

Simulation-Based Approach to Efficient Commonsense Reasoning in Very Large Knowledge Bases

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Abstract

Cognitive systems must reason with large bodies of general knowledge to perform complex tasks in the real world. However, due to the intractability of reasoning in large, expressive knowledge bases (KBs), many AI systems have limited reasoning capabilities. Successful cognitive systems have used a variety of machine learning and axiom selection methods to improve inference. In this paper, we describe a search heuristic that uses a Monte-Carlo simulation technique to choose inference steps. We test the efficacy of this approach on a very large and expressive commonsense KB, Cyc. Experimental results on hundreds of queries show that this method is highly effective in reducing inference time and improving question- answering (Q/A) performance.

Introduction¹

Deductive reasoning is an important component of many cognitive systems. Modern cognitive systems need large bodies of general knowledge to perform complex tasks [Lenat & Feigenbaum 1991, Forbus *et al.* 2007]. However, efficient reasoning systems can be built only for small-to-medium sized knowledge bases (KBs). Very large knowledge bases contain millions of rules and facts about the world in highly expressive languages. Due to the intractability of reasoning in such systems, even simple queries are timed-out after several minutes. Therefore, researchers believe that resolution-based theorem provers

are overwhelmed when they are expected to work on large expressive KBs [Hoder & Voronkov 2011].

The goal query in knowledge-based systems (KBS) is typically provable from a small number of ground atomic formulas (GAFs) and rules. However, unoptimized inference engines can find it difficult to distinguish between a small set of relevant rules and the millions of irrelevant ones. Hundreds of thousands of axioms that are irrelevant for the query can inundate the reasoner with millions of paths. Therefore, to make the search more efficient in such a KBS, an inference engine is expected to assess the utility of further expanding each incomplete path. A naive ordering algorithm can cause unproductive backtracking. To solve this problem, researchers have developed two types of search control knowledge: (i) Axiom/premise selection heuristics: These heuristics attempt to find the small number of axioms that are the most relevant for answering a set of queries, and (ii) Certain researchers have worked on *ordering heuristics* for improving the order of rule and node expansions.

In the current work, we describe a simulation-based approach for learning an ordering heuristic for controlling search in large knowledge-based systems (KBS). The key idea is to simulate several thousand paths from a node. New nodes are added to a search tree, and each node contains a value that predicts the expected number of answers from expanding the tree from that node. These values are simply the average number of answers from all simulated paths that visit that node. The search tree expansion guides simulations along promising paths, by selecting the nodes that have the highest potential values.

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The algorithm produces a highly selective and asymmetric search tree that quickly identifies good axiom sequences for queries. Moreover, the evaluation function is not handcrafted: It depends solely on the outcomes of the simulated paths. This approach has the characteristics of a statistical anytime algorithm: The quality of evaluation function improves with additional simulations. The evaluation function is used to order nodes in a search. Experimental results show that: (i) this approach helps in significantly reducing inference time and, (ii) by guiding the search toward more promising parts of the tree, this approach improves the question-answering (Q/A) performance in time-constrained cognitive systems.

This paper is organized as follows: We start by discussing relevant previous work. Our approach to using simulations to learn a search heuristic is explained next. We conclude after analyzing the experimental results.

Related Work

Learning of search control knowledge plays an important role in the optimization of KBS for at least two reasons: First, the inference algorithms of KBS (e.g., backward chaining, tableaux algorithms in description logic (DL)), typically represent their search space as a graph. Hundreds of rules can apply to each node in a large KBS, and researchers have shown that the specific order of node and rule expansion can have a significant effect on efficiency [Tsarkov & Horrocks 2005]. Further still, first-order logic (FOL) theorem provers have been used as tools for such reasoning with very expressive languages (e.g., OWL DL, the Semantic Web Rule Language (SWRL)), where the language does not correspond to any decidable fragment of FOL, or where reasoning with the language is beyond the scope of the existing DL algorithms [Tsarkov *et al.* 2004, Horrocks & Voronkov 2006]. Researchers have also examined the use of machine learning techniques to identify the best heuristics for problems [Bridge *et al.* 2014]. There has been work as well on premise selection algorithms [Hoder & Voronkov 2011, Sharma & Forbus 2013, Meng & Paulson 2009, Kaliszyk *et al.* 2015, Kaliszyk & Urban 2015, Alama *et al.* 2014]. In contrast, we focus on designing ordering heuristics that will enable the system to work with all axioms. [Taylor *et al.* 2007] use reinforcement learning to guide inference, but they do not discuss how their approach applies to deep inference. In [Tsarkov & Horrocks 2005], the authors proposed certain rule-ordering heuristics (e.g., preference between \exists and \cup rules), and expansion order heuristics (e.g., a descending order of frequency of the usage of symbols). In contrast, we believe that rule-ordering heuristics should be based on the search state. In other recent work [Sharma *et al.* 2016, Sharma & Goolsbey 2017, Sharma & Goolsbey

2018], researchers have used different machine learning techniques to improve the efficiency of theorem provers. Our approach is different from all aforementioned research because none have shown how Monte Carlo tree search/UCT-based approach can be used to improve reasoning in a very large and expressive KBS. The work in other fields [Chaudhuri 1998, Hutter *et al.* 2014, Brewka *et al.* 2011] is also less relevant because it does not address the complexity of reasoning needed for large and expressive KBS.

Background

We assume familiarity with the Cyc representation language [Lenat & Guha 1990]. In Cyc, concepts are represented as collections. For example, “Cat” is a set of cats and only cats. Concept hierarchies are represented by the “genls” relation. For example, (genls Telephone Artifact-Communication) holds. The “isa” relation is used to link things to any kind of collections of which they are instances. For instance, (isa MicrosoftInc PubliclyHeldCorporation) holds. For any entity e , Cyc keeps track of the most specific collections of which it is an instance. This set is referred to as MostSpecificCollections (e).

Reasoning with Cyc representation language is difficult due to the size of the KB and the expressiveness of the language. The Cyc representation language uses full first-order logic with higher order extensions. Some examples of highly expressive features of its language include: (a) Cyc has more than 2000 rules with quantification over predicates, (b) It has 267 relations with variable arities, and (c) Although first-order logic with three variables is undecidable [Tsarkov *et al.* 2004], Cyc has several thousand rules with more than three variables. The number of rules in Cyc with three, four, and five variables is 48160, 23813 and 14014 respectively. Moreover, 29716 rules have more than five variables. In its default inference mode, the Cyc inference engine uses the following types of rules/facts during inference: (i) 28,429 role inclusion axioms (e.g., $P(x, y) \rightarrow Q(x, y)$); (ii) 3,623 inverse role axioms (e.g., $P(x, y) \rightarrow Q(y, x)$), (iii) 494,045 concepts and 1.1 million concept inclusion axioms (i.e., “genls” facts); (iv) 817 transitive roles; (v) 120,547 complex role inclusion axioms (e.g., $P(x, y) \wedge Q(y, z) \rightarrow R(x, z)$); (vi) 77,170 axioms of the type $P(x, \dots) \rightarrow Q(w, \dots)$ (these axioms are not included in role inclusion, complex role inclusion or concept inclusion axioms mentioned above); and (vii) 35,528 binary roles and 10,508 roles with arities greater than two. The KB has 27.3 million assertions and 1.14 million individuals.

To efficiently search in such a large KBS, inference engines often use control strategies. They define: (i) set of

support, i.e. the set of important facts about the problem; and (ii) set of usable axioms, i.e. the set of all axioms outside the set of support. At every inference step, the inference engine has to select an element from the set of usable axioms and resolve it with an element of the set of support. To perform efficient search, a heuristic control strategy measures the “weight” of each clause in the set of support, picks the “best” clause, and adds to the set of support the immediate consequences of resolving it with the elements of the usable list [Russell & Norvig 2003]. Cyc uses a set of heuristic modules to identify the best clause from the set of support. If S is the set all of all states, and A is the set of actions (i.e. inference steps), then a heuristic module is a tuple $h_i: (w_i, f_i)$, where f_i is a function $f_i: S \times A \rightarrow R$, which assesses the quality of an inference step, and w_i is the weight of h_i . The net score of an inference step is $\sum_i w_i f_i(s, a)$ and the inference step with the highest score is selected. Cyc uses several heuristics including the success rate of rules, decision trees [Sharma *et al.* 2016], regression-based models [Sharma *et al.* 2016], and a large database of useful rule sequences [Sharma & Goolsbey 2017]. We can define a policy that uses these heuristics:

$$\pi_{\text{BASELINE}}(s) = \operatorname{argmax}_a \sum_i w_i f_i(s, a) \quad \dots\dots (1)$$

In (1), we use all heuristics mentioned above to calculate the score of an inference step. In its default inference mode, Cyc uses a policy function, $\pi_{\text{BASELINE}}(s)$, to guide the search. This is used as the “baseline” in the experiments discussed below.

We consider the problem of finding proofs for first-order formulas in large KBs. The search begins with a root state s_0 .² At each turn, the inference engine selects an action $a_t \in A(s_t)$, where s_t is the current state, and $A(s)$ is the set of inference steps applicable to the state s . This sequential sampling of states and actions continues, without backtracking, until the search finishes upon reaching a terminal state with outcome z . The aim of the reasoner is to maximize z . A policy π is a function that maps states to actions. $\pi(s)$ is defined as $\max_a Q(s, a)$ where $Q(s, a)$ is used to denote the value of selecting action a in state s . It is simply the expected reward of action a :

$$Q(s, a) = \frac{1}{N(s, a)} \sum_{i=1}^{N(s)} I_i(s, a) \cdot z_i$$

² In search problems, an agent needs to find the correct move for each position encountered during search. Therefore, each node generated in a search graph is a *state*, and is represented by a set of features (discussed below).

where $N(s, a)$ is the number of times action a has been selected in state s , $N(s)$ is the total number of times the simulation has passed through state s , z_i is the outcome of the i th simulation, and $I_i(s, a)$ is 1 if action a was selected in state s in the i th simulation, and 0 otherwise [Browne *et al.* 2012].

Simulation-Based Learning

The basic premise of this approach is that we can learn to search for answers in large expressive KBS by taking random samples in the search space and these samples could be used to approximate the true value of choosing an inference step. Monte Carlo tree search (MCTS) algorithms use Monte Carlo simulations to evaluate the quality of nodes in a search tree. The search tree contains a node for each state s that has been generated during simulations. Each state s in the tree stores three types of values: $N(s)$, $N(s, a)$ and $Q(s, a)$ for every action a that applies to state s . The generation of search trees is guided by the outcomes of previous explorations, and the estimates progressively become more accurate [Browne *et al.* 2012, Gelly & Silver 2007].

Input: A state s

A depth cutoff, d

1. Create a root node with state s .
2. While within computational budget, do
 - a. $s' \leftarrow \text{TreePolicy}(s, d)$
 - b. $z \leftarrow \text{DefaultPolicy}(s')$
 - c. $\text{UpdateValues}(s', z)$

Figure 1: High-Level Description of the Simulation Algorithm

Figure 1 shows the high-level approach of the simulation algorithm. The algorithm takes a state and depth cutoff as input. The state contains information about the query that has to be answered. The algorithm can be divided into two distinct phases: (i) a *tree policy* is used until depth d : During this stage, the algorithm selects actions according to knowledge contained with the search tree (ii) When the depth of a node is greater than d , then a *default policy* is used to complete the simulation. Finally, the outcome of the simulation is “backed up” through the selected nodes to update their statistics.

Tree policy: In step 2(a) of the algorithm in Figure 1, we use the UCT algorithm to build a tree over the state space with the current state as the root node. The execution of the *TreePolicy* uses the following mechanism: If there exists an action in $A(s)$, the set of possible actions in state s , which has never been selected, the algorithm defaults to selecting it before any sampled action. Otherwise, the UCT algorithm selects an action that maximizes the upper confidence interval given by

$$Q^*(s, a) \leftarrow Q(s, a) + c \sqrt{\frac{\log N(s)}{N(s, a)}} \dots(2)$$

The first term in (2), $Q(s, a)$, favors actions that have led to better outcomes in the past. The second term provides a balance between *exploiting* actions that are currently believed to be optimal and *exploration* of other actions that currently appear sub-optimal but may turn out to be better in the long run [Gelly & Silver 2011, Balla & Fern 2009, Finnsson & Bjornsson 2008]. When an action is chosen, $N(s, a)$ increases; therefore it is less likely to be chosen in future simulations. On the other hand, $N(s)$ increases, and all other actions become more likely to be selected. The value of the exploration parameter c helps us in biasing the search toward or against exploration. In this paper, we report results of several experiments that show how performance changes with c . The tree policy is used to generate a tree until depth d .

Default policy: Our algorithm uses a *default policy* for expanding nodes that have depth greater than the pre-specified depth limit. Cyc's existing mechanism for selecting inference steps (discussed above) is used as the default policy. The default policy is executed for a fixed duration of time (set to 30 seconds).

Updating Values: In step 2(c) of the algorithm shown above, the algorithm reaches a terminal state and observes the number of answers obtained from the simulation. If R is the number of answers obtained from the simulation, then the following updates are made for any state action pair on the simulation path:

$$\begin{aligned} N(s, a) &\leftarrow N(s, a) + 1 \\ N(s) &\leftarrow N(s) + 1 \\ Q(s, a) &\leftarrow Q(s, a) + \frac{1}{N(s, a)} * [R - Q(s, a)] \end{aligned} \dots(3)$$

Search Space Formulation

We now define a search space that can be used by the UCT algorithm. We used 2,698 features to represent an abstract

state in search space. These features were identified by selecting the commonly occurring types in the most specific collections of entities in the KB [defined as `MostSpecificCollections()` on page 2]. The features can be grouped into three types: (i) 2,664 features were used to represent whether a certain argument of the focal literal³ is a sub-type of a given collection⁴; (ii) 33 features were used to represent whether a certain argument of the focal literal is an instance of a given collection⁵; and (iii) the depth of the sub-goal in the tree. Each node in the search space is described by a vector of 2,698 features. Edges in our search space correspond to resolution steps that transform one node into another. Let us consider an example. During training, an agent might create a root node with a query Q1 from the training set⁶.

$$\text{(relationAllExists parts Nivalenol Carbon)} \dots(Q1)$$

During the MCTS simulation, the UCT algorithm might lead the algorithm to choose the inference step A1 shown below:

$$\begin{aligned} &(\text{memberOfList ?element ?list}) \wedge \\ &(\text{completeAtomicComposition-List ?compound ?list ?coefficients}) \\ &\rightarrow (\text{relationAllExists parts ?compound ?element}) \dots(A1) \end{aligned}$$

The selection of inference step A1 will lead to a child state with the query Q2:

$$\begin{aligned} &(\text{memberOfList Carbon ?list}) \wedge \\ &(\text{completeAtomicComposition-List Nivalenol ?list ?coefficients}) \dots(Q2) \end{aligned}$$

The tree expansion will continue with the state discussed above. Let us assume that the search ends with just one answer at the terminal nodes. Then R would be set to 1, and $Q(s, a)$ values for the nodes in the simulation path would be updated by the equations shown in (3).

The Monte Carlo tree search continues for a given number of simulations, and it learns the relation contribution of each feature to the likelihood of deriving an answer. The action value function $Q(s, a)$ is approximated by a partial tabular representation $\tau \subseteq S \times A$, where S and A are the sets of all states and actions respectively. τ contains the search tree of all visited states and it is a subset of all

³ In a conjunctive or a disjunctive query, the inference engine might decide to resolve one of the literals in the query. The literal that is resolved is called the focal literal.

⁴ An example of the feature for query Q1 would be that second and third arguments of the focal literal are sub-types of "Trichothecene" and "NonMetal" respectively.

⁵ An example of this feature for the query Q1 would be that the first argument of the focal literal is an instance of `TransitiveBinaryPredicate`.

⁶ `(relationAllExists parts A B)` means that for any instance A1 of A, there exists an instance B1 of B, such that `(parts A1 B1)` holds.

(state, action) pairs. Unfortunately, this tabular representation does not allow for easy generalization between states. Therefore, we consider a simple k-nearest neighbor algorithm to generalize from similar states. We define the following:

$$Q_{NN}(s, a) = \frac{1}{k} \sum_{i=1}^k Q(s(i), a),$$

where $s(i) \in NN(k, s) \quad \dots(4)$

In (4), $NN(k, s)$ denotes the k-nearest neighbor of state s , where we use the Manhattan distance to compute the distance between two states.

Given (4), we can define a heuristic module with the following cost and policy function:

$$f_{MCTS}(s, a) = Q_{NN}(s, a) \quad \dots(5)$$

$$\pi_{MCTS}(s) = \operatorname{argmax}_a Q_{NN}(s, a) \quad \dots(6)$$

This heuristic module uses the k-nearest neighbor algorithm on the output of the Monte Carlo tree search algorithm, and to evaluate the quality of inference steps. In the next section, we use this heuristic module to order inference steps and discuss its performance.

Experimental Results

The selection of benchmark problems for training models and evaluating algorithms is a critical aspect of research. Our decision to select problem instances was based on following principles: (a) Artificially generated problems have played an important role in the development of SAT algorithms. However, the generation of artificial problem instances has not received sufficient attention in the commonsense reasoning community. Therefore, we focused on the problems from the real world. These queries were created by the knowledge engineers and programmers to test the performance of different applications and the inference engine⁷. Query Q1 discussed above is an example of a query that is part of our test sets. (b) We believe that heuristics and algorithms should be tested using the most difficult problems. The Cyc KB has thousands of queries of various levels of difficulty. Some queries are quite simple, and can be answered in a few milliseconds (e.g., (isa BarackObama Person)). On the other hand, some require generation of a large search space, and cannot be answered in several minutes. In this work, we have included problems from the latter group, and the

⁷ The query parameters (e.g., the number of desired answers) were set by the knowledge engineers and programmers. In most cases, we were expected to find one answer for a fully bound query (e.g., query Q1 discussed above).

results from the baseline experiments show that many queries cannot be answered within 10 minutes. Moreover, the Cyc KB is the largest and most expressive knowledge base that is amenable to deductive reasoning⁸. Therefore, our algorithm has been tested on one of the most difficult reasoning problems.

We divided the queries into four parts. One of the four parts was used as a test set, while the queries from the remaining three were used for training purposes⁹. This process was repeated with each of the four parts to produce four experiments. In each experiment, we tried to answer the following questions:

- How does search performance change with the number of simulations?
- How does search performance change with the value of c ?

The results of these four experiments are shown in Figures 2-5. We compared the performance of $\pi_{BASELINE}(s)$ and $\pi_{MCTS}(s)$ in these experiments. In the results, speedup in experiment e is defined as:

$$\text{Speedup}(e) = \text{Time}(\pi_{BASELINE}, e) / \text{Time}(\pi_{MCTS}, e)$$

where $\text{Time}(\pi, e)$ refers to the time required by the inference engine to answer queries in the experiment e when it uses the search policy π . The graphs also show how the proportion of queries that could be answered changes with the value of ‘ c ’ and the number of simulations.

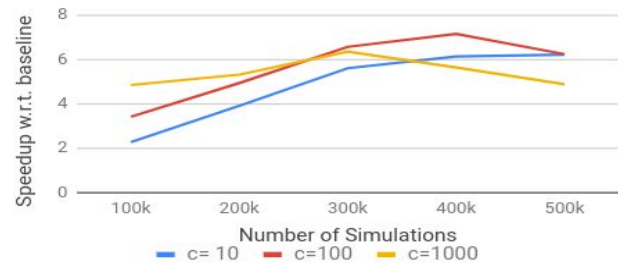


Figure 2a: Effect of exploration factor (' c ') and number of simulations on search performance ('Speedup') in Experiment 1.

The experimental data reported here was collected on a 4-core 3.40 GHz Intel processor with 32 GB of RAM. Due to the large time requirements of some of these queries, we

⁸ KBs like ConceptNet might have more GAFs than the Cyc KB, but they do not have axioms for deductive reasoning. Researchers have shown that Cyc-based problems are 1-3 orders of magnitude larger than other problems [see Table 1 in Hoder & Voronkov 2011].

⁹ For example, in experiment 2, query set 2 was used for testing purposes, whereas queries from sets 1, 3 and 4 formed the training set.

restricted the cutoff time for each query to 10 minutes. In Table 1, we show the parameter values for the best results obtained for each of the four experiments. For example, in the first experiment we could answer 46% of 266 queries in the baseline experiment. The best results from MCTS simulation was obtained when c was set to 100, and we allowed 400,000 simulations to learn the Q-values. This led to a speedup of 7.1 and we could answer 92% of all queries.

The results demonstrate the following:

- The search policy learned from MCTS simulations leads to significant speedup compared to the baseline.
- Moreover, we see that MCTS-based learning has also led to significant improvement in the Q/A performance.
- For small number of simulations (~100k), higher values of c (i.e. $c=1000$) lead to the best performance. However, the performance asymptotes soon. And the best performance is obtained for small to medium values of c (i.e. $c=10$ or 100).

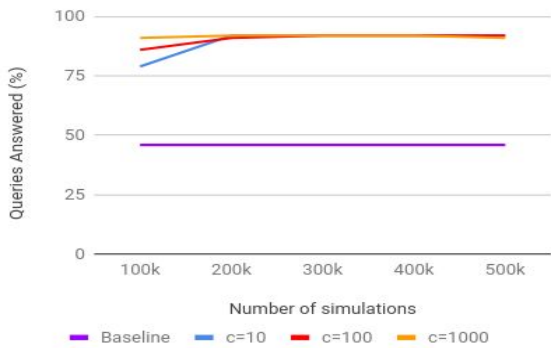


Figure 2b: Effect of exploration factor (c) and number of simulations on Q/A performance in Experiment 1.

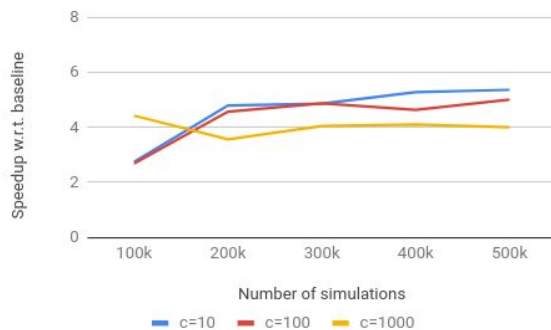


Figure 3a: Effect of exploration factor (c) and number of simulations on search performance ('Speedup') in Experiment 2.

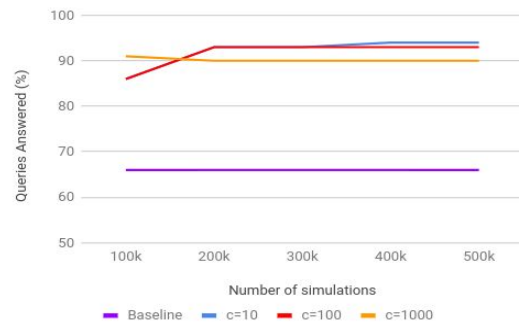


Figure 3b: Effect of exploration factor (c) and number of simulations on Q/A performance in Experiment 2.

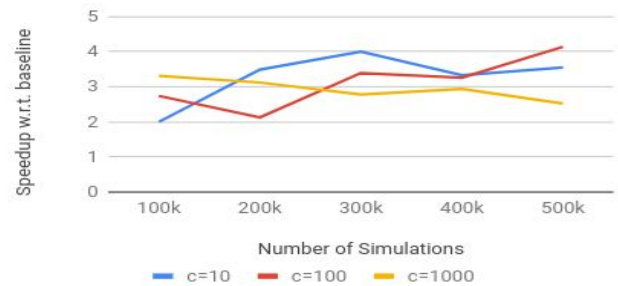


Figure 4a: Effect of exploration factor (c) and number of simulations on search performance ('speedup') in Experiment 3.

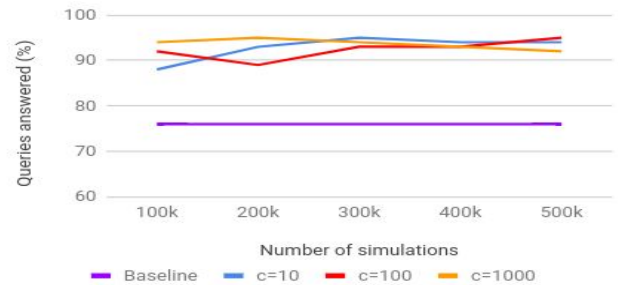


Figure 4b: Effect of exploration factor (c) and number of simulations on Q/A performance in Experiment 3.

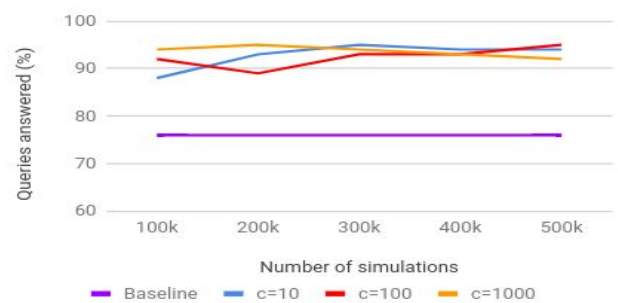


Figure 5a: Effect of exploration factor (c) and number of simulations on search performance ('Speedup') in Experiment 4.

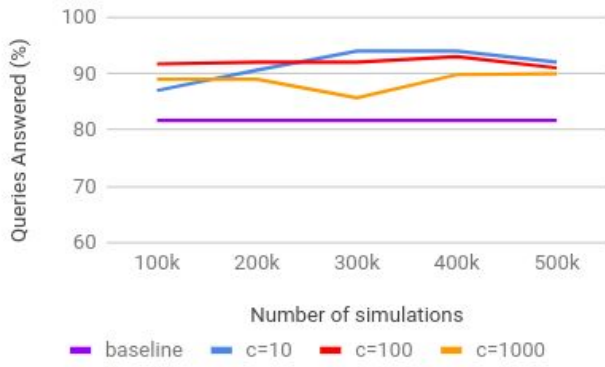


Figure 5b: Effect of exploration factor ('c') and number of simulations on Q/A performance in Experiment 4.

E	π	#Q	%A	c	TS	S	I(%)
1	B	266	46	-	-	-	-
	MCTS	266	92	100	400k	7.1	100
2	B	254	66	-	-	-	-
	MCTS	254	94	10	500k	5.4	42
3	B	261	76	-	-	-	-
	MCTS	261	94	100	500k	4.1	24
4	B	241	82	-	-	-	-
	MCTS	241	94	10	300k	3.3	14

Table 1: The experiment numbers are shown in the first column (labeled 'E'), and the second column shows the search policy that was used in the experiment: baseline(B) or MCTS. The third column (labeled #Q) shows the number of queries in each of the experiments. The proportion of queries answered is shown in the fourth column. The next column (labeled 'c') shows the value of c that led to these results. The sixth column (labeled 'TS') shows the number of simulations used in the Monte Carlo search. The column labeled 'S' shows the speedup obtained in the experiment. Finally, the last column (labeled I(%)) shows the improvement in the number of queries answered w.r.t. to the baseline.

We also divided the query by the "degree of difficulty" as measured by the time required to answer them by the baseline version of the inference engine. The speedup and improvement in the Q/A performance for the best MCTS

settings¹⁰ are shown in Table 2. For example, there were 597 queries that needed between 0 and 100 seconds in the baseline version. The best speedup obtained from MCTS simulations for these 597 queries was 1.23 and there was no change in the number of answerable queries..

Time (sec.)	#Q	S	I(%)
0-100	597	1.23	0
101-200	50	3.33	-2
201-300	38	13.79	0
301-400	9	11.79	0
401-500	1	18.2	0
>500	327	6.44	14600

Table 2: Column 1 shows the time requirements for the query in the baseline version. The second column shows the number of queries in the group. The third column shows the speedup w.r.t. to the baseline. And the fourth column (labeled I(%)) shows the percent improvement in the number of queries that were answered.

Conclusions

Deductive reasoning is an important issue for building large cognitive systems. To make deductive reasoning more efficient, in this work, we have proposed a sample-based search paradigm for learning search control knowledge. In this approach, we learn from simulated episodes that can be sampled from the model. Results for hundreds of queries from a very large and expressive KB show that this approach can lead to a significant reduction in inference time. It can also lead to notable improvement in Q/A performance. These results suggest several areas for future work: (i) First, we want to test these methods on a larger set of queries to ensure their generality, (ii) since feature selection plays an important role in the performance of learning algorithms, we will experiment with other schemes of feature selection, and (iii) we will design techniques to make Monte Carlo searches more efficient by including more domain knowledge in the simulation algorithm.

¹⁰ As discussed above, Table 1 shows the best MCTS settings obtained by us in the experiments.

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