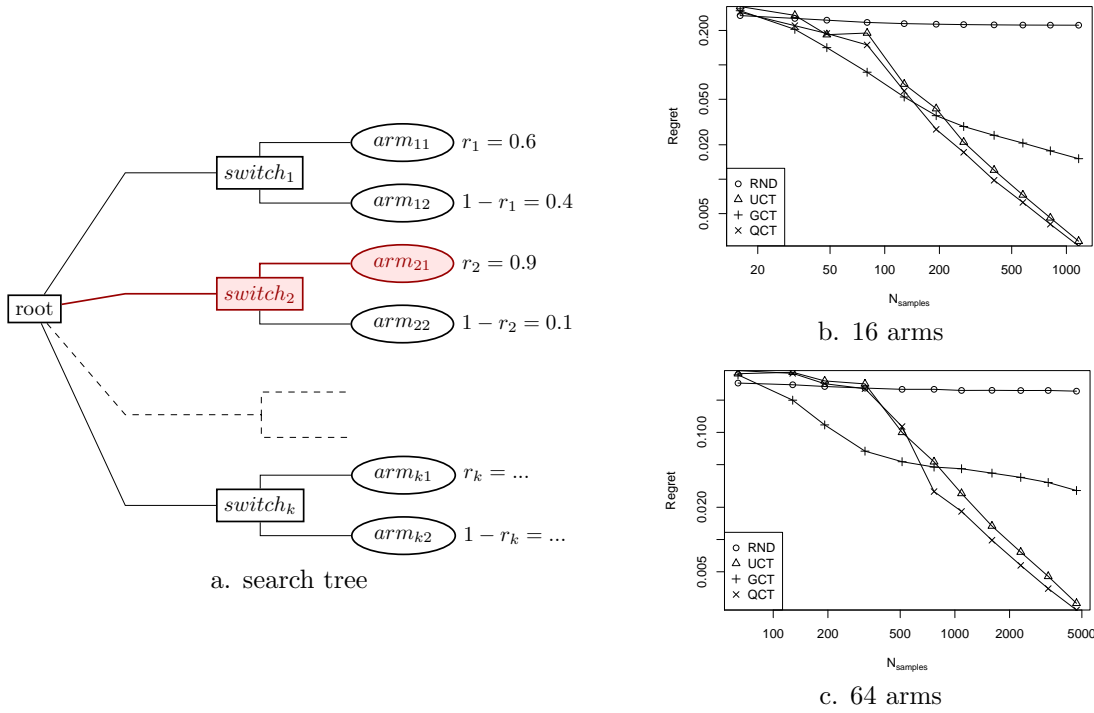
Figure 2: MCTS: a path to the best arm

is 0.5. Thus, a uniform sampling scheme results in the same average reward for all edges at the root, and an adaptive sampling scheme, such as UCT, has to be used.

Figure 3.2 shows a sketch of the search tree (Figure 3.2.a) and the dependency of the regret vs. the number of samples for trees with root degree 16 (Figure 3.2.b) and 64 (Figure 3.2.c). The dependencies look differently from Multi-armed bandit instances, but the algorithms exhibit a similar relative performance: either GCT or QCT is always better than UCT, QCT dominates UCT everywhere except for small numbers of instances. The advantage of QCT grows with the number of arms.

3.3 The sailing domain

Figures 3–6 show results of experiments on the sailing domain. Figure 3 shows the regret vs. the number of samples, computed for a range of values of C_p. Figure 3.a shows the median cost, and Figure 3.b — the minimum costs. UCT is always worse than either $\frac{1}{2}$-greedy (GCT) or QCT, and is sensitive to the value of C_p: the median cost is much higher than the minimum cost for UCT. For both $\frac{1}{2}$-greedy and QCT, the difference is significantly less prominent.

Figure 4 shows the regret vs. the exploration factor for different numbers of samples. QCT is always better than UCT, and $\frac{1}{2}$-greedy is better than UCT expect for a small range of values of the exploration factor C_p.

Figure 5 shows the cost vs. the exploration factor for lakes of different sizes. The relative difference between the sampling schemes becomes more prominent when the lake size increases.

Figure 6 compares QCT with UCT with a different exploration factor at the root (CCT). C_p for the rest of the steps was chosen to ensure the best performance from earlier experiments on the domain. Both algorithms exhibit similar dependency, but as the number of samples grows, QCT achieves smaller average regrets and is less sensitive to the choice of the value for C_p at the first step.
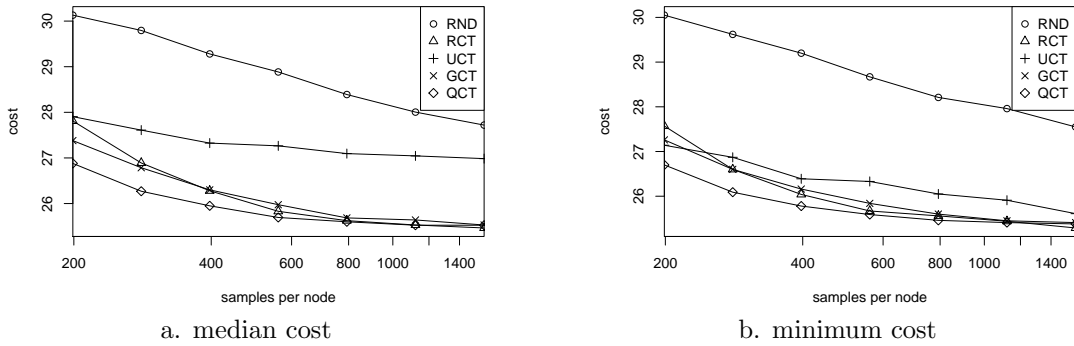
<div style="text-align:center">a. median cost   b. minimum cost</div>

Figure 3: The sailing domain, 6×6 lake, cost vs. number of rollouts

4 Summary and Future Work

The Monte Carlo tree search algorithms presented in the paper differ from UCT at the first step of the rollout, when the 'simple' selection regret is minimized instead of the cumulative regret. Both the theoretical analysis and the empirical evaluation provide evidence for better general performance of the proposed algorithms.

The improvement is inspired by the notion of value of information (VOI), but VOI is used implicitly in the analysis of the algorithm, rather than computed or learned explicitly in order to plan the rollouts. A further improvement can be achieved by computing or estimating the VOI of the rollouts and choosing a rollout that maximizes the VOI. Using VOI to guide Monte Carlo sampling instead of relying on the sample means of different actions is particularly beneficial when different actions have qualitatively different distributions: for example, when the distribution variance varies significantly between the actions.

VOI of a rollout can be computed when the sample distribution of an action is known up to the parameters, such as the normal distribution with an unknown mean and/or variance. Alternatively, the value of information can be estimated from the set of samples, and the need to assume a particular shape of the distribution can be lifted. In one realization of the latter approach the VOI of performing an action is estimated as *the value of perfect information learned from the outcome of earlier samples of the action divided by the number of samples*. Early experiments with this approach showed the best performance for sets of Bernoulli arms, and even a more prominent improvement for mixed arms (e.g. Bernoulli, triangularly distributed, and fixed arms. Sample-based VOI estimation requires keeping more information than an algorithm based only on the sample mean, but the overhead is small and justified by the improvement.

Acknowledgments

References

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[2] Sébastien Bubeck, Rémi Munos, and Gilles Stoltz. Pure exploration in finitely-armed and continuous-armed bandits. *Theor. Comput. Sci.*, 412(19):1832–1852, 2011.
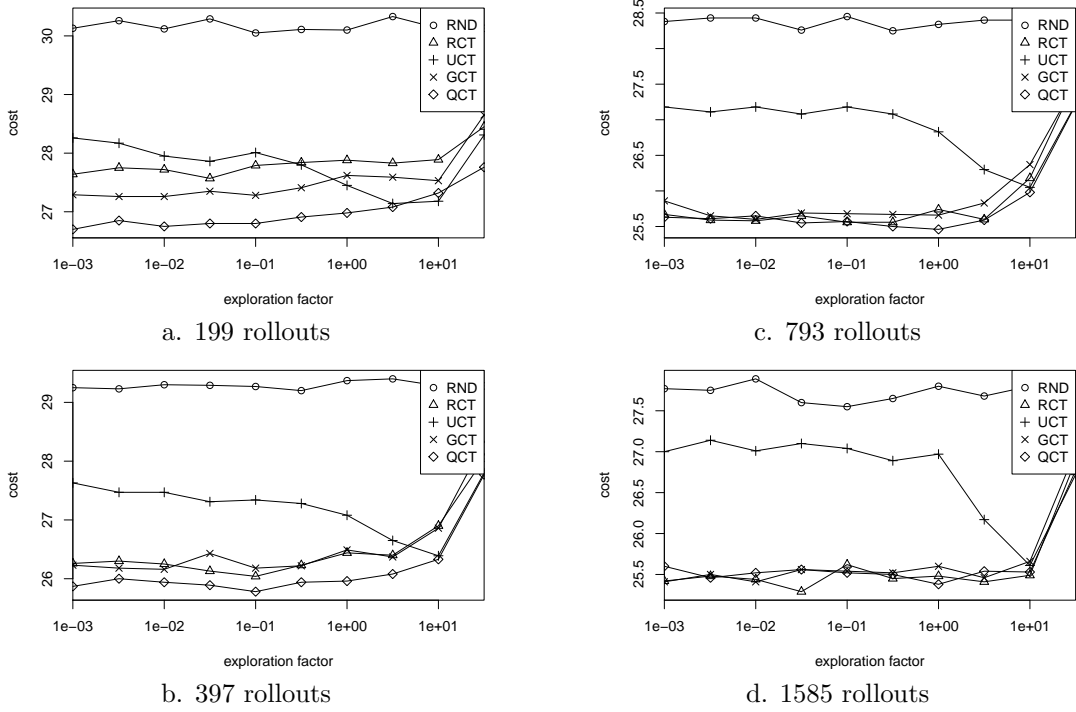
a. 199 rollouts

b. 397 rollouts

c. 793 rollouts

d. 1585 rollouts

Figure 4: The sailing domain, 6×6 lake, cost vs. factor

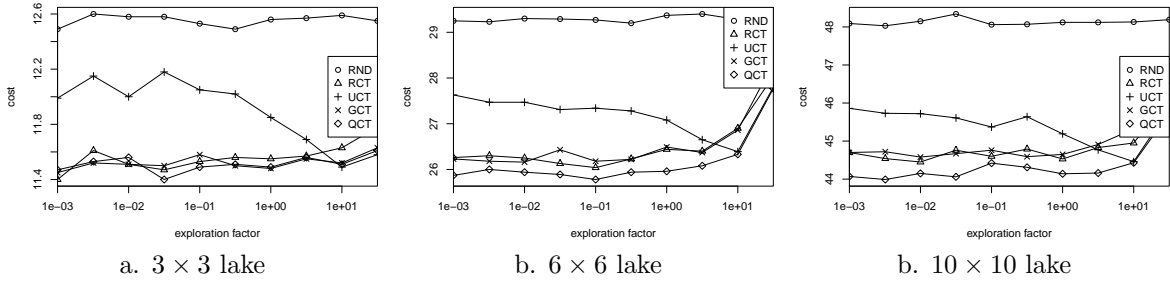a. 3×3 lake

b. 6×6 lake

b. 10×10 lake

Figure 5: The sailing domain, 397 samples, cost vs. factor

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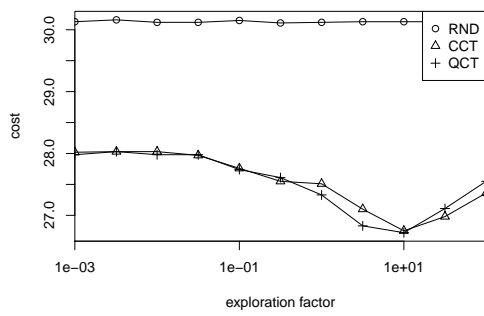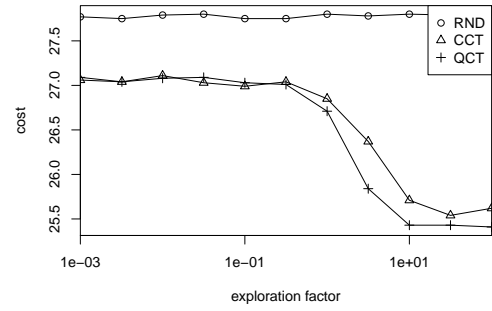
a. 199 rollouts
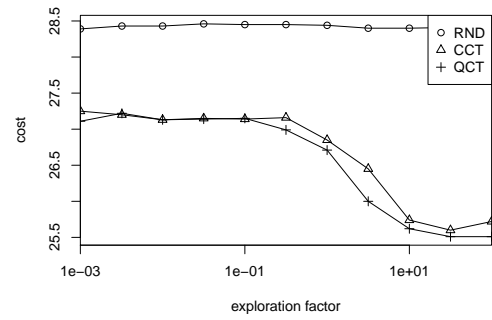
c. 793 rollouts
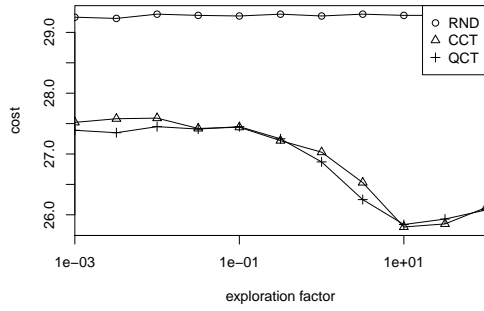
b. 397 rollouts

d. 1585 rollouts

Figure 6: The sailing domain, log vs. sqrt, 6×6 lake

8