Scallop: From Probabilistic Deductive Databases to Scalable Differentiable Reasoning

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Abstract

Deep learning and symbolic reasoning are complementary techniques for an intelligent system. However, principled combinations of these techniques are typically limited in scalability, rendering them ill-suited for real-world applications. We propose Scallop, a system that builds upon probabilistic deductive databases, to bridge this gap. On synthetic tasks involving mathematical and logical reasoning, Scallop scales significantly better without sacrificing accuracy compared to DeepProbLog, a principled neural logic programming approach. Scallop also scales to a real-world Visual Question Answering (VQA) benchmark that requires multi-hop reasoning, achieving 84.22% accuracy and outperforming two VQA-tailored models based on Neural Module Networks and transformers by 12.42% and 21.66% respectively.

1 Introduction

Integrating deep learning and symbolic reasoning in a principled manner into a single effective system is a fundamental problem in artificial intelligence [6]. Despite the great potential in terms of accuracy, interpretability, and generalizability, it is challenging to scale differentiable reasoning in the combined system while preserving the benefits of the neural and symbolic sub-systems [18].

In this paper, we propose Scallop, a systematic and effective framework to address this problem. The key insight underlying Scallop is a principled relaxation of exact probabilistic reasoning via a parameter $k$ that specifies the level of reasoning granularity. We observe that scalability is primarily hindered by reasoning about all proofs in computing the probability of each outcome. For a given $k$, Scallop only reasons about the top-$k$ most likely proofs, which asymptotically reduces computational cost while providing formal accuracy guarantees relative to the exact instantiation. Scallop thereby generalizes exact probabilistic reasoning and enables easy exploration of a rich space of tradeoffs. This tradeoff mechanism allows to drastically speed up the stochastic training of the involved neural components without sacrificing generalization ability.

The main technical contribution of Scallop concerns computing the set of top-$k$ proofs associated with each discrete fact efficiently, during the evaluation of a logic program, and correctly, by maintaining all and only the top-$k$ proofs. Scallop achieves this goal by formulating the problem in the framework of provenance for deductive databases [3]. The framework provides the theory and algorithms for tagging discrete facts derived by a logic program with information—in our case the set of top-$k$ proofs. Concretely, Scallop targets Datalog [11], a syntactic subset of Prolog. Although not Turing-complete, Datalog supports recursion and is expressive enough for a wide variety of applications.

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We evaluate Scallop on diverse tasks that involve combining perception with reasoning. On a suite of synthetic tasks that involve mathematical and logical reasoning over hand-written digits, Scallop scales significantly better without sacrificing accuracy compared to DeepProbLog [16], a principled neural logic programming approach. We also create and evaluate on a real-world task called VQAR (Visual Question Answering with Reasoning) which augments the VQA task with an external common-sense knowledge base for multi-hop reasoning. The goal is to answer a programmatic question with the correct subset of objects in a real-world image.

Scallop’s differentiable symbolic reasoning pipeline enables it to achieve 84.22% test accuracy, outperforming two VQA-tailored neural models based on Neural Module Networks and transformers by 12.42% and 21.66% respectively.

2 Background

We recap Datalog, the logic programming language that underlies Scallop, and present its probabilistic extensions that we leverage for inference and training tasks.

### Syntax of Datalog

A Datalog program $\bar{\mathcal{P}}$ consists of a set of input facts $\bar{\mathcal{F}}$, a set of rules $\mathcal{R}$, and a query $\mathcal{Q}$. The building block is an atom $a(t_1, \ldots, t_n)$ which consists of an $n$-ary predicate $a$ and a list of terms $t_1, \ldots, t_n$ as arguments. A fact $g$ is an atom which all the argument terms are constants; it may be an input fact (EDB) or a derived fact (IDB). Datalog rules are of the form $\alpha \leftarrow \alpha_1, \ldots, \alpha_m$ meaning that atom $\alpha$ in the head is true if all atoms $\alpha_i$ in the body are true. Multiple rules sharing a single head predicate denote disjunction (or union).

### Semantics of Datalog

Datalog programs can be executed using a bottom-up evaluation strategy. Starting from the input facts $\mathcal{F}$, we repeatedly apply the rules $\mathcal{R}$ in any order to derive new facts until a fixed point is reached. Upon completion, we obtain all the output facts $g$ of the query $\mathcal{Q}$. For example, with $\mathcal{F} = \{\text{left(o}_1, o_2), \text{below(o}_2, o_3)\}$ and $\mathcal{Q} = \text{left(o}_1, O)$, the execution of program $(\mathcal{F}, \emptyset, \mathcal{Q})$ produces $\{\text{left(o}_1, o_2)\}$. We denote the execution result as $\text{Exec}(\mathcal{P}) = \{g\}_{i=1}^n$. 

wish to compute the Proof Construction. Pr(\(\text{denoted}\) approximation. A key observation is that, when the inference system is used in a learning setting, Top-\(k\) disjunction respectively. Given two sets of proofs \(S\) during the bottom-up execution with tagged provenance. We initially tag each input fact \(f\) proof of (probabilistic) input facts \(q\) relational facts, \(J\) probabilistic reasoning. A probabilistic Datalog program \(P\) states that the digit \(f\) by associating a probability \(p\) and propagate proofs during execution from known facts to newly derived facts. When \(g\) is derived from a conjunction on \(f_1\) and \(f_2\), we combine the sets of proofs \(S_{f_1}\) and \(S_{f_2}\) to produce \(S_g\). The resulting \(S_g\) contains a single proof \(\{f_1, f_2\}\), as both \(f_1\) and \(f_2\) must be true for \(g\) to be true. More formally, we define two binary operations \(\otimes\), and \(\oplus\) corresponding to conjunction and disjunction respectively. Given two sets of proofs \(S_1\) and \(S_2\), we have
\[
S_1 \otimes S_2 = \{ F \mid F = F_1 \cup F_2, (F_1, F_2) \in S_1 \times S_2, F \text{ contains no disjunction conflict} \}.
\]
\[
S_1 \oplus S_2 = S_1 \cup S_2.
\]
With \(\oplus\) and \(\otimes\), the collection of sets of proofs \(P(P(F))\) forms a semiring (Appendix B.1), which we call the proof semiring. However, the complexity of \(S_g\) renders the computation infeasible.

**Top-\(k\) Proof Construction.** The probabilistic nature of our problem setting opens up room for approximation. A key observation is that, when the inference system is used in a learning setting,
We extend and evaluate on a suite of 6 synthetic tasks from DeepProbLog (DPL), as shown in Table 1. Accuracy. We next evaluate the tradeoff between the training runtime vs. testing accuracy in Scallop, as shown in Figure 4. With k = 1, Scallop learns the fastest in the beginning, but its high variance prevents it from converging to an optimal solution; with k = 5, it has much less variance and converges the fastest despite being slower in the beginning. All Scallop experiments converge within 30 minutes, while it takes DPL 14 hours to achieve the same accuracy (95.56%).

### Table 1: Testing accuracy of Scallop and DeepProbLog (DPL) on a suite of 6 synthetic tasks.

<table>
<thead>
<tr>
<th>Task</th>
<th>Goal Predicate</th>
<th>#Out</th>
<th>Max #Proofs</th>
<th>Scallop</th>
<th>DPL</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>sum2(3 7 10)</td>
<td>19</td>
<td>10</td>
<td>97.46%</td>
<td>96.90%</td>
</tr>
<tr>
<td>T2</td>
<td>sum3(3 7 5 15)</td>
<td>28</td>
<td>75</td>
<td>95.31%</td>
<td>95.47%</td>
</tr>
<tr>
<td>T3</td>
<td>sum4(5 7 5 17)</td>
<td>37</td>
<td>670</td>
<td>95.67%</td>
<td>96.07%</td>
</tr>
<tr>
<td>T4</td>
<td>sort2(5 7 0.1)</td>
<td>2</td>
<td>55</td>
<td>91.75%</td>
<td>94.99%</td>
</tr>
<tr>
<td>T5</td>
<td>sort3(7 4 2 1, 2, 0)</td>
<td>6</td>
<td>220</td>
<td>93.20%</td>
<td>94.57%</td>
</tr>
<tr>
<td>T6</td>
<td>sort4(7 5 5 5 3, 1, 2, 0)</td>
<td>24</td>
<td>715</td>
<td>95.31%</td>
<td>96.29%</td>
</tr>
</tbody>
</table>

We thereby introduce a top-k proof inference algorithm. With a user-specified hyper-parameter k ≥ 1, we perform top-k filtering at each step of the proof construction. We define two new operations, ⊗(k) and ⊕(k):

\[
S_1 \otimes(k) S_2 = \text{Top}_k(S_1 \otimes S_2), \quad S_1 \oplus(k) S_2 = \text{Top}_k(S_1 \oplus S_2).
\]

Intuitively, whenever ⊗ or ⊕ is performed, we rank proofs by their likelihood and preserve only the top-k proofs. This allows us to discard the vast majority of proofs and thus make inference tractable. An example run-through of top-3 natural join (⊗(3)) is depicted in Figure 3, where we perform a normal ⊗ operation followed by a top-3 filtering. As before, we construct a top-k proof semiring (Appendix E.2), with which we can express the resulting approximated beam of proofs \(\tilde{S}_q = \oplus_F \text{derives } q (\otimes_F S_f)\). Note that the size of \(\tilde{S}_q\) is bounded by \(k, |\tilde{S}_q| = O(k)\), reducing the exponential complexity of exact inference to a near constant one.

### Learning

We want to train a perception model \(M_\theta\) that takes in an input \(x\) and produces a probabilistic database \((F, J)\) such that after execution of \((R, Q)\), can derive the ground truth \(y\) as the output. Note that the probability of the input facts in the probabilistic database is generated by the perception model \(M_\theta\). Therefore each input probability \(p_i = \Pr(f_i)\) is also associated with their gradients \(\nabla_{\Pr(f_i)}\) with respect to the model parameters \(\theta\). To back-propagate the gradients through the inference process, similar to DeepProbLog [16], Scallop adopts a gradient semiring augmented WMC procedure. The beam of proofs \(S_q\) will be transformed into a weighted Conjunctive Normal Form (CNF) formula, where for each variable, \(f_i\), we attach the dual number \((\Pr(f_i), \nabla_{\Pr(f_i)})\) as its weight. As a result, the associated differentiable probability of each query result \(q_i\) will be \((\Pr(q_i), \nabla_{\Pr(q_i)})\), as computed by WMC. The result of the execution \(y' = \{q_i, (\Pr(q_i), \nabla_{\Pr(q_i)})\}_{i=1}^n\) along with the ground truth \(y\) is passed to the given loss function \(\mathcal{L}\). We, therefore, aim to minimize the following objective function: \(J(\theta) = \frac{1}{|D|} \sum_{(x,y) \in D} \mathcal{L}(y', y)\).
4.2 Visual Question Answering

Dataset. The VQAR dataset contains (a) 80,178 images from GQA [12], (b) object feature vectors + bounding boxes, (c) scene graphs with 500 object names, 609 attributes, and 229 relationships, (d) a shared knowledge graph with 6 rules and 3K knowledge triplets from CRIC [10], and (e) 4M programmatic queries and answer pairs. We further categorize these queries into different levels of difficulty by the number of occurring clauses from C2 to C6, where C2 is the simplest and C6 is the hardest. We formulate VQAR as a multi-label classification task. For each datapoint \((x, y)\) in our VQAR dataset, the input \(x\) consists of (a) the shared knowledge graph \(KG\), (b) a programmatic query, and (c) the object feature vectors and bounding boxes. The ground truth \(y\) is the set of objects that the given programmatic query identifies. All of our evaluated models but LXMERT share this same set of input and output. The accuracy is measured by Recall@5.

Setup of Scallop. We use a perception module consisting of three MLP-classifiers, \(M_\theta = (M_n, M_a, M_r)\), which predict names, attributes, and relations respectively. All predictions along with the entire \(KG\) form the probabilistic database. Over the database, we perform Datalog execution on the given programmatic query to obtain the set of identified objects. To compare the predicted set of objects and the ground truth set, we utilize binary cross-entropy as the loss function. The goal is to train the three classifiers in Scallop end-to-end and find the correct objects according to the question.

Baseline 1: DeepProbLog. It is prohibitively slow to train with DPL from scratch—a regular training sample from C6 can take DPL more than 100 hours to run. Therefore, instead of training with DPL, we use the perception model \(M_\theta\) trained with Scallop to test DPL’s inference capability. With 10 seconds timeout, DPL times out on 68.66% of the testing samples, while Scallop finishes all with an average running time under 0.3 seconds per sample.

Baseline 2: Neural Module Network. We compare against RVC [10], a Neural Module Network approach for VQA with external common-sense knowledge. This method first pretrains a TransE embedding [3] for the knowledge graph. Then, to mimic the reasoning process, it trains a set of neural modules that perform knowledge retrieval, scene graph traversal, and logical operations. The modules are assembled according to the programmatic query and can leverage object-based features.

Baseline 3: LXMERT. We also compare to LXMERT [20], a recent transformer-based approach that emphasizes its transfer learning ability. LXMERT takes in a natural language question corresponding to the given programmatic query. As this model cannot explicitly use a knowledge base, we leverage the implicit relations learned through pre-training over a variety of image-language tasks: MS COCO [15], Visual Genome [2], and GQA [12]. Finally, we fine-tune LXMERT on our VQAR training set.

5 Conclusion and Future Work

We proposed Scallop, a framework for scaling differentiable reasoning based on Datalog, motivated by real-world applications that necessitate combining perception and reasoning. The key idea underlying Scallop is to relax exact probabilistic reasoning via a tunable parameter that specifies the level of reasoning granularity. In future, we plan to develop expressive extensions to Scallop, target more challenging neuro-symbolic applications, and optimize the end-to-end pipeline on modern hardware.

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References


**A Illustrative Overview**

We illustrate our approach using two tasks: a simple task called sum2 and the real-world VQAR task.

**A Simple Task.** The sum2 task from [16] concerns classifying sums from pairs of hand-written digits, e.g., \(2 + 7 = 10\). As depicted in Figure 5, we specify this task using a neural and a symbolic component, following the style of DeepProbLog [16]. The neural component is a perception model that takes in an image of hand-written digit [14] and classifies it into discrete values \{0, ..., 9\}. The symbolic component, on the other hand, is a logic program in Datalog for computing the resulting sum. The interface between the neural and symbolic components is a probabilistic database which associates each candidate output of the perception model with a probability. For instance, the fact \(0.85 :: \text{d}(0,3)\) denotes that image 0 is recognized to be the digit 3 with probability 0.85.

Evaluating the logic program on the probabilistic database yields a weighted boolean formula for each possible result of the sum of two digits, i.e., values in the range \{0, ..., 18\}. Each clause of such a formula represents a different proof of the corresponding result. For instance, the bottom left of Figure 5 shows the formula representing all 9 proofs of the ground truth result 10. Each such formula is input to an off-the-shelf weighted model counting (WMC) solver to yield the probability of the corresponding result, e.g., \(0.7261 :: \text{sum}(2, 7, 10)\).

The scalability of this approach is limited in practice by WMC solving whose complexity is at least \#P-complete [19]. We observe that computing only the top-\(k\) most likely proofs bounds the size of each formula to \(k\) clauses, thereby allowing to trade diminishing amounts of accuracy for large gains in scalability. Moreover, stochastic training of the deep perception models itself can tolerate noise in data. As we show later in our experiments, the additional noise introduced by the top-\(k\) approximation can be well-compensated for by the stochastic training algorithm.

Scallop embodies this insight by introducing a parameter \(k\) which can be task-dependent, and even for a particular task, tuned differently for learning and inference. A higher \(k\) leads to slower inference, but accelerates the convergence of learning, especially for complex or sparse feedback; thus, Scallop enables to achieve the best of both worlds by employing a higher \(k\) during training, and a lower \(k\) thereafter. While Scallop’s inference time is under 0.1 second per task for the sum2 task regardless of the choice of \(k\), the difference is much more pronounced for the sum3 task of adding three digits: 0.05 seconds for \(k = 1\) versus 6.15 seconds for \(k = 15\).

**Visual Question Answering.** We next illustrate applying Scallop to a complex real-world task, Visual Question Answering (VQA) [2], which is widely studied in the deep learning literature. The task concerns answering a given question using knowledge from a given image of a scene. Since we are interested in tasks that combine perception with reasoning, we extend the VQA task with multi-hop reasoning over an external common-sense knowledge base. The resulting task, which we
call VQAR, improves upon the VQA task in two important ways: it generalizes the VQA task by allowing questions that require external knowledge, and it allows to precisely control the reasoning complexity through the number of hops needed to answer them.

We thereby develop a new dataset consisting of real-world images of scenes and object identification questions that necessitate varying hops of reasoning in a fixed external knowledge base.

It is natural to express the VQAR task using a combination of neural and symbolic modules akin to the sum2 task. As Figure 6 illustrates, these modules are more complex, reflecting the real-world nature of this task. The neural module is a perception model that takes the object feature vectors (extracted by pre-trained vision models) and outputs a scene graph comprising the predicted name and attribute distributions of each object, and relationships between the objects—all of which are uniformly represented as a probabilistic database. For instance, the tuple 0.83 :: name(o12, giraffe) denotes that name of object o12 is classified as giraffe with probability 0.83.

Likewise, the symbolic module uniformly represents both the logic representation of the question and the external knowledge base as a logic program in Datalog. Evaluating the program on the probabilistic database yields the answer, e.g., target(o12). The example in Figure 6 highlights the need for external knowledge: although the question refers to the concept of an “animal” that is missing in the scene graph, Scallop is able to derive the conclusion name(o12, animal) without changing the perception model. The derivation involves two-hop reasoning—two applications of the recursive rule name(O, N) :- name(O, N'), is_a(N', N). Evaluating this rule on facts from the scene and knowledge graphs:

\[
\begin{align*}
\text{name}(o12, \text{giraffe}) & \quad \text{is_a}(\text{giraffe}, \text{mammal}) \\
\text{name}(o12, \text{mammal}) & \quad \text{is_a}(\text{mammal}, \text{animal}) \\
\text{name}(o12, \text{animal}) &
\end{align*}
\]

While more sophisticated models can learn the representation of concepts such as animal from a large corpus, relying on such pretrained representation sacrifices the benefits of symbolic reasoning, such as interpretability, data efficiency, and generalization to unseen concepts.

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2 In contrast, prior works such as the GQA dataset [12] are limited to varying the reasoning complexity in the question alone, which renders the question unwieldy.

3 We presume that the input question is in programmatic form because existing models for semantic parsing achieve high accuracy in translating from natural language text to programmatic form [4].
B  Theoretical Guarantee

B.1 Proof Semiring

Definition B.1 Given a program $P = (F, R, J, Q)$, the collection of sets of proofs $S$ is defined to be

$$\{ S \mid S \in \mathbb{P}(P(F)) \text{, } \forall F \in S, \text{ } F \text{ is a proof} \}.$$ 

Note that $F$ being a proof implies that there is no disjunction conflict in $F$. That is,

$$\forall f_1, f_2 \in F, j \in J, f_1 \in j \implies f_2 \notin j$$

Definition B.2 The two binary operators $\oplus$ and $\otimes$: $S \times S \rightarrow S$ are defined as

$$S_1 \oplus S_2 = S_1 \cup S_2,$$

$$S_1 \otimes S_2 = \{ F \mid F = F_1 \cup F_2, (F_1, F_2) \in S_1 \times S_2, \text{ } F \text{ contains no disjunction conflict} \}.$$ 

Theorem B.3 $(S, \oplus, \otimes, \emptyset, \{ \emptyset \})$ forms a commutative semiring, which we call Proof Semiring.

Proof We show that (1). $\emptyset$ is a $\oplus$ identity, (2). $\{ \emptyset \}$ is a $\otimes$ identity, (3). $\oplus$ and $\otimes$ are commutative and associative, (4). multiplication is distributive, and (5). multiply by $\emptyset$ annihilates the operand. 

1. $\emptyset$ is a $\oplus$ identity. Given $S \in S$,

$$\emptyset \oplus S = S \cup \emptyset = S = \emptyset \cup S = \emptyset \oplus S.$$ 

2. $\{ \emptyset \}$ is a $\otimes$ identity. Given $S = \{ F_1, F_2, \ldots, F_n \} \in S$, we have

$$\emptyset \otimes \{ \emptyset \} = \{ F_1 \cup \emptyset, F_2 \cup \emptyset, \ldots, F_2 \cup \emptyset \} = S$$

3. $\oplus$ is commutative: Given $S_1$ and $S_2$,

$$S_1 \oplus S_2 = S_1 \cup S_2 = S_2 \cup S_1 = S_2 \oplus S_1.$$ 

$\otimes$ is commutative: Given $S_1$ and $S_2$,

$$S_1 \otimes S_2 = \{ F_1^1 \cup F_2^2, \ldots \} = S_2 \otimes S_1$$

$\oplus$ is associative: Given $S_1, S_2, S_3 \in S$,

$$S_1 \oplus (S_2 \oplus S_3) = S_1 \cup (S_2 \cup S_3) = (S_1 \cup S_2) \cup S_3.$$ 

$\otimes$ is associative: Given $S_1, S_2, S_3 \in S$ and $S_i = \{ F_i^1, F_i^2, \ldots, F_i^m \}$, we denote

$$F_{x,y,z} = \begin{cases} 
F_x^1 \cup F_y^2 \cup F_z^3 \\ \emptyset 
\end{cases}$$

if no disjunction conflict

otherwise,

where $x \in 1 \ldots n_1, y \in 1 \ldots n_2, z \in 1 \ldots n_3$. We then have

$$S_1 \otimes (S_2 \otimes S_3) = \{ F_{111}, F_{112}, \ldots, F_{n_1n_2n_3} \}$$

$$= (S_1 \otimes S_2) \otimes S_3$$

4. Distributive. Given $S_1, S_2$, and $S_3 \in S$ similar to above, we have

$$S_1 \otimes (S_2 \oplus S_3) = S_1 \otimes (S_2 \cup S_3) = (S_1 \otimes S_2) \cup (S_1 \otimes S_3)$$

$$= (S_1 \otimes S_2) \oplus (S_1 \otimes S_3)$$

5. Multiplying $\emptyset$ annihilates the operand:

$$S_1 \otimes \emptyset = \emptyset.$$ 

Therefore $(S, \oplus, \otimes, \emptyset, \{ \emptyset \})$ forms a semiring.

Theorem B.4 $S$ is naturally ordered and $\omega$-complete \[\blacksquare\].

Proof We define a partial order $\leq$ such that $S_1 \leq S_2 \iff S_1 \subseteq S_2$. Therefore our $S$ is naturally ordered. In addition, our chain has a strict upper bound which is $\mathbb{P}(F)$, as $\forall S \in S, S \subseteq \mathbb{P}(F)$. Hence $S$ is also $\omega$-complete. \[\blacksquare\]
Theorem B.5 The end result $S_q$ can be expressed as

$$S_q = \bigoplus_{F \text{ derives } q} \left( \bigotimes_{f \in F} S_f \right).$$

Proof Under the provenance semiring framework [11], we define a $S$-Relation $R : G \rightarrow S$, such that

$$R(f) = \{ \{ f \} \} = S_f, \forall f \in F.$$  

With $S$ being a commutative $\omega$-continuous semiring, $Q$ being a datalog query, and our $S$-Relation $R$, by Definition 5.1 [11], we have

$$Q(R)(t) = \bigoplus_{\tau \text{ yields } t} \left( \bigotimes_{t' \in \text{leaves}(\tau)} R(t') \right),$$

where $\tau$ ranges over all $Q$-derivation trees for $t$. In our case, we seek the result $t = q$, which is, $S_q = Q(R)(q)$. At the same time, we know that $\tau$ is a derivation tree for $q$ and its leaf nodes $t'$ are from our input facts $F$. Note that $\text{leaves}(\tau)$ is simply a proof $F$ in our case and each $t' \in \text{leaves}(\tau)$ is an input fact $f \in F$. Therefore we know that $t' \in F$ and $R(t') = S_{t'}$. At last, we can express $S_q$ as

$$S_q = Q(R)(q) = \bigoplus_{F \text{ derives } q} \left( \bigotimes_{f \in F} S_f \right),$$

as expected. \[\square\]

Proposition B.6 $|S_q| = \mathcal{O}(2^{|F|}).$

Proof (Sketch) Theoretically, $2^{|F|}$ is the absolute upper bound as there could be at most $2^{|F|}$ proofs, given by that each input fact $f \in F$ can be in or not in a proof. \[\square\]

In reality, this upper bound can rarely be achieved. The actual size of $S_q$ is always determined by various factors including input facts, rules, and disjunctions.

B.2 Top-$k$ Proof Semiring

We repeat our definitions of $\oplus^{(k)}$ and $\otimes^{(k)}$ here:

Definition B.7 With a $\text{Top}_k : S \rightarrow S$ defined as keeping the top-$k$ proofs, we define

$$S_1 \otimes^{(k)} S_2 = \text{Top}_k(S_1 \otimes S_2),$$

$$S_1 \oplus^{(k)} S_2 = \text{Top}_k(S_1 \oplus S_2).$$

Proposition B.8 The approximated set of proofs $\tilde{S}_q$ can be expressed as

$$\tilde{S}_q = \bigoplus_{F \text{ derives } q} \left( \bigotimes_{f \in F} S_f \right).$$

Proof (Sketch) First show that $S$ still form a semiring under $\oplus^{(k)}$ and $\otimes^{(k)}$ with the exact same proof as in Theorem A.3. Then follow Theorem A.5 to show that this expression still holds. \[\square\]

Proposition B.9 $|\tilde{S}_q| = \mathcal{O}(k).$

Proof (Sketch) This follows directly from the definition of $\oplus^{(k)}$ and $\otimes^{(k)}$ as at each step the size of the resulting set of proofs is capped by $k$. \[\square\]

B.3 Approximation Analysis

Proposition B.10 We give an approximation error bound

$$|\Pr(S_q) - \Pr(\tilde{S}_q)| \leq \sum_{F \in S_q \setminus \tilde{S}_q} \Pr(F).$$
This is a loose bound given by the difference between $S_q$ and $\tilde{S}_q$. Equality happens when all the proofs in $S_q$ are disjoint.

**Proposition B.11** For a program $P = (F, R, J, Q)$, if $J = \emptyset$, then we have $\tilde{S}_q = \text{Top}_k(S_q)$.

The proof of this proposition can be found in Theorem 1 of [8]. Under that setting, there is no $J$ and therefore $J = \emptyset$. At the same time the top-$k$ derivation tree is equivalent to our top-$k$ proof.
C VQAR Dataset Collection

C.1 Dataset Generation

We focus on the task of multi-hop VQA with external common-sense knowledge. For this purpose, we generate an object retrieval VQA dataset, called VQAR, by building upon two existing datasets, GQA [12] and CRIC [10]. These datasets comprise real-world images from the Visual Genome and have complementary qualities necessary for our task. In particular, we use curated scene graphs of the images from the GQA dataset, and we use curated knowledge graphs related to visual questions from the CRIC dataset.

Scene and Knowledge Graphs. Starting with the image and scene graph pairs from the GQA dataset, we further pre-process the scene graphs to generate cleaner questions, as follows. We only include the top 500 most frequently occurring object names, which covers more than 88% of all object occurrences. We retain 609 attributes and 229 relationships after normalizing their names. Finally, we ensure that every image has more than 5 objects so that its scene graph is complex enough. After pre-processing, we are left with 80,178 images with their scene graphs.

The knowledge graph provided by the CRIC dataset comprises triplets of the form \(\langle e_1, r, e_2 \rangle\), where \(e_1\) and \(e_2\) are two entities, and \(r\) describes a relationship between them, e.g., \(\langle\text{giraffe}, \text{is\_a}, \text{animal}\rangle\). We represent each type of relationship as a separate binary relation. There are 10 different types of relationships, such as \(\text{is\_a}\), \(\text{used\_for}\), and \(\text{capable\_of}\). We considered two alternatives to CRIC: OK-VQA [17] and KB-VQA [21]. OK-VQA includes common-sense knowledge as part of the question itself, and thus precludes multi-hop reasoning. KB-VQA comprises over 160M probabilistic common-sense knowledge triplets drawn from Wikilinks, but is noisy.

Programmatic Query Generation. Existing programmatic VQA questions typically seek aggregated results which makes them liable to exploitable bias. For instance, a binary choice question may be answered by an educated guess without using reasoning. We therefore generate object identification queries that require reasoning to varying degrees. Such queries are harder to exploit, since objects vary from scene to scene.

We use GQA’s domain specific language to generate programmatic queries for our purpose. Such a query is composed of a functions sequence that successively identify a set of objects, where the final set of objects are the targets to our query. We define a suite of 9 such functions as shown in Table 3. Consider for instance the RELATE function. Viewing the scene graph as a relation \(\langle\text{subject, predicate, object}\rangle\), this function identifies the object, given the subject and predicate. Then, the natural language question in Figure 6 corresponds to the following programmatic query:

\[\text{[INITIAL, RELATE(left), FIND HYPERNYM(animal), FIND ATTR(tall)]}\]

The number of clauses \(n\) determines the degree of multi-hop reasoning in the query, which we call a query of type \(C_n\). Thus, the above example is a query of type \(C_4\). Furthermore, such queries are straightforward to translate into Datalog, allowing them to be executed using Scallop. The Datalog counterpart of the above query is also shown in Figure 6.

Our query generation procedure always starts with the INITIAL function which refers to all objects in the scene graph. It then traverses through the scene graph and the knowledge graph to identify valid clauses to append to the query. Lastly, we execute the resulting query using Scallop to obtain the ground truth answer. We control the difficulty of the query by the number of its clauses.

Since we are not targeting the natural language questions, we only generate these questions in functional program form. For each image, we generate 10 different question and answer pairs for each clause length 2 to 6, to obtain 4 million data points in total. We split them into training (60%),

<table>
<thead>
<tr>
<th>Category</th>
<th>Function Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scene Graph</td>
<td>INITIAL, FIND NAME, FIND ATTR, RELATE, RELATED REVERSE</td>
</tr>
<tr>
<td>Knowledge Graph</td>
<td>FIND KG, FIND HYPERNYM</td>
</tr>
<tr>
<td>Logic Operators</td>
<td>AND, OR</td>
</tr>
</tbody>
</table>

Table 3: Basic functions used to generate questions in VQAR.
validation (10%), and testing (30%) sets, and ensure that all the questions about the same image occur within the same split to test generalizability.
D Experiments

D.1 Machines

All experiments are conducted on a machine with two 20-core Intel Xeon CPUs, four GeForce RTX 2080 Ti GPUs, and 768 GB RAM.

D.2 Synthetic Experiment Setup

Models. Our perception model uses two convolutional layers and two fully connected layers, which takes in the MNIST image as input, and output a distribution on 10 possible numbers, 0-9. This model is trained from scratch in an end-to-end fashion.

Training Hyper-parameters. The learning rate for both DeepProbLog and Scallop is 0.01; the batch sizes for Scallop is 64, and 2 for DeepProbLog, as batch size 64 for DeepProbLog converges too slow. We set the epoch size to 20, where both of the methods converge before 5 epochs.

Evaluation Metric. Our evaluation metric is accuracy. If the predicted outcome is the same as the correct one, the accuracy is 1, otherwise, the accuracy is 0.

D.3 VQAR Experiment Setup

Models. Our perception model uses pre-trained fixed-weight Mask RCNN and ResNet models, which take as input an image and produces feature vectors (along with bounding boxes). Then, input facts representing names, attributes, and object relationships are extracted by 3 separate trainable MLP classifiers. We note that these classifiers integrated with our reasoning engine are trained from scratch in an end-to-end fashion. We also note that to ensure a fair comparison, the visual input (features + bounding boxes) we feed to all baselines (including LXMERT) are the same.

Baselines. We use three baselines that are representative of different state-of-the-art approaches to combining perception and reasoning: (1). Neural Module Network (NMN), which uses a set of neural modules, one per basic function, (2). DATALOG-RL, a reinforcement learning approach supervised by a discrete logic reasoning engine, (3). DeepProbLog, a probabilistic logic programming approach, and (4). LXMERT, a transformer based approach.

Dataset. To evaluate performance, we sample 50K tasks from the training split, 5K from the validation split, and 5K from the testing split. To measure generalizability and sample complexity, we sample 10 to 10K tasks of type C2 for training, and 1K tasks each of type C2 to C6 for testing.

Training Hyper-parameters. All the models converge under 20 training epochs. The learning rate is tuned and is 0.0001 for Scallop, NMN, and DPL, 0.00001 for LXMERT. We select the loss function to be binary cross-entropy loss, except DPL that only supports cross-entropy loss. With batch size 16 and $k = 10$, Scallop achieves the best accuracy in reasonable training time. All the optimizers are Adam.

Model Size Comparison. The model for Scallop, datalog-RL and DeepProbLog are the same, so they share the same model size: 10.91MB for attribute classification, 14.67MB for name classification, 17.78MB for relation classification. The neural modular networks method contains 8 modular network. The and or modules are 0.02MB, the find_name and find_attribute modules are 9.63MB, the find_hypername and find_KG are 8.61MB, the relate and relate_reverse modules are 18.06MB. The LXMERT method uses a large pretrained module, which is 836MB.

Evaluation Metric. Since our tasks essentially involve object retrieval, any ground truth label is a set of object IDs that satisfy the constraints stated in the question. For set comparison, we select the recall@5 rate as the evaluation metric. It assesses the recall on the top 5 probable predictions.

D.4 More VQAR experiments

Top-k selection. We compare the performance of Scallop under different choices of $k$: 1, 5, 10, and 15. We train on 10K C2 tasks and test on 1K tasks of varying clause length. As shown in Figure ??, We observe that the recall@5 score increases as $k$ grows, as expected. However, the larger the $k$, the longer it takes to process a single task at training time. Our running time increases modestly from $k = 1$ to $k = 10$, and more dramatically when $k = 15$. We thus confirm that Scallop can strike a
balance between efficiency and accuracy by tuning the $k$ value, and that exact probabilistic reasoning is not required to obtain good performance on VQAR tasks.

**Ablation Study: Datalog Reinforcement Learning (DATALOG-RL).** In this study, we remove the differentiability in Scallop's learning pipeline. Instead, we sample a discrete scene graph, run it through the standard Datalog execution, and use the overlap in predicted objects as a reward to estimate the gradient using REINFORCE [22]. This method does not scale with the training dataset of 50K tasks, so we only perform the generalizability experiments (Figure 7).

**Results.** Table 2 and Figure ?? compares the performance of Scallop, NMN, and LXMERT based on 50K training tasks. Scallop significantly outperforms both in terms of accuracy and data efficiency. Figure 7 shows that Scallop generalizes to answer more difficult questions (1K from each of C2-C6) even when trained on only the easiest ones (10K C2). Figure 8, on the other hand, shows the testing accuracy (on 1K C2) when trained on varying dataset sizes (10, 100, 1000, and 10,000 C2). We observe that Scallop has the best data efficiency. Finally, with DATALOG-RL we observe that the addition of differentiable reasoning is crucial to Scallop’s learning performance.

### D.5 DeepProbLog

We give a more fine-grained analysis of the DeepProbLog performance. In particular, we investigate the relation between timeout rate and query complexity. Again, our timeout is set to 10 seconds.

<table>
<thead>
<tr>
<th>Test Dataset</th>
<th>Timeout Rate w/ KG</th>
<th>Timeout Rate w/ Rela</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000 C2</td>
<td>100%</td>
<td>21.43%</td>
</tr>
<tr>
<td>1000 C3</td>
<td>91.55%</td>
<td>73.09%</td>
</tr>
<tr>
<td>1000 C4</td>
<td>88.79%</td>
<td>70.74%</td>
</tr>
<tr>
<td>1000 C5</td>
<td>88.54%</td>
<td>62.27%</td>
</tr>
<tr>
<td>1000 C6</td>
<td>87.85%</td>
<td>75.20%</td>
</tr>
</tbody>
</table>

Table 4: Success Rates of DeepProbLog
Table 5: DeepProbLog timeout rate on 1000 tasks of types C2-C6.

<table>
<thead>
<tr>
<th>Dataset (Clause-(\tau))</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Timeout rate (%)</td>
<td>54.5%</td>
<td>69.7%</td>
<td>74.4%</td>
<td>70.7%</td>
<td>74.0%</td>
</tr>
</tbody>
</table>

In the above table, column 2 shows DeepProbLog’s timeout rate when at least one KG-related clause is presented in the programmatic query. It is worth noting that DeepProbLog performs the worst on the C2 dataset. In C2, the KG-related clause is the only clause in the programmatic query other than the first INITIAL clause. This implies that there is no constraint posed around the KG clause, leading to a huge amount of possible proofs, and in turn causing the timeout.

Column 3 shows DeepProbLog’s timeout rate when at least one relation-related clause is presented in the programmatic query. As one would expect, the more relation is included in the query, the deeper the reasoning will need to be. The table clearly shows that DeepProbLog, without approximation strategy, suffers from handling deep reasoning chain, as that would lead to an exponential amount of proofs.
E Implementation Details

The Scallop implementation is composed of compilation, runtime, and weighted model counting. The compilation part takes in a Datalog program and compiles it into a positive relational algebra form. Then, the runtime executes the generated relational algebra expression and generates the query output with its top-k proofs. Last, the weighted model counting process takes in the query output with the fact probability and calculates the corresponding output probability with gradients. We implement Scallop in Rust for better efficiency.

E.1 Compilation

The compilation process takes in the high-level datalog program and compiles it into an executable form. First, the compiler preprocesses the program, ensures no parsing errors and type errors occur in the given program. Then, it analysis the datalog program and convert it into a mid level positive relational algebra form, which contains **empty**, **union**, **projection**, **selection**, **natural join** and **renaming**. These mid-level relational algebra forms will be further compiled into **join** and **disjunction**, which are directly executable by the runtime.

E.2 Runtime

The runtime execution adopts a bottom-up evaluation strategy with a tagging system for the provenance semiring. It starts with all the input facts tagged with themselves as proofs and keeps applying the rules in the **join** and **disjunction** form until a fixpoint is reached. Whenever a **join** happens on tuple \( t_1 \) tagged with \( F_1 \), and tuple \( t_2 \) tagged with \( F_2 \), the generated tuple is tagged with \( F_1 \otimes F_2 \), where the \( \otimes \) is easily configurable. The story is similar for **disjunction** case. In terms of optimization, we adopt the leap join strategy rather than the naive join to increase the evaluation efficiency.

E.3 Weight Model Counting

The weighted model counting algorithm is the same as DeepProbLog. We depend on the sentential decision diagram to realize the weighted model counting process. To realize the gradient calculation, we also implemented a semiring system to carry the additional information during weighted model counting.
F Synthetic Task Details

F.1 Sum n numbers

The sum n numbers task is an extension from the original MNIST digit recognition task. Instead of recognizing a single digit from the image, this task takes in n images, and recognizes the sum of all the input images. For example, \( \text{sum}([2, 7]) \) is corresponding to a sum2 task. In a scallop program, we have the rule 
\[
\text{sum}(I_1, I_2, DA + DB) : \text{digit}(I_1, DA), \text{digit}(I_2, DB),
\]
where \( I_j \) are the image ids in the MNIST dataset. This rule propagates the probability from low level perception in \( \text{digit}(3) \) and \( \text{digit}(7) \) to the high level answer \( \text{sum}([2, 7]) \). We list the code for sum n digit tasks below.

\[
\text{Sum2} \\
\{ \\
\text{decl digit(Symbol, Int).} \\
\text{decl sum(Symbol, Symbol, Int).} \\
\text{sum(imgA, imgB, DA + DB) :- digit(imgA, DA), digit(imgB, DB).}
\}
\]

Figure 10: sum 2 numbers.

\[
\text{Sum3} \\
\{ \\
\text{decl digit(Symbol, Int).} \\
\text{decl sum(Symbol, Symbol, Symbol, Int).} \\
\text{sum(imgA, imgB, imgC, DA + DB + DC) :- } \\
\text{digit(imgA, DA), digit(imgB, DB), digit(imgC, DC).}
\}
\]

Figure 11: sum 3 numbers.

\[
\text{Sum4} \\
\{ \\
\text{decl digit(Symbol, Int).} \\
\text{decl sum(Symbol, Symbol, Symbol, Symbol, Int).} \\
\text{sum(imgA, imgB, imgC, imgD, DA + DB + DC + DD) :- } \\
\text{digit(imgA, DA), digit(imgB, DB), digit(imgC, DC), digit(imgD, DD).}
\}
\]

Figure 12: sum 4 numbers.

F.2 Sort-n-numbers

The sort n numbers task is another extension from the original MNIST digit recognition task. In this task, the input are n images in the MNIST dataset, and the desired output is to sort them in order. For example, \( \text{sort}(2, [3, 0, 1]) \) means the given input \( [3, 0, 1] \) has the order 0, 1 from small to large. In the scallop program to sort two numbers, we have the corresponding rules: 
\[
\text{sort}(0, DA), \text{sort}(1, DB), DA <= DB. \\
\text{sort}(0, DA), \text{sort}(1, DB), DA > DB. \\
\text{sort}(0, DA), \text{sort}(1, DB), DA = DB.
\]

This means, if the first number is smaller or equal to the second number, then we give them the order \( (0, 1) \), else we give them the order \( (1, 0) \). We manually assign the order if two numbers are the same. The corresponding scallop programs are shown below:

\[
\text{Sort2} \\
\{ \\
\text{decl digit(Symbol, Int).} \\
\text{decl sort_2(Int).} \\
\text{sort_2(0) :- digit(0, DA), digit(1, DB), DA <= DB.} \\
\text{sort_2(1) :- digit(0, DA), digit(1, DB), DA > DB.}
\}
\]

Figure 13: sort 2 numbers.
Sort3 {
  decl digit(Symbol, Int).
  decl sort_3(Int).
  decl digit_abc(Int, Int, Int).

digit_abc(DA, DB, DC) :- digit(0, DA), digit(1, DB), digit(2, DC).
sort_3(0) :- digit_abc(DA, DB, DC), DA <= DB, DB <= DC. // 0, 1, 2
sort_3(1) :- digit_abc(DA, DB, DC), DA <= DC, DC < DB. // 0, 2, 1
sort_3(2) :- digit_abc(DA, DB, DC), DB < DA, DA <= DC. // 1, 0, 2
sort_3(3) :- digit_abc(DA, DB, DC), DB <= DC, DC < DA. // 1, 2, 0
sort_3(4) :- digit_abc(DA, DB, DC), DC < DA, DA <= DB. // 2, 0, 1
sort_3(5) :- digit_abc(DA, DB, DC), DC < DB, DB < DA. // 2, 1, 0
}

Figure 14: sort 3 numbers.

Sort4 {
  decl digit(Symbol, Int).
  decl sort_4(Int).
  decl digits(Int, Int, Int, Int).
digits(D0, D1, D2, D3) :- digit(0, D0), digit(1, D1), digit(2, D2), digit(3, D3).
sort_4(0) :- digits(D0, D1, D2, D3), D0 <= D1, D1 <= D2, D2 <= D3. // 0, 1, 2, 3
sort_4(1) :- digits(D0, D1, D2, D3), D0 <= D1, D1 <= D3, D3 < D2. // 0, 1, 3, 2
sort_4(2) :- digits(D0, D1, D2, D3), D0 <= D2, D2 < D1, D1 <= D3. // 0, 2, 1, 3
sort_4(3) :- digits(D0, D1, D2, D3), D0 <= D2, D2 <= D3, D3 < D1. // 0, 2, 3, 1
sort_4(4) :- digits(D0, D1, D2, D3), D0 <= D3, D3 < D1, D1 <= D2. // 0, 3, 1, 2
sort_4(5) :- digits(D0, D1, D2, D3), D0 <= D3, D3 < D2, D2 < D1. // 0, 3, 2, 1
sort_4(6) :- digits(D0, D1, D2, D3), D1 <= D0, D0 <= D2, D2 <= D3. // 1, 0, 2, 3
sort_4(7) :- digits(D0, D1, D2, D3), D1 < D0, D0 <= D3, D3 < D2. // 1, 0, 3, 2
sort_4(8) :- digits(D0, D1, D2, D3), D1 <= D2, D2 < D0, D0 <= D3. // 1, 2, 0, 3
sort_4(9) :- digits(D0, D1, D2, D3), D1 <= D2, D2 <= D3, D3 < D0. // 1, 2, 3, 0
sort_4(10) :- digits(D0, D1, D2, D3), D1 <= D3, D3 < D0, D0 <= D2. // 1, 3, 0, 2
sort_4(11) :- digits(D0, D1, D2, D3), D1 <= D3, D3 < D2, D2 < D0. // 1, 3, 2, 0
sort_4(12) :- digits(D0, D1, D2, D3), D2 < D0, D0 <= D1, D1 <= D3. // 2, 0, 1, 3
sort_4(13) :- digits(D0, D1, D2, D3), D2 < D0, D0 <= D3, D3 < D1. // 2, 0, 3, 1
sort_4(14) :- digits(D0, D1, D2, D3), D2 < D1, D1 < D0, D0 <= D3. // 2, 1, 0, 3
sort_4(15) :- digits(D0, D1, D2, D3), D2 < D1, D1 <= D3, D3 < D0. // 2, 1, 3, 0
sort_4(16) :- digits(D0, D1, D2, D3), D2 <= D3, D3 < D0, D0 <= D1. // 2, 3, 0, 1
sort_4(17) :- digits(D0, D1, D2, D3), D2 <= D3, D3 < D1, D1 < D0. // 2, 3, 1, 0
sort_4(18) :- digits(D0, D1, D2, D3), D3 < D0, D0 <= D1, D1 <= D2. // 3, 0, 1, 2
sort_4(19) :- digits(D0, D1, D2, D3), D3 < D0, D0 <= D2, D2 < D1. // 3, 0, 2, 1
sort_4(20) :- digits(D0, D1, D2, D3), D3 < D1, D1 < D0, D0 <= D2. // 3, 1, 0, 2
sort_4(21) :- digits(D0, D1, D2, D3), D3 < D1, D1 <= D2, D2 < D0. // 3, 1, 2, 0
sort_4(22) :- digits(D0, D1, D2, D3), D3 < D2, D2 < D0, D0 <= D1. // 3, 2, 0, 1
sort_4(23) :- digits(D0, D1, D2, D3), D3 < D2, D2 < D1, D1 < D0. // 3, 2, 1, 0
}

Figure 15: sort 4 numbers.
G VQAR Dataset Details

G.1 VQAR Stats

Figure 16: This is the distribution of functions in queries. We only introduce AND and OR for the questions with more than 5 clauses.

Figure 17: This is the distribution of knowledge graph related function number in queries. FIND_HYPERNAME and FIND_KG are the two basic functions that requires look into the knowledge graph. When the question has more clauses, it is more likely include knowledge base related clauses.

Figure 18: This is the distribution of relation related function number in queries. RELATE and RELATE.Reverse are the two basic functions that requires look into the knowledge graph. When the question has more clauses, it is more likely include knowledge base related clauses.

G.2 VQAR Examples

We show 6 images in our VQAR dataset in Figures 19, 20, 21, 22, 23, and 24 each paired with 2 question and answer pairs. For each question, we show its original Programmatic Query as well as the transformed Datalog Query. The object IDs are shown on the bounding boxes (in white) on the image.

Then the program is $P^x_θ = (KG_F \cup F_n \cup F_a \cup F_r, KG_R, J_n, Q)$. Note the universal knowledge graph $KG_F$ is the same across different tasks.
Programmatic Query

Datalog Query
Answer

Figure 19: VQAR Example 1

Programmatic Query

Datalog Query
Answer

Figure 20: VQAR Example 2

Programmatic Query

Datalog Query
Answer

Figure 21: VQAR Example 3
Programmatic Query

Datalog Query

Answer

Figure 22: VQAR Example 4

Figure 23: VQAR Example 5

Figure 24: VQAR Example 6