Measurable Monte Carlo Search Error Bounds

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Abstract

Monte Carlo planners can often return sub-optimal actions, even if they are guaranteed to converge in the limit of infinite samples. Known asymptotic regret bounds do not provide any way to measure confidence of a recommended action at the conclusion of search. In this work, we prove bounds on the sub-optimality of Monte Carlo estimates for non-stationary bandits and Markov decision processes. These bounds can be directly computed at the conclusion of the search and do not require knowledge of the true action-value. The presented bound holds for general Monte Carlo solvers meeting mild convergence conditions. We empirically test the tightness of the bounds through experiments on a multi-armed bandit and a discrete Markov decision process for both a simple solver and Monte Carlo tree search.

1 Introduction

Monte Carlo (MC) methods are powerful tools for solving decision problems when environment dynamics are not fully known. Monte Carlo solvers sample experiences from a generative model of the environment to estimate the values of different actions. On and off-policy solvers based on Monte Carlo sampling have been proposed for single-step and sequential decision problems [1]. Monte Carlo tree search (MCTS) is a planning method for Markov decision processes (MDPs) that uses MC sampling to build a search tree over possible trajectories of states and actions. MCTS has been a critical component of several recent advances in sequential decision making and reinforcement learning [2], [3]. Recent work has explored integration of MCTS in self-driving vehicle systems [4], [5]. Despite the popularity of MC methods, practical understanding of their behavior remains limited.

Monte Carlo solvers typically select actions to sample according to a non-stationary search policy that converges during search to the optimal policy. For many MC algorithms, regret and convergence rate bounds have been defined in terms of unknown parameters of the true action value distributions and asymptotic solver behavior in the limit of infinite samples [1]. For example, the upper confidence tree (UCT) MCTS algorithm, has known bounds on the probability of several different measures of error defined in terms of the difference between the converged Monte Carlo estimate and the true action value [6]. While these expressions provide understanding of the general behavior of this algorithm, they cannot generally be calculated. The non-stationary payout distributions encountered during search make defining general error bounds with finite samples difficult.

Monte Carlo solvers reduce the expected error due to bias in the baseline policy at the cost of expected error from sample variance [7]. Expected variance error tends to decrease with the number of samples. Sampling enough experience is critical to ensuring an accurate value estimate and action recommendation. Many Monte Carlo algorithms are run online with arbitrary, heuristic stopping conditions such as reaching a sample limit. Results from such solvers do not provide a meaningful

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measure of confidence on the returned estimates. Monte Carlo search using informative baselines, for example a policy trained with reinforcement learning, can introduce excess variance error to the baseline, resulting in worse performance. Finite-sample error bounds can provide a more principled stopping criteria for Monte Carlo search.

In this work, we present empirical bounds on error probability for general Monte Carlo solvers. The proposed bound limits the probability that an action recommended by a convergent Monte Carlo search is worse than any other action considered in the search by a given margin. A corollary bound limits the probability that an action value estimate overestimates the true value by more than a given margin. These bounds can be applied to any Monte Carlo method solving a non-stationary bandit problem or MDP that satisfies mild convergence conditions. Unlike previously known bounds, the presented bounds can be numerically calculated at any point during search using known, empirical values. They can then be used as a confidence measure for the returned recommendations or as a principled stopping criteria.

Numerical experiments tested the tightness of the bounds on a multi-armed bandit and a discrete action space MDP. A simple, fixed-depth Monte Carlo sampler was tested on both problems and UCT-MCTS was additionally tested on the MDP. We examined the effect of various problem and solver configurations on bound tightness. Results show that the bounds generally hold with the bound gap decreasing with sample count.

2 Related Work

Multi-armed bandit problems have been extensively studied by the statistics and learning communities [8]. Many algorithms have been proposed to approximately solve the bandit problem and foundational algorithms, such as UCB1, have been extensively studied [9]. Similarly, many MCTS methods have been proposed to solve MDPs, with UCT being a well-studied foundational algorithm [6]. Since their introduction, these algorithms have had several convergence guarantees and non-asymptotic performance bounds proved, often in terms of the true action value or other unknown parameters. As new Monte Carlo algorithms are developed, the theoretical performance analysis similar to these foundational works tends to be presented [10].

Much of the analysis to-date has focused on the behavior of specific algorithms. Shah, Xie, and Xu [10] present non-asymptotic analysis of UCT with improved regret-bounds, and additionally propose a modified, fixed-depth tree search with policy-improvement guarantees. Similarly, James, Konidaris, and Rosman [11] analyze the effects of value function smoothness and baseline policies on UCT. Prior work in statistical analysis of random processes provide foundational measures toward generally applicable non-asymptotic bounds. Several prior works develop empirical Bernstein-type bounds based on sample variance. Early work proved bounds for sums of independent, identically distributed random random variables based on sample mean and variance [12], [13]. Further work extended these ideas to functions over martingales [14], [15] with some restrictions. This work draws on the insights of these analyses to develop the proposed empirical bounds.

3 Empirical Monte Carlo Bounds

This section presents bounds on the sub-optimality of a Monte Carlo search. The bound applies to searches over multi-armed bandits with non-stationary payout distributions and Markov decision problems (MDPs). The bounds hold for any Monte Carlo method meeting the following two convergence conditions.

Convergence Conditions

1. Solver Convergence: The expected value of the search policy increases with the number of searches, such that \( \mathbb{E}[V^n] \geq \mathbb{E}[V^m] \) for \( n \geq m \).

2. Positive Search Bias: The search samples actions with higher values more often, such that \( \mathbb{E}[T(a_i)] \geq \mathbb{E}[T(a_j)] \), where \( T(a) \) gives the number of times \( a \) was sampled and \( Q(s, a_i) \geq Q(s, a_j) \).

For MDPs, we additionally assume that the search simulates trajectories from a given starting state \( s \) to some potentially variable depth \( h \) and uses a baseline estimator to bootstrap the value of the
We can define the set of actions considered in the Monte Carlo search to be a subset of the complete action space $A_T \subseteq A$. The set of samples for action $a_i \in A_T$ is represented as $C_i \leftarrow (\hat{Q}_i^{(1)}, \ldots, \hat{Q}_i^{(n)})$. The value estimate of action $a_i$ is then $\bar{Q}_i = \frac{1}{|C_i|} \sum_{q \in C_i} q_i$. It is assumed that the sample values are bounded by some non-zero constant $a$ almost surely as $|\hat{Q}_i^{(k)}| \leq a \forall i, k$.

**Theorem 1.** Let a Monte Carlo solver satisfy the convergence conditions for a problem with sample values bounded by $b$. For a search that returns action value estimates over two actions $\bar{Q}_i - \bar{Q}_j = \delta$, the probability that the true optimal action value gap $\bar{Q}_i - \bar{Q}_j \leq -\epsilon$ is no greater than

$$\exp \left( -\frac{n_i n_j (\delta + \epsilon - \zeta_i - \zeta_j)^2}{2(n_i \hat{\sigma}_i^{2,\alpha} + n_j \hat{\sigma}_j^{2,\alpha})} \right) + \alpha \tag{1}$$

The variance term is defined for bounded random variables as

$$\hat{\sigma}^{2,\alpha} \leftarrow b^2 \left( \frac{1}{b} V_i^{\frac{1}{2}} + \sqrt{\ln \alpha \over n} \right)^2 \tag{2}$$

where $V_i$ is the sample variance over $n$ samples and $b$ is the sample range. Taking the minimum of eq. (2) over $\alpha$ gives the tightest bound. In the bandit setting, the bias term $\zeta \leftarrow 0$, since the values are sampled directly from the true distributions. In the MDP setting, the error bound term $\zeta$ in corollary 1.1 is defined as

$$\zeta = \frac{1}{|C_i|} \sum_k \gamma^{H_k} \epsilon_k \tag{3}$$

where $k$ indexes the samples of $C_i$, $H_k$ is the depth of the Monte Carlo rollout, $\gamma \in [0, 1]$ is a discount factor, and $\epsilon_k$ is an upper bound on the error of the baseline value estimate at the end of the trajectory. At worst, $\epsilon_k \leftarrow \max(Q_{\text{max}} - \bar{Q}_k, \bar{Q}_k - Q_{\text{min}})$, where $\bar{Q}_k$ is the value of the baseline estimate at the end of the trajectory $k$. The error is zero for trajectories reaching termination.

The presented bound is entirely empirical and requires no knowledge of unobserved parameters to compute. Intuitively, it provides a limit on how likely it is that action considered in a Monte Carlo search is better than another action with a higher estimated value. The bound does not provide general guarantees on action optimality, for example in problems with continuous action spaces. As can be seen, the probability decays exponentially with the number of trajectories sampled for the given action. For MDPs, the search-bias decreases with the depth $H$ of each trajectory sample as $\gamma^H$.

A useful corollary to corollary 1.1 gives the probability that an estimated action value is overestimated by more than $\epsilon \geq 0$. Like theorem 1, the inequality of corollary 1.1 can be calculated using only known empirical values.

**Corollary 1.1.** Let a Monte Carlo solver satisfy the convergence conditions for a problem with sample values bounded by $b$. For a search that returns action value estimate $\bar{Q}_i = q_i$, the probability that the true optimal action value is overestimated as $\bar{Q}_i - Q_i \geq \epsilon$ is no greater than

$$\exp \left( -\frac{n_i (|\epsilon - \zeta|)^2}{2\hat{\sigma}_i^{2,\alpha}} \right) + \alpha \tag{4}$$

where $n_i$ is the number of trajectories sampling $a_i$, $\hat{\sigma}^{2,\alpha}$ is an upper bound on the value variance with significance level $\alpha \in (0, 1)$, and $\zeta$ is an upper bound on the expected bias of the baseline value estimate. $|x|^+ \text{ represents the max}(0, x) \text{ function.}$

Equation (4) only provides a meaningful bound for $\epsilon > 0$.

### 3.1 Proofs

This section provides a proof of theorem 1, which also proves corollary 1.1, which can be shown to be a special case. We first present several lemmas. The first lemma presents a bound on the difference in expected error of action value estimates generated by a Monte Carlo search.
Lemma 1. Given a convergent Monte Carlo search over an MDP returning estimates $\bar{Q}_i$ and $\bar{Q}_j$ and true action values $Q_j \geq Q_i$, the expected error is

$$E[\bar{Q}_i - Q_i] - E[\bar{Q}_j - Q_j] \leq \frac{1}{|C_i|} \sum_k H_k \epsilon_k^{0} - \frac{1}{|C_j|} \sum_l H_l \epsilon_l^{0}$$

where $k$ and $l$ index the samples of $C_i$ and $C_j$ respectively, and $\epsilon_i^{0}$ is the expected error of the baseline estimate at the end of the trajectory.

A proof of lemma 1 is given in section 3.3. The next lemma shows that an appropriate upper bound on the conditional likelihood of an estimator of an unknown parameter is also an upper bound on a probability of the parameter.

Lemma 2. Let $\theta$ be a population parameter and let $\tilde{\theta}$ be a potentially biased estimator of that parameter with variance $\sigma^2$. If the probability

$$P(\tilde{\theta} \geq a | \theta = b) \leq c(\sigma^2)$$

where $c(\sigma^2)$ is a function that increases monotonically with $\sigma^2$, then the inequality

$$P(\theta \geq b | \tilde{\theta} = a) \leq c(\sigma^2)$$

also holds.

Lemma 2 follows from the Bayesian Cramér-Rao inequality [16], [17], which, for appropriate priors, implies

$$\text{Var}[\theta | X] \leq \text{Var}[\tilde{\theta} | X]$$

for distributional parameter $\theta$, estimator $\tilde{\theta}$, and data $X$. The final lemma bounds the true variance of an expectation estimator around the sample variance.

Lemma 3. Let $\hat{X} = \frac{1}{n} \sum_i^n X_i$ be an estimator of the mean over $n$ random variables with variance $\sigma^2$. Given a estimate $\bar{x} = \frac{1}{n} \sum_i^n x_i \sim X_i$ and sample variance $V_n = \frac{1}{n} \sum_i^n (x_i - \bar{x})^2$, the variance is bounded as

$$\sigma^2 \leq \frac{b^2}{n} \left( \frac{1}{b} V_n^{\frac{1}{2}} + \sqrt{\ln \alpha \frac{n}{n-1}} \right)^2$$

where $b = \max_i x_i - \min_i x_i$ is the range of the sample values and $\alpha \in (0, 1)$ is a significance level.

Lemma 3 follows from the sample variance penalty for empirical Bernstein bounds stated in theorem 10 of the work by Maurer and Pontil [12].

3.2 Proof of Theorem

Proof. The proof begins by constructing a bound on the likelihood of search results as

$$P(\bar{Q}_i - \bar{Q}_j \geq \delta | Q_i - Q_j = \epsilon)$$

$$= P(\bar{Q}_i - \bar{Q}_j - E[\bar{Q}_i - \bar{Q}_j] \geq \delta - E[\bar{Q}_i - \bar{Q}_j])$$

$$= P(\bar{Q}_i - \bar{Q}_j - E[\bar{Q}_i - \bar{Q}_j] \geq \delta + \epsilon - E[\bar{Q}_i - \bar{Q}_j] + E[\bar{Q}_j - Q_j])$$

$$\leq P(\bar{Q}_i - \bar{Q}_j - E[\bar{Q}_i - \bar{Q}_j] \geq \delta + \epsilon - \sum_{i \in C_i} H_i \epsilon_i^{0} + \sum_{j \in C_j} H_j \epsilon_j^{0})$$

$$\leq P(\bar{Q}_i - \bar{Q}_j - E[\bar{Q}_i - \bar{Q}_j] \geq \delta + \epsilon - \sum_{i \in C_i} H_i \epsilon_i^{0} - \sum_{j \in C_j} H_j \epsilon_j^{0})$$

where the conditional dependence term is omitted after eq. (10) for clarity. The inequality of eq. (13) follows from lemma 1. The expected baseline estimator error $\epsilon_i^{0}$ is not generally known, though its magnitude can be limited by a term $\epsilon_i^{U} \geq |\epsilon_i^{0}|$. Since the bound on error magnitude is applied symmetrically, the probability is only bounded by the worst case, resulting in eq. (14).

We can use this term to construct a Chernoff-Hoeffding inequality bounding the sub-optimality as

$$P(Q_j - Q_i \geq \epsilon | \bar{Q}_i - \bar{Q}_j = \delta) \leq \exp \left( \frac{2n_i n_j (\delta + \epsilon - \zeta^{+})^2}{n_i \sigma_i^2 + n_j \sigma_j^2} \right)$$

(15)
where $\sigma^2$ gives the variance of the value estimators. We apply the inequality of eq. (15) to bound the sub-optimality by applying lemma 2. By applying the variance upper bound of lemma 3 to eq. (15) with the union bound, we arrive at

$$\leq \exp \left( -\frac{2n_i n_j (|\delta + \epsilon - |\zeta| + )^2}{n_i \sigma_i^2 + n_j \sigma_j^2} \right) + \alpha$$

which concludes the proof.

Corollary 1.1 can be proved for action $a_i$ by applying the above procedure to the special case where the values of $a_j$ are known to be 0.

3.3 Proof of Lemma 1

**Proof.** Define $\phi$ to be a policy that follows the Monte Carlo sampling strategy until a depth $h$ and then follows the optimal policy. Using this policy, we can define the expected error of an action value estimate to be

$$E[\bar{Q}_i - Q_i] = E \left[ \frac{1}{n} \sum_{i \in Ch} \bar{v}_i - Q_i \right]$$

$$= E \left[ \frac{1}{n} \sum_{i \in Ch} \bar{v}_i - Q_i^\phi \right] + E[Q_i^\phi - Q_i]$$

$$= \frac{1}{n} \sum_{i \in Ch} \gamma^H_i E \left[ (\bar{v}_i - v_i) \right] + E[Q_i^\phi - Q_i]$$

$$= \frac{1}{n} \sum_{i \in Ch} \gamma^H_i \epsilon_i^0 + E[Q_i^\phi - Q_i]$$

where $v_i$ and $\bar{v}_i$ are the true and estimated values at the end of the sample trajectory, respectively. Intuitively, this is a decomposition of the expected error to the error of the baseline estimator and the expected error caused by the Monte Carlo sampling procedure.

Under the Monte Carlo convergence conditions, the negative sampling bias decays in expectation with increased samples and higher value actions are sampled more frequently, giving

$$0 \geq E[Q_j^\phi - Q_j] \geq E[Q_i^\phi - Q_i]$$

for $Q_j \geq Q_i$. Using the definition in eq. (20) and the inequality in eq. (21), we can write the difference in the expected error terms as

$$E[\bar{Q}_i - Q_i] - E[\bar{Q}_j - Q_j] = \sum_{i \in Ch_i} \gamma^H_i \epsilon_i^0 - \sum_{j \in Ch_j} \gamma^H_j \epsilon_j^0 + E[Q_i^\phi - Q_i] - E[Q_j^\phi - Q_j]$$

$$\leq \sum_{i \in Ch_i} \gamma^H_i \epsilon_i^0 - \sum_{j \in Ch_j} \gamma^H_j \epsilon_j^0$$

which concludes the proof.

4 Experiments

Experiments were conducted to evaluate the tightness of the presented bounds. We tested two problems: a simple multi-armed bandit and a grid-world MDP. We calculated the bounds under various conditions using a simple Monte Carlo estimator for both problems. For the MDP, we also tested MCTS with upper confidence tree (UCT) sampling. All testing was done in the Julia language using the POMDPs.jl framework [18]. Minimization of the $\alpha$ terms in the bounds was done with Nelder-Mead optimization [19].

Each trial, the Monte Carlo solver draws $n$ samples of actions from a discrete distribution over the complete action space. Distribution weights for each action $w_i$ are calculated from the softmax over the value estimates as

$$w_i \leftarrow \frac{\exp Q_i \tau^{-1}}{\sum_i \exp Q_i \tau^{-1}}$$

(24)
Figure 1: Bandit Results: Figure (a) shows the error probability for the bandit problem. Figure (b) shows the sub-optimality probability for the same. In both figures, the x-axis gives the total number of samples in the search. Solid lines show the mean bound with one standard-error bars, and the dashed lines show the true values. Curves for high and low payout variance are shown.

where $\tau$ is a temperature parameter, which was set to 10 for experiments in this work. Actions that have not yet been sampled have $q_i \leftarrow \infty$. In the MDP setting, after sampling the first action, the remaining actions are selected according to an $\epsilon$-greedy baseline policy, up to a specified depth $h$. Source code for the experiments is provided in the supplementary materials.

4.1 Multi-Armed Bandit

The bandit problem had 10 arms, each with a Gaussian payout distribution. The tests were run in episodes, with each episode having differently parameterized distributions. The payout mean values were sampled from a uniform distribution on $[-1, 1]$. Each payout distribution had the same variance $\sigma^2$ each episode. To test the bound performance under low and high variance, runs were conducted with with payout variance set to 0.5 and 0.75. The bandit expected payouts were estimated with the Monte Carlo solver for varying numbers of samples $n$.

For each episode, the error probability bound was calculated for the two actions with the highest estimated values. The sub-optimality bound was calculated for the best action for each sampling level and variance. The margin was $\epsilon = 0.1$ for both experiments. We calculated the true rates of error and sub-optimality in excess of $\epsilon$ across episodes. The average upper bound calculated for each trial and one standard error bounds are plotted along with the true rate curves in fig.1. The x-axis plots the total number of samples for the the search, not necessarily the samples over the measured action.

As can be seen, both the error and sub-optimality bounds decay exponentially with the number of samples drawn. The bound is fairly loose with a low number of samples, but decays exponentially and reaches near 0 gap at approximately 10,000 samples. Higher payout variance increases both the true rates and the upper bound values for the error probability and sub-optimality.

4.2 Gridworld MDP

In the gridworld MDP task, an agent is required to navigate through a discrete, 2D world from a random initial position to a goal destination. There are two goal locations generating positive rewards of 10 and 3, and two penalty locations giving negative rewards of -10 and -5. The episode terminates when the agent reaches any of the four reward-generating locations. Each step, the agent takes an action to attempt to move in one of the four cardinal directions. The agent successfully moves in the intended direction with a probability of 0.7 and moves randomly otherwise. The grid tested was $10 \times 10$. The time discount was set to $\gamma = 0.95$.

We used offline value iteration to learn a baseline policy and approximate optimal action values. The offline solver terminated after an update step with a Bellman residual less than $10^{-6}$. The simple Monte Carlo solver used an $\epsilon$-greedy baseline policy select actions after the initial step. The bootstrap value estimates were generated by the baseline policy with additive uniform noise bounded between $[-0.1, 0.1]$. We ran the tests with the solver searching to depths of 5, 10, and 25. As with the bandit
problem, we calculated the error and sub-optimality rates for the top performing actions. The results are shown in fig. 2.

![Figure 2: Gridworld Simple MC Results](image)

Figure 2: Gridworld Simple MC Results: Figure (a) shows the error probability for the gridworld MDP with a simple MC solver. Figure (b) shows the sub-optimality probability for the same. In both figures, the x-axis gives the total number of samples in the search. Solid lines show the mean bound with one standard-error bars, and the dashed lines show the true values. Curves for searches to depth 5, 10, and 25 are shown.

As with the bandit results, both the error and sub-optimality bounds decay exponentially with the number of samples drawn. At low samples, the bounds are tighter for the MDP than for the bandit problem, due to the higher true error rates. Conversely, at 10,000 samples, the bounds are not as tight. The effects of leaf-node error are shown by the trends in the search depth, with deeper searches tending to produce tighter bounds as a result of the reduction of the magnitude of the $\zeta$ terms.

We tested the tightness of the bounds on the popular MCTS-UCT algorithm, using the MCTS.jl implementation. We tested the performance with max depth was set to 5, 10, and 25 steps for each search. The UCT exploration constant was set to 1.0. As with the simple solver, leaf node values were estimated by the baseline policy with additive uniform noise. The results are shown in fig. 3.

The same trends can be observed in the MCTS results as in the simple Monte Carlo search results, however, the bounds are significantly looser at high sample counts in the MCTS tests. This is likely due to the influence of several shallow searches early in the search leading to higher magnitude $\zeta$ terms. In both results, the sample count of the action with the highest estimated value tended to be much higher than that of the second-highest.

These results suggest several adaptations to MCTS methods to improve expected error bounds. For a given number of samples, tighter error bounds can be achieved when the sample counts of the compare actions are comparable. For situations where accurate action selection from a discrete set is important, this suggests that increased exploration at the end of search may improve error performance. Deeper searches tend to result in better estimates than shallow searches. This suggests modifications to either increase search depth or to more heavily weight samples from longer trajectories in the value estimate.

5 Conclusions

In this work, we presented empirical bounds on the error probability for convergent Monte Carlo solvers over non-stationary bandit problems and Markov decision processes. We demonstrated that these bounds hold for a multi-armed bandit and a discrete gridworld MDP. Results showed that the bounds are loose for low sample numbers, but decay exponentially as samples increase. These bounds can serve as principled stopping criteria for Monte Carlo methods. We anticipate that these measures may be especially useful to methods that use an informed baseline such as offline policy improvement and performance verification of safety-critical systems.

The current work only tested these bounds for simple bandits and MDPs. Future work shall explore their performance in other, more complex tasks such as MCTS for partially observable MDPs [20].
Figure 3: Gridworld UCT-MCTS Results: Figure (a) shows the error probability for the gridworld MDP with the UCT-MCTS solver. Figure (b) shows the sub-optimality probability for the same. In both figures, the x-axis gives the total number of samples in the search. Solid lines show the mean bound with one standard-error bars, and the dashed lines show the true values. Curves for searches with maximum depth 5, 10, and 25 are shown.

Even with a moderate number of samples, the bounds were sometimes loose. Future work will look to specialize the general form presented in this work to produce tighter bounds for specific algorithms. The current work also only considered arithmetic mean estimators. Future work will extend the bounds to more general estimators.

Other forms of the presented bound shall be investigated to provide tighter bounds, possibly with more restrictive conditions. For example, several prior works have proved variants of the central limit theorem for non-stationary Markov chains [21]–[24]. Future work will investigate application of this to achieve tighter general bounds through the Berry-Esseen theorem [25], [26].

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