MULTIPROVER: Generating Multiple Proofs for Improved Interpretability in Rule Reasoning

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Abstract
We focus on a type of linguistic formal reasoning where the goal is to reason over explicit knowledge in the form of natural language facts and rules (Clark et al., 2020). A recent work, named PROVER (Saha et al., 2020), performs such reasoning by answering a question and also generating a proof graph that explains the answer. However, compositional reasoning is not always unique and there may be multiple ways of reaching the correct answer. Thus, in our work, we address a new and challenging problem of generating multiple proof graphs for reasoning over natural language rule-bases. Each proof provides a different rationale for the answer, thereby improving the interpretability of such reasoning systems. In order to jointly learn from all proof graphs and exploit the correlations between multiple proofs for a question, we pose this task as a set generation problem over structured output spaces where each proof is represented as a directed graph. We propose two variants of a proof-set generation model, MULTIPROVER. Our first model, Multilabel-MULTIPROVER, generates a set of proofs via multi-label classification and implicit conditioning between the proofs; while the second model, Iterative-MULTIPROVER, generates proofs iteratively by explicitly conditioning on the previously generated proofs. Experiments on multiple synthetic, zero-shot, and human-paraphrased datasets reveal that both MULTIPROVER models significantly outperform PROVER on datasets containing multiple gold proofs. Iterative-MULTIPROVER obtains state-of-the-art proof F1 in zero-shot scenarios where all examples have single correct proofs. It also generalizes better to questions requiring higher depths of reasoning where multiple proofs are more frequent.

1 Introduction
Formal reasoning over explicit multi-sentence knowledge (Newell and Simon, 1956) has often proved to be challenging (Musen and Van Der Lei, 1988), owing to the difficulty in creating logical forms from such sentences, thereby restricting the application of semantic parsers (Zettlemoyer and Collins, 2005; Berant et al., 2013; Berant and Liang, 2014). Thus, in a recent work, Clark et al. (2020) bypass the creation of intermediate logical forms and show that transformers (Vaswani et al., 2017) can act as “soft theorem provers” by answering questions over natural language (English) rule-bases, consisting of facts and rules. In order to reliably interpret these predicted answers, Saha et al. (2020) propose PROVER, a transformer-based model that generates the corresponding proof graph, thus emulating formal reasoning closely. Consider the two example rule-bases with two questions and corresponding proofs in Figure 1, where a proof is a directed graph consisting of the relevant facts and rules from the corresponding rule-base. PROVER shows good single-proof generation accuracy but is designed and trained in a way to generate only a single proof for each question. This is not ideal because formal proofs are not always unique and there may be multiple correct ways of arriving at the answer. For example, Q1 and Q2 in Figure 1 have three and four correct proofs respectively. Hence, in order to enhance the human-interpretability of linguistic formal reasoning systems, it is desirable to develop methods that can generate multiple proofs, each providing a different rationale for the predicted answer. Such interpretable methods, while possessing the flexibility of operating over natural language, can also aid in verifying claims when constructing proofs from scratch is tedious or infeasible.

We find that PROVER (Saha et al., 2020), when trained on all proofs as independent training examples (Eq. 2) and extended to generate top-$p$ proofs during inference (Eq. 3), fails drastically, achieving a low proof precision of 34%. The subsequent proofs are often incorrect because it is not
Rules:
R1: White, round things are furry.
R2: All blue, young things are big.
R3: If something is white and young, then it is blue.
R4: If Dave is round then Dave is white.
R5: If something is blue and white then it is round.
R6: If Harry is big and Harry is white then Harry is red.
R7: All furry, red things are young.
R8: Red things are round.
R9: If something is blue then it is red.

Facts:
F1: Bob is big.
F2: Bob is blue.
F3: Bob is furry.
F4: Bob is young.
F5: Dave is red.
F6: Fiona is white.
F7: Harry is big.
F8: Harry is red.
F9: Harry is white.
F10: Harry is quiet.

Q1: Harry is furry. [Answer: T]

Figure 1: Two rule-bases with rules, facts, questions, answers and all possible proofs. The first question has three correct proofs while the second question has four correct proofs. MULTIPROVER answers both questions correctly and also generates all the corresponding proofs accurately for each question.

trained jointly with all proofs and hence, is unable to exploit the inter-proof correlations and also does not learn the correct number of proofs for a question. Thus, we propose MULTIPROVER, a transformer-based model that can generate a set of proof graphs with appropriate cardinality for a given question. Since multiple proofs can be generated in any arbitrary order, we pose this task as a set generation problem over graphs and train MULTI-PROVER jointly with a permutation-invariant Hungarian Loss (Zhang et al., 2019a,b) over all proofs.

A proof graph is generated through a node module which selects the relevant facts and rules as part of the proof and an edge module which determines the edges between the chosen nodes. Similar to PROver, we first enforce multiple structural constraints during training and inference to ensure that a generated proof is valid. Next, in order to generate a set of proofs jointly, we propose our first model, Multilabel-MULTI-PROVER, a multi-label classification framework which performs implicit conditioning among the proofs and predicts p binary labels for each node and edge, denoting its presence or absence in each of the p proofs that we want to generate. It is efficient in terms of the number of parameters and training time and also achieves a better proof F1 than PROVER. However, the lack of explicit conditioning between the proofs is not ideal because a question with multiple proofs often has certain common sub-graphs across the proofs. E.g., all the 3 proofs for Q1 in Figure 1 have the sub-graph \( \{ F_{10} \rightarrow R_1 \} \) common. Thus, in order to exploit these correlations which Multilabel-MULTI-PROVER cannot capture explicitly, we further propose an improved variant of MULTI-PROVER, named Iterative-MULTI-PROVER, which generates an appropriate number of proofs by stacking multiple node and edge encoders, each of which generates one proof at each time step by conditioning on the previously generated proofs. This enables the model to better learn the correlations between multiple proofs for a given question. To capture the set-based nature of the task, we train MULTI-PROVER using a permutation-invariant Hungarian Loss (Sec. 3.5), which solves an assignment problem between a set of predicted and gold proofs.

Empirical evaluation on synthetic and human paraphrased QA rule-bases (Clark et al., 2020) show that both of our MULTI-PROVER models achieve a significantly higher proof F1 compared to PROVER while retaining the QA accuracy. Further, on a challenging hand-authored zero-shot dataset, where all examples have single gold proofs, Iterative-MULTI-PROVER achieves state-of-the-art proof F1. It also generalizes better to questions requiring higher depths of reasoning with more multiple proofs. Overall, our contributions are:

- We address a new and challenging problem of generating a set of multiple logical proof graphs for reasoning over natural language rule-bases by proposing two set-based joint models, Multilabel-MULTI-PROVER and Iterative-MULTI-PROVER. \(^1\)
- Iterative-MULTI-PROVER’s joint training and explicit conditioning helps it to better learn the relative importance of rules and facts for a particular question and uncover common subgraphs across multiple proofs. Thus, compared to Multilabel-MULTI-PROVER and PROVER, it is able to transfer well in zero-shot settings because it learns to assign a soft prior over the rule-base.

\(^1\)Our code and models are publicly available at https://github.com/swarnaHub/multiPROVER.
tions requiring higher depths of reasoning where the presence of multiple proofs is frequent.

2 Related Work

The task of rule reasoning (Clark et al., 2020) is related to other recently proposed tasks on QA (Weston et al., 2015; Yang et al., 2018; Lin et al., 2019; Tafjord et al., 2019; Richardson et al., 2020) and NLI (MacCartney and Manning, 2014). However, most of these tasks require implicit reasoning rules as opposed to explicit ones and the focus is either on broad language understanding or on single rule application. Below we discuss MULTI PROVER’s relation to multiple areas of NLP and ML.

Structured Explanations: There is useful previous work on generating interpretable and explainable models (Doshi-Velez and Kim, 2017; Rudin, 2019; Hase and Bansal, 2020; Jacovi and Goldberg, 2020) for NLP. Explanations in NLP take three major forms – (1) extractive rationales or highlights (Zaidan et al., 2007; Lei et al., 2016; Yu et al., 2019; DeYoung et al., 2020) where a subset of the input text explain a prediction, (2) free-form or natural language explanations (Camburu et al., 2018; Rajani et al., 2019; Zhang et al., 2020; Kumar and Talukdar, 2020) that are not constrained to the input, and (3) structured explanations that range from semi-structured text (Ye et al., 2020) to chain of facts (Khot et al., 2020; Jhamtani and Clark, 2020; Gontier et al., 2020) to explanation graphs (based on edges between chains of facts) (Jansen et al., 2018; Jansen and Ustalov, 2019; Xie et al., 2020).

Generating Multiple Outputs: Generating a set of proofs can be viewed as a task of generating multiple structured outputs (Prasad et al., 2014). Multiple prior studies focus on generating diverse unstructured texts (Gimpel et al., 2013; Dai et al., 2017; Xu et al., 2018; Raffel et al., 2020), which broadly span two categories – (1) using improved decoding techniques like beam search with intersibling ranking penalty (Li et al., 2016), iterative beam search (Kulikov et al., 2018), diverse beam search (Vijayakumar et al., 2018), and sentence codes (Shu et al., 2019), (2) varying the hidden representations or using multiple decoders (Dai et al., 2017; Jain et al., 2017; Shen et al., 2019). Our baseline, PROVER-top-p, which extends PROVER to generate top-p proofs during inference falls in the first category while MULTI PROVER falls in the second category, where the multiple node and edge encoders vary the node and edge representations for generating multiple proofs.

Machine Learning over Sets: Set-based ML models (Zaheer et al., 2017; Lee et al., 2018; Zhang et al., 2019a; Kosiorek et al., 2020) have a wide range of applications including generating multiple image captions (Vinyals et al., 2015), generating diverse translations (Cho et al., 2014; Bahdanau et al., 2015), enumerating rules in a logical inference system (Gao et al., 2019). Set problems are challenging because the number of valid solutions for a set of size n are n!, which increases faster than exponential in n and ignoring the set structure produces sub-optimal solutions (Zhang et al., 2019a). Thus, we use a set-based Hungarian Loss (Zhang et al., 2019a,b) for capturing the permutation-invariant nature of generating a set of proofs.

3 Method

3.1 Task Description and Notations

The input to our task is a tuple of the form \((C, Q)\), where \(C\) is a rule-base context and \(Q\) is the question. We want to predict a binary answer \(A \in \{\text{True}, \text{False}\}\) for the question and generate a set of proof graphs \(P = \{P_1, \ldots, P_p\}\), each of which provides a diverse rationale for the answer (see Figure 1). The context \(C\) consists of a set of facts and rules, denoted by \(F\) and \(R\) respectively. Facts \(F = \{F_1, \ldots, F_j\}\) are unambiguous statements, while rules \(R = \{R_1, \ldots, R_k\}\) are logical statements, which can be used in conjunction with the facts to arrive at a logical conclusion. Each proof \(P_i = (V_i, E_i)\) is a directed graph, with a set of nodes \(V_i \subseteq N\) and a set of edges \(E_i \subseteq V_i \times V_i\), where \(N = F \cup R \cup \{\text{NAF}\}\) and \(k = |N|\). If a statement (E.g. “Anne is big”) cannot be deduced from the context, then Negation as Failure (NAF) contains the negation of that statement (E.g. “Anne is not big”), which is considered true in a closed-world assumption. See appendix for more details of the syntax of proof graphs.

3.2 Baseline PROVER Model

PROVER (Saha et al., 2020) builds on top of RoBERTa (Liu et al., 2019) and consists of a question answering (QA) module, a node module, and an edge module where the node and edge modules are used to predict a single proof graph. The input to RoBERTa is the concatenation of the facts, rules, and the question. The QA module takes
in the representation of the $[CLS]$ token and predicts a binary label for the question. The node module computes the node embeddings $N \in \mathbb{R}^{k \times d}$ consisting of the representations of each fact, rule, and NAF where $d$ is the embedding dimension. The $i^{th}$ row $n_i$ of $N$ denotes the embedding of node $i$. A node classifier takes in these embeddings to output the node probabilities $n_{pi} \in \mathbb{R}^k$ for each fact, rule, and NAF being present in the proof. The edge module computes the edge embeddings $E \in \mathbb{R}^{k^2 \times d}$ for every edge $(i, j)$ through the function $\phi(i, j) = [n_i; n_j; (n_i - n_j)]$ where $\phi$ is the concatenation operation and outputs probabilities $e_{pi,j} \in \mathbb{R}^{k^2}$ of each edge being present in the proof. PROVER is trained using the joint cross-entropy loss over the QA, node, and edge modules. The authors pose inference as an Integer Linear Program (ILP). Given a set of nodes and the edge probabilities from the trained model, the following global score over the edge probabilities is maximized, subject to multiple structural constraints $S$ that ensure the validity of a proof graph (like checking for graph connectivity).

$$\arg \max_{e_{pi,j} \in \{0,1\} \cdot S, i,j \neq j} \sum_{i,j} e_{pi,j} \cdot e_{pi,j} + (1 - e_{pi,j}) \cdot (1 - e_{pi,j})$$

**Extending PROVER to Generate Proof-Sets:**

Since Saha et al. (2020) focus on generating one proof per question, they also train their model with one gold proof per question. For multiple proof generation, an obvious extension is to treat each proof for a question as a separate training example. Formally, for each sample $l$, given a context $C^l$, a question $Q^l$, an answer $A^l$ and a set of gold proofs $P^l_i$, where $i \in \{1, \ldots, P_l\}$, the extended training dataset can be defined as:

$$\mathcal{D} = \bigcup_{i=1}^{L} \left\{ \left( Q^l, C^l, A^l, P^l_i \right) \right\}$$

Once PROVER is trained with this dataset, during inference, we generate top-$p$ proofs by first selecting the top-$p$ node sets according to Eqn. 3 and then choosing the corresponding edge sets using the optimization function in Eqn. 1.

$$\arg \max_{v \in \{0,1\}^k} \sum_{i=1}^k n_{pi} - v_i + (1 - n_{pi}) \cdot (1 - v_i)$$

The top-$p$ solutions of Eqn. 3 are $v^1, \ldots, v^p$, which indicate a node’s presence or absence in the proofs. Although simple, this approach has two major issues. First, the lack of coupling between the proofs can potentially confuse the model as there are multiple possible proofs for the same (question, context) pair. Second, inference is inflexible and always generates a fixed number of proofs for every example, thus leading to the generation of many incorrect proofs (Section 5.1). As shown in Figure 1, certain questions can have multiple possible proofs. Figure 2 demonstrates this phenomenon statistically – the datasets we experiment with (Clark et al., 2020) contain up to 13% of the samples with $>1$ correct proof. Thus, in the light of PROVER’s limitations, we propose two novel architectures of a proof-set generation model, MULTIPROVER.

### 3.3 Multilabel-MULTIPROVER

As described in the previous section, a desired property for generating a set of proofs is to have the proofs conditioned on each other as opposed to treating them independently. Thus, we propose *Multilabel-MULTIPROVER* (see Figure 3), which poses the problem of generating a set of proofs as a multi-label classification task over all the nodes and
We also have a parallel, the model is trained by padding empty proofACKS. First, since the proofs are generated in parallel from the same node embeddings and edge embeddings. Thus, it has the strengths of the connections between these nodes. However, it suffers from two major drawbacks. First, since the proofs are generated in parallel, the model is trained by padding empty proof.

This model is advantageous because there is implicit conditioning between the proofs as all the proofs are generated in parallel from the same node embeddings and edge embeddings. Thus, it has no additional time or memory overhead while also generating proof-sets better than PROVER (Section 5.1). However, it suffers from two major drawbacks. First, since the proofs are generated in parallel, the model is trained by padding empty proof.

As a motivating example for why explicit conditioning among proofs is necessary, consider the proofs for $Q_1$ in Figure 1 where the sub-graph $\{F_{10} \rightarrow R_1\}$ is common across all the proofs. $F_{10}$ and $R_1$ are essential for answering the question and hence conditioning on the previously generated proofs will help the model adjust the relevance of nodes and edges in the subsequent proofs. Quantitatively, we find that about 75% of the samples with 4 proofs have at least one node and one edge common across all the proofs (see Figure 5). Thus, we propose Iterative-MULTI PROVER (see Figure 4), which broadly consists of a base PROVER architecture, as in Figure 3 and an additional $p$ node and edge encoders for generating a maximum of $p$ proofs. The proofs are generated iteratively until an empty graph is generated to denote the end.

Base PROVER architecture computes the first level of node embeddings $N^1 \in \mathbb{R}^{k \times d}$ and edge embeddings $E^1 \in \mathbb{R}^{k^2 \times d}$. These are passed respectively through a node and edge classifier to generate the node probabilities $np^1 \in \mathbb{R}^k$ and edge probabilities $ep^1 \in \mathbb{R}^{k^2}$, corresponding to the first proof. In the next iteration, two transformer encoders generate the node and edge embeddings corresponding to the second proof. Specifically, we condition the generation of the next node embeddings $N^2$ on the previous node $(N^1)$ and edge $(E^1)$ embeddings simultaneously. Conditioning on both is crucial because $N^1$ captures the relevance of nodes for the first proof, while $E^1$ contains information about the strength of the connections between these nodes. We condition $E^2$ only on $E^1$, because the edge embeddings corresponding to the nodes predicted by
N^1 are already updated in E^1. Formally,

\[ T^1 = W^{(1)} E^1 W^{(2)}, W^{(1)} \in \mathbb{R}^{k \times k^2}, W^{(2)} \in \mathbb{R}^{3d \times d} \]

\[ N^1 = [N^1; T^1] W^{(3)}, W^{(3)} \in \mathbb{R}^{2d \times d} \]

\[ N^2 = \text{Transformer}(N^1); E^2 = \text{Transformer}(E^1) \]

These next set of embeddings, when passed through the respective node and edge classifiers, predict the node probabilities \( np^2 \in \mathbb{R}^k \) and edge probabilities \( ep^2 \in \mathbb{R}^{k^2} \), denoting the likelihood of their presence in the second proof. We repeat this process of stacking up the node and edge encoders for generating a maximum of \( p \) proofs. Given the node and edge probabilities corresponding to each proof and a QA probability from the QA module, we train Iterative-MULTI PROVER jointly with all proofs using the Hungarian Loss, described below.

### 3.5 Permutation-Invariant Hungarian Loss

Unlike words in text generation, proofs can be generated in any arbitrary order. Consequently, computing cross-entropy loss between the \( i^{th} \) predicted proof and the \( i^{th} \) gold proof, \( i \in \{1, ..., p\} \) will be sub-optimal. Thus, we use a permutation-invariant Hungarian Loss (Zhang et al., 2019a,b) which finds the most optimal assignment between the predicted proofs and the gold proofs such that the overall loss is minimized. Formally, the Hungarian loss \( \mathcal{L}_H \) and total loss \( \mathcal{L} \) are denoted as follows:

\[ \mathcal{L}_H = \min_{\pi} \sum_{i=1}^{p} CE(np^i, y_n^{\pi(i)}) + CE(ep^i, y_e^{\pi(i)}) \]

\[ \mathcal{L} = \mathcal{L}_{QA} + \mathcal{L}_H \]

where \( CE(., .) \) is the cross entropy loss, \( np^i \) and \( ep^i \) are the respective node and edge probabilities for the \( i^{th} \) predicted proof while \( y_n^{\pi(i)} \in \{0, 1\}^k \) and \( y_e^{\pi(i)} \in \{0, 1\}^{k^2} \) are the respective true node and edge labels for the gold proof \( \pi(i) \), where \( \pi \) is the most optimal permutation. The Hungarian Loss is implemented by first summing the node and edge cross-entropy loss matrices \( \mathcal{L}_N \in \mathbb{R}^{p \times p} \) and \( \mathcal{L}_E \in \mathbb{R}^{p \times p} \) respectively, each entry \((i, j)\) of which corresponds to the proof loss between the \( i^{th} \) predicted proof and \( j^{th} \) gold proof (see Figures 3 and 4). Then we find the best assignment between the gold and predicted proofs through the Hungarian algorithm (Kuhn and Yaw, 1955). Our final loss sums the Hungarian proof loss and the QA loss.

### 3.6 Integer Linear Program (ILP) Inference

Following PROVER, we generate valid proofs during inference using an ILP, subject to multiple global constraints (see Saha et al. (2020)). For each predicted proof, the predicted nodes and edge probabilities from MULTI PROVER, we obtain the corresponding predicted edges using Eqn. 1.

### 4 Experimental Setup

We experiment on synthetic, hand-authored zero-shot, and human paraphrased datasets, following Clark et al. (2020); Saha et al. (2020).

**Datasets:** The five synthetic datasets DU0-DU5 consist of 100k questions with their own train, validation and test splits (70/10/20) and reasoning depths up to \( D = 0, 1, 2, 3, 5 \). Each example in these datasets is annotated with all possible proofs. The second dataset is a Birds-Electricity dataset, consisting of 5k hand-authored samples aimed at evaluating the zero-shot performance of the models. Unlike the previous datasets, all examples in this dataset have a unique gold proof. Third, ParaRules is a human-paraphrased dataset, consisting of 40k examples with all possible proofs, where the facts and rules are paraphrased by crowdsworkers. Further details of the datasets and model’s hyperparameters can be found in the appendix.

**Evaluation Metrics:** Following PROVER, QA evaluation is done through accuracy. For proofs, we compute the following metrics: (1) **Node Precision, Recall, F1**, (2) **Edge Precision, Recall, F1**, (3) **Proof Precision, Recall, F1**, and (4) **Full Accuracy** (FA). For each sample, given a set of gold proofs and predicted proofs, node precision is computed as the fraction of predicted proofs where the predicted node set matches exactly with a gold proof’s node set. Similarly, node recall for each sample is computed as the fraction of gold proofs where the corresponding node sets match exactly. The overall node precision, recall, and F1 are the respective sample-wise precision, recall, and F1 scores averaged over all the samples. Edge metrics are computed similarly but with respect to the edges only and the proof metrics consider both nodes and edges in conjunction. Our final metric, full accuracy evaluates a sample as a whole and is given by the fraction of samples where the answer and all corresponding proofs are exactly correct.

### 5 Results and Analysis

#### 5.1 Comparison of PROVER variants with MULTI PROVER

In Table 1, we compare ML-MULTI PROVER and IT-MULTI PROVER with five variants of PROVER
we first predict the number of proofs by training. Table 1: Comparison of our MULTI-PROVER (Saha et al., 2020) and context and then generate those many top proof graphs, and (5) PROVER-top-p-threshold, another improved model over vanilla top-p, where we use the optimization score from Equation 3 to predict the number of proofs to generate, i.e., we stop generating proofs when the score difference between two consecutive proofs exceeds a certain threshold (tuned on the validation set). All models are trained on the DU5 train set and tested on the corresponding test set. Based on Figure 2 which shows that 98% of the dataset contains samples with \( p \leq 3 \) proofs, we set max-proofs, \( p = 3 \). 87% of the examples in the dataset have a single gold proof, thereby making PROVER a strong baseline.

We observe that PROVER-all has a slightly lower proof F1 than PROVER, because the model likely gets confused with multiple possible proofs for the same context and question. PROVER-top-p’s huge drop in precision is unsurprising because the subsequent non-empty proofs are always incorrect, causing full accuracy to drop to 0%. When we perform careful inference over PROVER either by predicting the number of proofs or by thresholding and do not generate a fixed \( p \) number of proofs for all examples, we observe a boost in precision over the vanilla top-p model, with very little drop in recall. However, PROVER continues to be a stronger baseline than all the top-p variants because of a lot of single-proof examples in the dataset.

Both MULTI-PROVER models improve significantly on the state-of-the-art proof F1, while retaining a near perfect QA accuracy. IT-MULTI-PROVER is a significantly stronger model because of its explicit conditioning mechanism and obtains up to a statistically significant\(^2\) \((p < 0.001) 4\%\) improvement on proof F1 and full accuracy. While our model is expected to improve the proof recall compared to PROVER and PROVER-all because of the generation of multiple proofs, the improvement in precision is particularly important as it shows that the subsequently generated proofs by IT-MULTI-PROVER are mostly correct. Similarly, its improvement in proof recall compared to PROVER-top-p also shows the strength of the model considering that PROVER-top-p generates the maximum number of proofs for every sample. Overall, IT-MULTI-PROVER outperforms all other models in all metrics. In summary, careful inference strategies over a single-proof generation model like PROVER are largely ineffective for generating multiple proofs and an effective proof-set generation model needs to exploit and learn the inter-proof correlations during the training phase itself. Our experiments on the ParaRules dataset demonstrate similar findings, details of which and the effect of varying \( p \) for MULTI-PROVER is in the appendix.

Iterative-MULTI-PROVER performs equally well on the subset of questions where the context has negations, achieving a high proof F1 of 90.8. As part of error analysis, we find that 58% of Iterative-MULTI-PROVER’s wrongly predicted proofs have more nodes and edges than those in the gold proof, suggesting that our model tends to overestimate the essential rules and facts and their inter-connections. In the following subsections, we analyze MULTI-PROVER’s generalization capabilities in three dif-

\(^2\)We use bootstrap test (Efron and Tibshirani, 1994) for calculating the statistical significance score.
The Birds-Electricity test-only dataset evaluates the generalization capabilities of the \textsc{PROVER} models on higher depth questions. Specifically, in Table 3, we compare the DU5-trained models of \textsc{PROVER}-all, \textsc{ML-MULTI\textsc{PROVER}} and \textsc{IT-MULTI\textsc{PROVER}} on the subset of DU5 test examples with varying depths of reasoning ($d$). Each row also shows the percentage of examples with multiple gold proofs (MP) which, unsurprisingly, increases as the depth increases. We observe that much of \textsc{IT-MULTI\textsc{PROVER}}’s improvement compared to \textsc{ML-MULTI\textsc{PROVER}} comes at higher depths where the presence of multiple proofs is a more frequent phenomenon. At depth-5, where 23% of the examples have > 1 correct proof, \textsc{IT-MULTI\textsc{PROVER}} obtains a 6% improvement over \textsc{ML-MULTI\textsc{PROVER}}. This shows that joint training with all proofs and explicit conditioning between them leads to better generalization at higher depths.

### 5.4 Generalization with Less Training Data

Collecting proofs for supervised training is expensive in most real-world scenarios. Hence, on top of the zero-shot and depth generalization results presented so far, we ask if our \textsc{MULTI\textsc{PROVER}} models can learn from less training data. Table 4 shows that these models obtain near perfect QA accuracy with only 40% of the training data (30k examples). However, proof generation proves to be challenging and only improves with sufficient training.
5.5 Comparison of MULTI PROVER with the Skyline Single-Proof Generation Model

We find that an ideal (skyline) single-proof generation model’s proof recall for the DUS5 dataset is upper-bounded by 92% as it contains about 87% of single-proof examples. This is computed by considering exactly 1 correct proof per question. Hence, we ask how well our MULTI PROVER models compare with this ideal performance (Figure 7).

Our results are encouraging, not only because IT-MULTI PROVER generates more correct proofs than all other models but also because it almost matches the performance of the skyline single-proof generation model. The PROVER model is 9.2% worse as compared to the skyline single-proof generation model while IT-MULTI PROVER reduces this gap to 3%. Given the dataset mostly contains single-proof examples, the skyline is a strong upper-bound on proof generation performance and IT-MULTI PROVER significantly reduces the gap. See appendix for ablations of IT-MULTI PROVER, including the effect of Hungarian Loss.

6 Qualitative Analysis of MULTI PROVER

Fig. 6 shows the sets of proofs correctly generated by Iterative-MULTI PROVER for two randomly chosen questions. For $Q_1$, it generates all the possible proofs by identifying the common subgraph

$F_0 \rightarrow R_0$, $Q_2$ is interesting, because (i) the single-node proof $F_2$ is significantly different from the other proofs in both structure and size, and (ii) the two larger proofs have two distinct common subgraphs. Here, PROVER performs a simple lookup in the rule-base to generate the proof $F_2$, thereby limiting our understanding of its reasoning capabilities. However, MULTI PROVER, through its ability to also generate the larger and more complex proofs enhances the transparency and verification of its reasoning abilities, and hence is a crucial step towards bridging the gap between neural and symbolic approaches.

7 Conclusion

We proposed Multilabel-MULTI PROVER and Iterative-MULTI PROVER, two variants of a proof-set generation model where the former performs implicit conditioning between the proofs to generate them in parallel while the latter generates a proof-set through explicit conditioning on the previously generated proofs. Both models obtain strong proof F1 improvements on synthetic and human-paraphrased datasets and Iterative-MULTI PROVER also obtains state-of-the-art proof F1 on a zero-shot dataset with single proofs. MULTI PROVER’s modeling is fairly generic and similar methods can be used in generating a set of structured explanations for other NLP tasks like multi-hop QA.
Ethical Considerations

Despite the overwhelming success of pre-trained language models for various NLP tasks, a common criticism is their lack of interpretability. Generating structured proofs from such models allows us to explain their reasoning capabilities and also bridges the gap between neural and symbolic systems. In this work, we take a step closer towards improving the interpretability of rule-based reasoning by generating a set of multiple proofs, each providing a diverse rationale for the reasoning process. We experiment with a wide variety of rule-bases ranging from synthetic to hand-authored to human-paraphrased rule-bases. Our results show good generalization performance of our models across three different aspects – (1) zero-shot settings, (2) questions requiring higher depths of reasoning, and (3) availability of less training data. We hope our models and findings will inspire future work on generating multiple structured explanations for different compositional reasoning tasks in NLP.

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A Appendix

A.1 Experimental Setup

MULTIPOVER is developed on top of the Hugging Face transformers library (Wolf et al., 2020).\(^3\) Experiments with PROVER (Saha et al., 2020) are performed using their publicly released code and hyperparameters.\(^4\) All MULTIPOVER hyperparameters are chosen based on the best Full Accuracy on the corresponding validation set. We use RoBERTa-large (Liu et al., 2019) as the pre-trained language model. The batch size and maximum sequence length are set to 8 and 300 respectively. We train all our models for a maximum of 7 epochs using an initial learning rate of 10\(^{-5}\), a weight decay of 0.1 and a dropout probability of 0.1. We use a random seed of 42 across all our experiments. All experiments are performed on one V100 Volta GPU. Batch size and learning rate are manually tuned in the range \([8,16]\) and \([10^{-5}, 2 \times 10^{-5}]\) respectively. For inference, we use PROVER's ILP optimization code, which is modeled using PuLP.\(^5\) In all the datasets, the maximum number of facts and rules corresponding to a context is 25.

A.2 Datasets

Our experiments are conducted on the datasets introduced in Clark et al. (2020).\(^6\) These consist of 5 datasets with synthetic rule-bases, DU0-DU5, a zero-shot test-only dataset called Birds-Electricity and a dataset with human-paraphrased rules called ParaRules. All datasets, except Birds-Electricity, have their corresponding train, validation and test splits.

**DU0-DU5:** Each of these consists of 100k questions with synthetic rule-bases and requires reasoning chains up to a maximum depth of \(D = 0, 1, 2, 3, 5\). The number of train, validation and test examples in each of the datasets are 70k, 10k and 20k respectively. Further, each question in the datasets is annotated with all possible proofs. The total number of proofs in the DU5 train set range from 1 to 1350, with a mean and median of 1.45 and 1 respectively.

**Birds-Electricity:** The Birds-Electricity dataset comprises of two test-only datasets where the contexts are about birds and electric circuits. The vocabulary of the entities, attributes and predicates, apart from \(i \in \mathcal{N}\) are all new at test time, thus providing a benchmark for testing the generalization capability of the models on out-of-distribution data. Another interesting aspect of this dataset is that all examples are annotated with a unique gold proof.

**ParaRules:** The ParaRules dataset is one where the facts and rules are paraphrased by humans into more natural language. It consists of a total of 40k questions, with 28k, 4k, and 8k questions in the train, validation and test splits respectively. This dataset tests the model’s ability to reason over more complex human-like language. Similar to the synthetic datasets, each example is annotated with all possible proofs.

A.3 Syntax of Proof Graph

Each proof \(\mathcal{P}_i = (\mathcal{V}_i, \mathcal{E}_i)\) is a directed graph, with a set of nodes \(\mathcal{V}_i \subseteq \mathcal{N}\) and a set of edges \(\mathcal{E}_i \subseteq \mathcal{V}_i \times \mathcal{V}_i\). Each node \(n_i \in \mathcal{N}\) is either a fact \(F \in \mathcal{F}\) or a rule

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\(^3\)https://github.com/huggingface/transformers

\(^4\)https://github.com/swarnaHub/PRover

\(^5\)https://pypi.org/project/PuLP/

\(^6\)https://rule-reasoning.apps.allenai.org/
$R \in \mathbb{R}$ from the context or a special NAF node, denoting “Negation as Failure”. A NAF node in a proof indicates the truthfulness of the negation of statement(s) that cannot be proved using the set of rules (under closed-world assumption). Edges in the graph can be directed either from a fact (or NAF) to a rule or between two rules. An edge from a fact to a rule means that the rule applies on the fact to generate a new fact. Similarly, an edge from a rule $R_1 \in \mathbb{R}$ to another rule $R_2 \in \mathbb{R}$ implies the application of $R_2$ on the fact generated by $R_1$.

Proofs are either successful or failed. A successful proof is one where the question statement can be logically reached (to be either proved or disproved) using the given rule-base while for failed proofs, no conclusion can be reached, in which case the shallowest branch of the proof tree that fails is generated. For more details and examples of proofs, we refer the readers to prior work (Saha et al., 2020; Clark et al., 2020).

### A.4 Ablation Analysis

In Table 5, we compare our baselines PROVER, PROVER-all and PROVER-top-$p$ variants with our MULTIPROVER models on the validation set of DU5 dataset. Additionally, we also show two ablations of IT-MULTI PROVER – in the first, we replace the Hungarian loss with a sequential loss, which computes the cross-entropy loss of the $i^{th}$ predicted proof with the $i^{th}$ gold proof and in the second, we condition the node embeddings on the previous node embeddings only instead of both node and edge embeddings. Except PROVER and PROVER-all, which generate a single proof, all other models generate a maximum of 3 proofs. PROVER-top-$p$ suffers from a significant drop in proof precision due to the generation of many incorrect proofs. Although carefully choosing the value of $p$ either by thresholding or through a classifier helps boost the proof precision, PROVER continues to be a superior baseline on this dataset due to a high skew towards single-proof examples. ML-MULTI PROVER improves upon PROVER’s proof F1 and full accuracy (FA) which are further bet-tered by IT-MULTI PROVER, owing to its explicit conditioning mechanism between the proofs. Replacing the Hungarian loss with a sequential loss leads to a significant drop in proof F1, thereby showing the effectiveness of modeling multiple proof generation as a set generation problem. Finally, conditioning the node embeddings on both node and edge embeddings leads to marginal improvement in proof F1. Overall, IT-MULTI PROVER outperforms all other models across all metrics.

### A.5 MULTI PROVER with Varying Maximum Number of Proofs

We analyze the effect of varying the maximum number of proofs $p$ on ML-MULTI PROVER and IT-MULTI PROVER in Table 6 and 7 respectively. All models are trained on the DU5 training set and evaluated on the corresponding validation set. The proof metrics start to decrease marginally with increase in $p$. Unlike Multilabel-MULTI PROVER, it is significantly robust to variation in $p$.

| $p$ | QA | P | R | F1 | Edge | P | R | F1 | Proof | P | R | F1 | PA |
|-----|----|---|---|----|------|---|---|----|------|---|---|----|---|
| 2   | 99.4| 90.5| 89.1| 89.2 | 89.3| 88.3| 88.4 | 88.8| 87.8| 87.9| 84.4 |
| 3   | 99.3| 89.9| 89.6| 89.3 | 88.3| 88.3| 88.0 | 87.7| 87.6| 87.3| 83.9 |
| 4   | 99.3| 89.1| 89.2| 88.8 | 87.8| 82.0| 87.8 | 87.2| 87.5| 87.1| 83.6 |
| 5   | 99.1| 88.6| 89.1| 88.5 | 87.2| 87.8| 87.2 | 86.6| 87.2| 86.6| 83.1 |

| $p$ | QA | P | R | F1 | Edge | P | R | F1 | Proof | P | R | F1 | PA |
|-----|----|---|---|----|------|---|---|----|------|---|---|----|---|
| 2   | 99.5| 90.0| 89.0| 89.0 | 89.2| 88.4| 88.3 | 88.6| 87.8| 87.7| 84.1 |
| 3   | 99.5| 90.6| 90.5| 90.1 | 89.9| 90.0| 89.5 | 89.4| 89.4| 89.0| 85.3 |
| 4   | 99.5| 90.2| 89.7| 89.5 | 89.5| 89.2| 89.1 | 89.1| 88.7| 88.6| 85.2 |
| 5   | 99.5| 90.1| 89.6| 89.4 | 89.5| 89.2| 89.1 | 89.0| 88.6| 88.5| 85.2 |

Table 6: Effect of varying maximum number of proofs ($p$) on Multilabel-MULTI PROVER. All models are trained on the DU5 training set and evaluated on the corresponding validation set. The proof metrics start to decrease marginally with increase in $p$.

Table 7: Effect of varying maximum number of proofs ($p$) on Iterative-MULTI PROVER. All models are trained on the DU5 training set and evaluated on the corresponding validation set. Unlike Multilabel-MULTI PROVER, it is significantly robust to variation in $p$. 
Table 8: Comparison of models trained on DU3 and ParaRules training sets and evaluated on ParaRules validation set. IT-MULTIPROVER outperforms all other models across all metrics.

| Node QA  | P  | R  | F1 | Edge QA  | P  | R  | F1 | Proof QA  | P  | R  | F1 | FA |
|----------|----|----|----|---------|----|----|----|----------|----|----|----|----|
| PROVER-all | 98.6 | 95.9 | 94.1 | 94.5 | 95.4 | 93.8 | 94.3 | 95.3 | 93.7 | 94.2 | 92.3 |    |
| PROVER-top-p | 98.6 | 39.3 | 96.6 | 96.4 | 96.4 | 96.2 | 96.2 | 96.2 | 96.0 | 96.0 | 95.2 |    |
| ML-MULTIPROVER | 98.9 | 97.3 | 97.2 | 97.2 | 97.2 | 97.0 | 97.0 | 96.8 | 96.7 | 96.7 | 96.1 |    |

Table 9: Comparison of models trained on DU3 and ParaRules training sets and evaluated on ParaRules test set. IT-MULTIPROVER outperforms all other models across all metrics.

| Node QA  | P  | R  | F1 | Edge QA  | P  | R  | F1 | Proof QA  | P  | R  | F1 | FA |
|----------|----|----|----|---------|----|----|----|----------|----|----|----|----|
| PROVER-all | 98.2 | 95.3 | 92.8 | 93.5 | 94.7 | 92.7 | 93.3 | 94.4 | 92.4 | 93.0 | 90.5 |    |
| PROVER-top-p | 98.2 | 38.7 | 95.9 | 54.3 | 38.3 | 95.5 | 53.9 | 38.2 | 95.3 | 53.8 | 00.1 |    |
| ML-MULTIPROVER | 98.3 | 96.0 | 95.6 | 95.7 | 95.9 | 95.5 | 95.6 | 95.5 | 95.2 | 95.2 | 93.8 |    |
| IT-MULTIPROVER | 98.3 | 96.8 | 96.2 | 96.3 | 96.5 | 96.3 | 96.3 | 96.2 | 96.0 | 96.0 | 94.5 |    |

Table 10: Comparative study of the number of parameters and training time per epoch (in hours) for PROVER-all (PR), ML-MULTIPROVER and IT-MULTIPROVER with varying number of maximum proofs (p).

| p | # Parameters | Time/epoch (in hours) |
|---|--------------|----------------------|
| 1 | 361M | PR 361M ML 488M | 5.0 3.4 3.6 |
| 2 | 361M | PR 361M ML 615M | 5.0 3.5 4.0 |
| 3 | 361M | PR 361M ML 742M | 5.0 3.6 4.6 |
| 4 | 361M | PR 361M ML 869M | 5.0 3.7 5.1 |
| 5 | 361M | PR 361M ML 996M | 5.0 3.8 5.7 |

A.6 Evaluation on Human-Paraphrased Rule-Bases

Following PROVER, we also test MULTIPROVER’s effectiveness in generating proofs for more human-like complex rule-bases. The ParaRules dataset is constructed by first creating a set of fact groups where each fact group consists of all facts in the theory concerning a particular person and then paraphrasing these fact groups into more complex language. E.g., a fact group “Alan is blue. Alan is rough. Alan is young.”, can be re-worded into “Alan is on the young side, but rough. He often feels rather blue.” Thus, unlike the DU datasets or the Birds-Electricity dataset where the proof graphs are composed of facts and rules, ParaRules proofs are composed of fact groups and rules. Following past work (Clark et al., 2020; Saha et al., 2020), we train our models combining the DU3 and ParaRules train sets, and evaluate on the ParaRules validation and test set in Tables 8 and 9 respectively. We find that similar conclusions to the DU5 dataset hold for this dataset as well – ML-MULTIPROVER achieves a better proof F1 and full accuracy than PROVER, which are further improved by IT-MULTIPROVER due to its explicit conditioning mechanism between the proofs.

A.7 Training Time and Size Comparison

Table 10 shows the number of trainable parameters and training time per epoch for the baseline model PROVER and our proposed models, ML-MULTIPROVER and IT-MULTIPROVER across varying number of maximum proofs (p) per sample. Since ML-MULTIPROVER adopts the same PROVER architecture but with multi-label classification, it has the same number of parameters as PROVER, which also remains unchanged irrespective of the maximum number of proofs. The number of parameters for IT-MULTIPROVER, how-
ever, increases with the increase in $p$ because of the presence of multiple node and edge encoders. While IT-MULTIPOVER has more parameters than PROVER, our empirical findings reveal that just having a similarly-sized, larger PROVER model will not be sufficient and exploiting the correlations between multiple proofs with a permutation-invariant loss is necessary for the task of generating a set of multiple proofs.

The training time of PROVER is more than that of ML-MULTIPOVER because the former treats each proof as a separate example, causing an increase in the training data size from 70k to 110k. ML-MULTIPOVER is the most time-efficient model and its running time only increases marginally with the increase in $p$. This is due to the additional node and edge classifications that the model has to perform corresponding to each additional proof. Unsurprisingly, IT-MULTIPOVER takes longer to train but encouragingly for $p \leq 4$, still has a comparable running time to PROVER.